Modeling and optimization of thermoelectric generator for waste heat recovery

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**NANYANG
TECHNOLOGICAL
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SINGAPORE

**MODELING AND OPTIMIZATION OF
THERMOELECTRIC GENERATOR FOR WASTE
HEAT RECOVERY**

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AND ELECTRONIC
ENGINEERING**
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Modeling and Optimization of Thermoelectric Generator for Waste Heat Recovery

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Table of Contents

ACKNOWLEDGEMENT.....	5
TABLE OF CONTENTS	7
SUMMARY	11
LIST OF FIGURES	13
LIST OF TABLES.....	16
LIST OF SYMBOLS	18
LIST OF ACRONYMS	21
CHAPTER 1 INTRODUCTION.....	23
1.1 Background.....	23
1.1.1 Energy market and potential for waste heat recovery.....	23
1.1.2 Review of existing waste heat recovery technology.....	27
1.1.3 Thermoelectric generators.....	30
1.2 Objectives and Contributions.....	30
1.3 Organization of the Thesis	32
CHAPTER 2 LITERATURE REVIEW ON THERMOELECTRIC GENERATOR	
35	
2.1 Introduction.....	35
2.2 State of art of thermoelectric material development.....	38
2.3 State of art of thermoelectric module development.....	42
2.4 State of art of thermoelectric generator system development.....	46
2.5 Summary	52

CHAPTER 3 THERMOELECTRIC ELEMENT AND THERMOELECTRIC MODULE MODEL DEVELOPMENT 53

3.1 Introduction.....	53
3.2 Governing equations and boundary conditions for thermoelectric elements.....	54
3.3 An improved analytical model regarding the thermoelectric elements	56
3.3.1 Prediction of the output performance	56
3.3.2 Thermal resistance network of a TEM.....	61
3.3.3 Finding TEG key parameters from various data source	62
3.4 Experimental validation of analytical model	66
3.5 3-D model development in ANSYS and comparison with improved analytical TEM model.....	69
3.6 Summary	72

CHAPTER 4 INTEGRATED HEAT EXCHANGER AND THERMOELECTRIC MODEL DEVELOPMENT 73

4.1 Introduction.....	73
4.2 Development of heat exchanger model.....	74
4.3 Integration of thermoelectric generator model	83
4.4 Validation of integrated thermoelectric generator model.....	87
4.5 Parametric study on different input and design parameters.....	90
4.6 Summary	94

CHAPTER 5 THERMOELECTRIC MODULE DESIGN AND OPTIMIZATION 95

5.1 Introduction.....	95
5.2 Thermal resistance network and boundary conditions.....	96
5.3 Parametric study of thermoelectric module height at original working condition	98

5.4 Parametric study of thermoelectric TEM design parameters under different boundary conditions.....	101
5.5 Parametric study at different fill factor	103
5.6 Summary	104
CHAPTER 6 CO-OPTIMIZATION OF THERMOELECTRIC AND HEAT EXCHANGER FOR WASTE HEAT RECOVERY	105
6.1 Introduction.....	105
6.2 Taguchi method.....	106
6.3 Taguchi method on automotive application	107
6.3.1 Problem description	107
6.3.2 Modeling results and SNR ratio.....	109
6.3.3 Analysis of variance	112
6.3.4 Comparison of original experiment and optimized design	117
6.4 Taguchi method on marine application	118
6.4.1 Problem description	118
6.4.2 Modeling results and SNR ratio.....	121
6.4.3 Analysis of variance	123
6.5 Summary	126
CHAPTER 7 CONCLUSIONS AND FUTURE RESEARCH	129
7.1 Conclusion	129
7.2 Recommendations for Future Works	130
7.2.1 Prototype development of TEG system	130
7.2.2 Improve heat transfer by heat pipe or phase change material.....	131
Appendix A: Derivation of efficiency and figure of merit.....	132

Appendix B: Solution of temperature field inside TE element.....	134
REFERENCE.....	136

Summary

Tremendous energy is dissipated as waste heat during industrial processes. Many waste heat recovery technologies have been proposed to convert some waste heat to useful energy. Among those waste heat recovery technologies, thermoelectric generator (TEG) has its distinct advantage of directly converting heat into electricity, reliability, long lifetime, no moving parts and no gas emissions. Thermoelectric materials have been investigated extensively in recent decades and the figure of merit ZT has been continuously enhanced. However, the thermoelectric module (TEM) and system development is rather stagnant, and the overall efficiency is quite low for practical applications. This has raised the urgent need for developing simulation and design tools for TEGs.

Design and optimization relies on effective simulation tool development. However, the simulation of TEG, consisting of TEM and heat exchanger (HEX), is a complex problem as it involves thermo-electric coupling effect, solid state heat transfer and convective heat transfer as HEXs are usually adopted. To address this issue, the first part of this thesis proposes a numerical model to simulate the TEM and its heat transfer system. Both 3-D computational fluid dynamics (CFD) model and 1-D numerical model are developed and validated against experiments and the models have proven to be accurate enough. After the numerical model is developed and validated by experiments, optimization and design work are conducted on both TEM and TEG.

Many previous optimization works assume fixed temperature boundary condition. However, this assumption is only applicable to limited practical circumstances. The effect of different boundary condition is not adequately investigated. This thesis studies the effect of different types of boundary conditions on the optimization of TEM and TEG, and it is found that the optimized geometry parameter, thermoelectric elements height, and cross-section area vary significantly under different boundary condition assumption. With this finding, the TEM and HEX are optimized simultaneously by Taguchi method taking into consideration the interactive effect. Also, the contributions of each factor to the output power variance are quantified.

This thesis provides a set of numerical models for TEG simulation, and an optimization

technique based on Taguchi method for preliminary design of TEG for waste heat recovery from exhaust gas. As low computation cost is required and the ability of considering different boundary conditions, the proposed numerical model and optimization method can be generalized to a broad range of waste heat recovery applications.

List of Figures

Figure 1.1 Keeling curve of carbon dioxide trend in atmosphere.....	23
Figure 1.2 Energy flow in Southeast Asia from energy source to end application. Source: The ASEAN energy system	26
Figure 1.3 Three key components of WHR	28
Figure 2.1 Definition of terms related with TEG.....	36
Figure 2.2 Typical waste heat and operating temperature [22].....	39
Figure 2.3 Thermoelectric material efficiency compared to generator system efficiency simulated for three potential applications	41
Figure 2.4 Diagram of a single TE couple [28]	42
Figure 2.5 output power of the TEG as function of TE element length under different ratio of cross-sectional area to thermoelements length [31].....	44
Figure 2.6 TEG output power for various leg lengths at different currents [32]	44
Figure 2.7 Nontraditional TEM design [34]	45
Figure 2.8 Diagram of Panasonic's TEG tube [44]	48
Figure 2.9 Solar-TEG system [52].....	51
Figure 3.1 TE element with a simple Dirichlet boundary condition.....	56
Figure 3.2 Discretization of TE element to find the open circuit voltage.....	57
Figure 3.3 Energy balance in TE elements	58
Figure 3.4 Thermal resistance network of a TEM	62
Figure 3.5 Modules contained in calculation sections	63

Figure 3.6 Outward appearance of TEM adopted in the experiments	67
Figure 3.7 Inward arrangement of the TEM adopted in the experiments. A total 127 TE couples of identical size of 2.5*2.5*1.5mm, where 1.5mm is the vertical length, integrate the module.....	67
Figure 3.8 Experimental setup for TEM level testing.....	68
Figure 3.9 Comparison of simulation and experiments at TEM level.	68
Figure 3.10 Temperature field calculated by ANSYS Mechanical. At hot side temperature of 750K, cold side temperature of 400K.	70
Figure 3.11 Electrical potential field calculated by ANSYS Mechanical. At hot side temperature of 750K, cold side temperature of 400K.....	70
Figure 4.1 Diagram of TEG system.....	73
Figure 4.2 Diagram of a TEM and HEX system	74
Figure 4.3 Straight fin HEX.....	75
Figure 4.4 Sudden expansion and contraction of flow channel	81
Figure 4.5 Sudden contraction of flow channel: (a) square reduction; (b) tapered reduction .	81
Figure 4.6 Sudden expansion of flow channel: (a) square expansion; (b) tapered expansion.	82
Figure 4.7 Parameter relationship in the integrated TEG model	84
Figure 4.8 Discretization of HEX flow channel after symmetric simplification.....	85
Figure 4.9 Energy flow in each zone	85
Figure 4.10 Flow chart of the integrated TEG model.....	86
Figure 4.11 Comparison of simulation and experiments	89
Figure 4.12 Temperature distribution of exhaust gas, TEG hot and cold surface, and cooling	

water with respect to their axial location of the HEX.....	93
Figure 4.13 Output power with various cooling water flow rates	94
Figure 5.1 Thermal resistance network of TEM model	97
Figure 5.2(a) Voltage, current and (b) power changes with TE element height under fixed T_H , $T_H=573K$, $T_C=303K$	100
Figure 5.3 (a) Voltage, current and (b) power changes with TE element height under constant temperature boundary condition; $Q_H=398W$, $T_C=303K$	101
Figure 5.4 Output power versus TE leg height under different fixed T_H , while $T_C=303K$	102
Figure 5.5 Output power versus TE leg height under different fixed Q_H , while $T_C=303K$...	102
Figure 5.6 Output power versus TE leg height under different FF . (a) Fixed T_H , and fixed T_C and (b) fixed Q_H and fixed T_C	103
Figure 6.1 Mean S/N ratio analysis in automotive application.....	115
Figure 6.2 Contribution of selected factors to the S/N ratio in automotive application	116
Figure 6.3 Effect of interactions in automotive application.....	116
Figure 6.4 Comparison of output power under the original and the optimal design parameters	118
Figure 6.5 Mean S/N ratio analysis in marine application.....	124
Figure 6.6 Contribution of selected factors to the S/N ratio in marine application	125
Figure 6.7 Effect of interactions in marine application	125

List of Tables

Table 1.1 Estimation of industrial waste heat recovery potential	24
Table 1.2 Most widely WHR technology for power generation [1]	29
Table 2.1 List of commercially available TEMs.....	42
Table 2.2 Selected commercial activities on TEG	46
Table 2.3 Investigation on TEG development in academia sector.....	49
Table 3.1 TE material properties used for ANSYS validation of the improved TEM analytical model.	71
Table 3.2 Comparison between results obtained by ANSYS Mechanical and by 1D analytical model.	71
Table 4.1 Calculation of Nu and f for laminar flow in a duct	80
Table 4.2 Input parameters for integrated TEG model validation [86].....	88
Table 4.3 Integrated TEG model parameters and configuration	92
Table 4.4 Output performance predicted by the integrated TEG model.....	93
Table 5.1 Input parameters for original working condition	98
Table 6.1 Selected factors and levels for automotive application.....	109
Table 6.2 Orthogonal array and simulation results in automotive application	111
Table 6.3 Response table for S/N ratios in automotive application	114
Table 6.4 Input parameters in marine application- baseline model	119
Table 6.5 Selected factors and levels in marine application	120
Table 6.6 Orthogonal array and simulation results in marine application	121

Table 6.7 Response table for S/N ratios in marine application.....	123
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List of Symbols

Latin letters

A	cross-section area (m ²)
D	hydraulic diameter of flow channel (m)
E	Open circuit voltage (V)
f	friction factor
g	standard gravity (m/s ²)
h	convective heat transfer coefficient (W/m ² K)
h_f	head loss due to friction (m)
I	electrical current (A)
j	current density (A /m ²)
k	thermal conductivity of fluid (W/m·K)
K	thermal conductance of TEM (W/ K)
l	length of TE legs (m)
L	length of flow channel (m)
Nu	Nusselt number
ΔP	pressure drop (Pa)

P	output power (W)
Pr	Prandtl number
q	heat flux density (W/m ²)
q_c	heat flux density by thermal conduction (W/m ²)
q_{cl}	heat flux density by thermal conduction from left (W/m ²)
q_{cr}	heat flux density by thermal conduction from right (W/m ²)
q_h	heat flux by convective heat transfer (W/m ²)
q_j	heat flux by Joule heating (W/m ²)
q_t	heat flux by Thomson effect
Q	heat flux (W)
R	<i>electrical resistance</i> (Ω)
Re	Reynold number
T	temperature (K)
v	fluid flow rate (m/s)
<i>Greek letters</i>	
α	Seebeck coefficient (V/K)
κ	thermal conductivity of TEM (W/m·K)

ρ	density (kg/m ³)
ρ_e	electrical resistivity ($\Omega\cdot\text{m}$)
π	Peltier coefficient
τ	Thomson coefficient (V/K)

Subscripts

C	cold side of TE leg
H	hot side of TE leg
n	n-type TE leg
p	p-type TE leg

List of Acronyms

HEX	Heat exchanger
PCM	Phase change material
TE	Thermoelectric
TEG	Thermoelectric generator
TEM	Thermoelectric module
WHR	Waste heat recovery
ZT	Figure of merit

CHAPTER 1 Introduction

1.1 Background

1.1.1 Energy market and potential for waste heat recovery

As shown in the Keeling curve, greenhouse gas emission has been increasing during the past decades. This is largely caused by burning of fossil fuels. One strategy to reduce the greenhouse gas emission is to improve the energy efficiency by waste heat recovery (WHR) [1].

Figure 1.1 Keeling curve of carbon dioxide trend in atmosphere

Besides the consideration for environment protection, there is also economic rationale for waste heat recovery. The energy flow in Southeast Asia from energy source to end application in 2011 is shown in Figure 1.2. The industrial and transportation consumption accounts for around 50% of total energy consumption. Most of energy source for transportation and industry is non-renewable like oil, coal and natural gas. During the process of burning fossil fuel, it is estimated that around 20% to 50% of industrial energy input is lost as waste heat.

The amount of waste heat in 2011 in Southeast Asia is assumed to be around 77 Mtoe (million tons of oil equivalent). This amount is equivalent to the power generated by 54 nuclear reactors (size of Daya Bay, China) by rough calculation. In the US [2], the industrial sector accounts for one third of total energy consumption in the country. The amount is estimated to be around 32 quadrillion Btu (1 Btu=1055 joules) per year and 1.68 billion tons of CO_2 emission per year. Table 1.1 summarizes the estimations of WHR potential by previous research. Blaney et al. [3] conducted a research in 1984 concluding that around 14.1 quadrillion Btu energy is lost, among them 1.6 quadrillion Btu energy could be recovered. Pelegriano et al. [4] conducted study in 2004 evaluating energy losses of manufacturing. From their perspective, around 20-50% of input energy, which is 1.6 quadrillion Btu, could be recovered through waste heat recovery effort. A study conducted in 2006 [5] estimated potential chemical energy contained in waste heat stream (uncombusted gas) is around 1.7 quadrillion Btu/yr. Johnson et al. [2] estimated that around 5 to 13 quadrillion Btu/yr energy is lost as waste heat in the industrial sector.

Table 1.1 Estimation of industrial waste heat recovery potential

Study	Estimation of Waste Heat Loss/recovery Potential
[6] Cook 1971	Waste heat losses in the USA total 50% of energy inputs
[3] Blaney 1984	Losses from exhaust gases from industrial processes and power generation sites total 14.1 quadrillion Btu/yr. About 1.5 quadrillion Btu/yr could be recovered at temperatures above 300°F.
[4] Pellegrino 2004	Waste heat could range from 20-50% of industrial inputs. Selected energy saving opportunities from waste heat recovery could total 1.6 quadrillion Btu/yr
[5] Viswanathan 2006	The chemical energy contained in exhaust gas streams totals about 1.7 quadrillion Btu/yr.

[2] Johnson 5 to 13 quadrillion Btu/yr of energy is lost as waste heat.
2008

Figure 1.2 Energy flow in Southeast Asia from energy source to end application. Source: The ASEAN energy system

Based on the temperature, waste heat source can be classified as high, medium and low temperature waste heat source [7] as follows:

High: 650 °C and higher

Medium: 232 °C to 650 °C

Low: 232 °C and lower

High temperature waste heat source has the advantage of highest quality, enabling higher efficiency power generation and higher heat transfer rate per unit area. However, high temperature also induces higher thermal stresses on heat exchanger materials and increased corrosions. Low temperature waste heat source has the largest quantity of WHR potential [7]: based on a reference temperature of 25 °C, in all industrial sector, roughly 60 % of waste heat is below 230 °C. But low temperature waste heat is very difficult to recover and the efficiency is relatively low. The medium temperature waste heat is more compatible with heat exchanger materials and more practical for power generation.

1.1.2 Review of existing waste heat recovery technology

Previous section shows that there is a significant amount of waste heat source available for waste heat recovery. Besides the waste heat source, there are other key components of the WHR process. Three key components in WHR are shown in Figure 1.3: 1) waste heat source. 2) WHR technology, and 3) the end use of recovered energy.

Figure 1.3 Three key components of WHR

Most commonly investigated WHR technologies are summarized and listed in Table 1.2 [7]. These technologies can be classified into two different types in terms of the form of working process. The first type includes: ORC, Kalina Cycle and traditional steam cycle. This type of WHR firstly exploits the waste heat to create mechanical energy and then drives an electric generator to produce electricity. Another type includes: TEG, piezoelectric generation, and these technologies can directly generate electricity from waste heat. The thermodynamic limitations are critical when selecting appropriate WHR technologies, since the efficiency of WHR is heavily dependent on the temperature of waste heat source. Generally, the power generation efficiency increases with higher temperature.

Table 1.2 Most widely WHR technology for power generation [1]

WHR technology	Temperature range	Typical source of waste heat	Capital cost (\$/kW)
Traditional Rankine Cycle	Medium, High	Exhaust from gas turbines, reciprocating engines, incinerators, and furnaces	\$1100 -- 1,400/kW
Organic Rankine cycle (ORC)	Low, Medium	Gas turbine exhaust, boiler exhaust, heated water, cement kilns	\$1,500 -- 3,500/kW
Kalina Cycle	Low, Medium	Gas turbine exhaust, boiler exhaust, cement kilns	\$1100 -- 1,500/kW
Thermoelectric Generation (TEG)	Medium, High	Gas turbine exhaust, solar thermal, heated water	\$20,000 -- 30,000/kW
Piezoelectric generation	Low	Not yet demonstrated in industrial application	NA

Traditional steam cycle uses the waste heat to generate steam and then drive the steam turbine. The traditional steam Rankine cycle is the most efficient option for WHR when the temperature of waste heat source ranges from 340-370°C. When the temperature is lower, steam Rankine will be less cost-effective, since lower temperature may not provide sufficient energy to superheat the steam. Organic Rankine cycle (ORC) works similar to traditional steam Rankine cycle. But instead of steam, ORC uses an organic, high molecular mass fluid with a liquid-vapor phase change as working fluid. These organic fluids usually have lower boiling temperature, which allows ORC to recover waste heat from a lower temperature

source [8]. Kalina cycles is also a thermodynamic process for converting thermal energy to mechanical power [9]. Unlike the Organic Rankine cycle, Kalina cycle uses a solution of two different fluids (usually ammonia and water) with different boiling temperatures. Since the mixture can boil at a range of temperature, Kalina cycle can extract more heat compared with a pure working fluid at certain temperature range [9].

1.1.3 Thermoelectric generators

TEG is a solid-state device that directly converts heat into electricity based on the Seebeck effect, which was discovered by Thomas Johann Seebeck in 1821 [10]. Historically, due to the low efficiency, TEG was only used in small-scale applications like thermocouples, thermometers, and space applications. In the 1990s, using the thermoelectric effect in WHR applications began to draw lots of attention with the development of nanotechnology on thermoelectric materials.

TEG is a solid-state device that can directly convert heat energy into electricity by means of charge carriers, which work similar to working fluid. Unlike the WHR technologies that transform waste heat into mechanical energy and then convert it into electricity, TEG has the unique advantage of no moving parts, and therefore no noise, long lifetime and high reliability. In the case of passenger ships, automobiles, reducing the noise level is especially important. Also, maintenance on remote applications, like sea and space, is expensive, therefore the high reliability of TEG has a unique advantage, making this technology ideal for marine, space, and automotive WHR. However, compared with other WHR technologies, TEG has not yet been widely implemented in practical applications, and only a few prototypes have been reported in the literature [11, 12].

1.2 Objectives and contributions

While the thermoelectric materials have been continuously developed for several decades, the simulation and design of TEMs and systems have been relatively stagnant with quite low efficiencies. This has raised urgent needs to build efficient

tools for simulation and design of TEGs. Accordingly, the major objectives of this study are summarized as follows:

- (1) A reliable TE model is the prerequisite for the investigation and preliminary design of TEG. This study aims to propose a multi-physics TE model with high accuracy and low complexity, which can be used for material selection and preliminary design of TEG.
- (2) Lots of previous TE studies focus on the model level and simplify the heat transfer systems of TEG. However, the heat transfer system design heavily interacts with the TEG design. This study aims to build an HEX model and system level TEG with high accuracy and low computational complexity.
- (3) The TEM is the most critical part of a TEG system. The optimization design theory of TEM has yet been adequately investigated. This study aims to propose a design tool for preliminary parameter selection and design of TEG that can be used in different engineering conditions.
- (4) Different HEX designs provide different thermal boundary conditions for TEM designs, and different TEM designs also affect the optimal HEX selection. This thesis aims to provide a systematic approach to co-optimize the TEM and HEX.

According to the aforementioned objectives, the major contributions of this thesis are summarized as follows:

- (1) In this thesis, a multi-physics TE model is proposed, which is based on fundamental TE transportation equations and first law of thermodynamics. An experimental setup is built to verify this model and the model is proved to be accurate. This TE model will be the basis for TEG modeling and design.
- (2) This study proposes a system level numerical model for TEG, which consists of TE and HEX model. This numerical model enables the feasibility study and preliminary simulation and design of TEG.
- (3) Optimization and design of TEM is conducted at different thermal boundary conditions: Dirichlet condition, Neumann boundary condition, and Robin boundary condition. This study compares the difference on optimal design parameter selection under different boundary conditions.

-
- (4) System level optimization is conducted by simultaneously considering TEM and HEX design parameters. The effect of TEM and HEX design parameters on output power are investigated by the Taguchi method. Using this method, key design parameters and interactive effect between design parameters have been identified.

1.3 Organization of the Thesis

The thesis consists of seven chapters, which have been organized as follows:

Chapter 1 briefly introduces the background of the study, including potentials for WHR, current WHR, including TEG. The objectives and major contributions are also presented.

Chapter 2 presents a detailed and in-depth literature review related to the research topics of this thesis. The chapter begins with the fundamental of the TE principle, and introduces the transportation equations, features, current device and system development status.

Chapter 3 introduces an improved TEM model, which is capable of solving both steady state and transient TE governing equations. The TE transportation equations are established to describe the energy flow within the TE material and the first law of thermodynamics is also applied. Following that, the governing equations are solved under different assumptions and boundary conditions. An experimental setup is built to verify the accuracy of the model in terms output power. Besides, a 3-D numerical model is developed in well prove software ANSYS to validate the analytical model in terms of heat flux.

Chapter 4 focuses on the HEX model development and the integration of TEG system model consisting of TEM and HEX model. The HEX model incorporates empirical heat transfer equations to calculate the rate of heat transfer rate in HEXs. Following that, the HEX model is integrated with the TEM model, which is developed in Chapter 3.

In Chapter 5, the TEM optimization in terms of output power is carried out under different thermal boundary conditions. Different combinations of thermal boundary conditions, including Dirichlet condition, Neumann boundary condition, and Robin boundary condition are imposed based on actual engineering problems to investigate their effect in module geometry optimization.

In Chapter 6, an optimization scheme for the TEG system is proposed. The optimization scheme uses a Taguchi statistical method which analyzes the effect of each design parameter (namely TEM height, TEM fill-ratio, TEM A_n/A_p ratio, the HEX length and the HEX material). In the Taguchi analysis, a L_{27} orthogonal array with five design parameters at three levels has been considered for both automotive and the marine applications.

Chapter 7 summarizes the key conclusions of this thesis. Some potential research topics related to this thesis are also recommended for future work.

CHAPTER 2 Literature Review on Thermoelectric Generator

2.1 Introduction

TEG has been used in space applications as radioisotope thermoelectric generator (RTEG) for decades [10]. However, because of its low efficiency, it was used as temperature sensor or remote sensor power supply only, until the efficiency greatly improved in the recent years [13]. During the past two decades, a wide variety of new TE materials exhibiting high efficiency over a wide temperature range have been discovered. With the development of high efficiency TE materials, recovering energy from various heat sources by TEG technology becomes possible and many researches and efforts have been devoted to TEG development. In this chapter, a thorough literature review is carried out on the knowledge of TEG and the design of TEG including the small scale TEM and the aggregate level TEG system.

The rest of this chapter is organized as follows. Section 2.2 briefly introduces the current status of TE material development. Section 2.3 reviews the TEM development status, including basic TEM structure, different module design, the efficiency of current TEMs. Section 2.4 provides an in-depth review of the existing research on TEG system developments. Section 2.5 summarizes the current literature and points out the existing challenges, which will be extensively discussed and addressed in the following chapters of the thesis.

The main terms related with TEGs from small size to system size are defined in Figure 2.1.

Figure 2.1 Definition of terms related with TEG

A single TE pillar is called TE leg or TE element. TE leg is usually manufactured in cuboid shape. TE elements have n-type and p-type legs depending on the TE material properties [10].

A pair of TE legs is called TE couple, where the n-type and p-type legs are connected by metal conductors. Between the TE elements and the metal conductors, a barrier layer is usually inserted to avoid the diffusion of TE material into the metal conductors [14].

Several TE pair connected in electrically serial is called TEM. In some literature and industry reports, TEM may also be referred as TE device (TED) [15]. TEM is made modular for maintenance, easy replacement, and scalability. The output power of a single commercial TEM usually ranges from several watts to 50 watts.

Several TEMs mounted together on an HEX and used for generating power is called TEG, or referred as TEG system. The TEG system is a complete system that can be directly connected to a waste heat source for power generation. The output power of current TEG systems can range from several hundred of watts [16] to tens of kilowatts [17].

The term “thermoelectric effect” actually encompasses three separately effects:

Seebeck effect, Peltier effect, and Thomson effect [18]. Seebeck effect is the direct conversion of temperature difference into electricity. The Seebeck effect is described locally by the creation of an electromotive field:

$$E = \alpha \Delta T \quad (2.1)$$

where α is the Seebeck coefficient, ΔT is the temperature difference between hot and cold side of a TE element.

The Peltier effect is a phenomenon that is produced in the junctions of two different conductors. At the electrified junction, heat flux is found to be greater or less than pure Joule heating value. The difference between the actual value and what would be expected in a homogeneous conductor due to simply Joule heating, depends on the magnitude and direction of the current, temperature and materials of both sides. This phenomenon is called the Peltier effect, named after the French physicist Jean Charles Athanase Peltier. It can be expressed as [10]:

$$q_{pel} = (\pi_p - \pi_n)J \quad (2.2)$$

where π_p , π_n , are Peltier coefficients at two sides of the junction, J is the current density, and q_{pel} is the heat flux at junction due to Peltier effect.

In a conductor rod with a temperature difference applied at two sides, if an electric current flows through this rod, the heat developed is greater or less than pure Joule heating. This difference depends on the magnitude and direction of the current, the temperature, and the material. This phenomenon is called Thomas effect. Thomas effect is caused by the variance of Seebeck coefficient inside the TE material, and it could be regarded as a continuous version of the Peltier effect. Heat produced due to Thomson effects is calculated as:

$$q_{tho} = -\tau J \bullet \nabla T \quad (2.3)$$

where τ is the Thomson coefficient, q_{tho} is the heat flux at junction due to Thomson effect, J is the current density, T is the temperature in the TE material.

The aforementioned Peltier, Seebeck and Thomson effects are essentially a single effect that manifests differently. The equations describing their relationships are named as Kelvin equations in memory of Lord Kelvin (William Thomson) who found the relation between Seebeck and Peltier effects and derive the relation from the thermodynamic law [10]. Those relations are as follows:

First Kelvin relation [19]:

$$\tau = \frac{d\pi}{dT} - \alpha \quad (2.4)$$

where the α is the Seebeck coefficient.

The first Kelvin relation describes the relationship between Thomson, Peltier and Seebeck coefficients.

The second Kelvin relation is the relationship between Seebeck coefficient and Peltier coefficient [19]:

$$\pi = T\alpha \quad (2.5)$$

Substituting the second Kelvin relation into the first Kelvin relation, the following relation between Seebeck coefficient and Thomson effect is obtained as:

$$\tau = T \frac{d\alpha}{dT} \quad (2.6)$$

The state of the art of TE material, TEM, TEG system research and developments is discussed in the following sub-section.

2.2 State of art of thermoelectric material development

TE materials can be classified by their material structure and composition. One commonly adopted classification is: chalcogenide, clathrate, skutterudite, half-Heusler, silicide, and oxide [20]. Chalcogenide material is one of the most widely used TE materials. Bismuth telluride and lead telluride both belong to Chalcogenide

material [20]. Bismuth telluride materials are dominating the commercial low temperature TEM market, while lead telluride has better performance at higher temperatures (500-600°C). Material development of clathrates and skutterudites usually nanostructuring, to block phonon transportation and optimize electron concentration.

TE material properties such as Seebeck coefficient, thermal resistance and electrical resistance vary with temperature. Therefore, based on their optimum working temperature, TE materials are usually classified as low temperature TE materials (<500K), middle temperature TE materials (500–900 K) and high temperature TE materials (>900 K) [21]. Some of the most investigated TE materials are listed in

Figure 2.2 [22].

Figure 2.2 Typical waste heat and operating temperature [22]

The figure of merit is an important parameter that describes the performance of a certain TE material. It is defined as [23]:

$$ZT = \frac{\alpha^2 T}{\rho \kappa} \quad (2.7)$$

where α is the Seebeck coefficient, ρ is the electrical resistivity, and κ is the thermal conductivity of a single TE leg. Figure of merit is highly related with the efficiency of a TE device. A larger ZT is always preferred.

For the low temperature range (<500K), Bi_2Te_3 alloys have shown the greatest ZT for both n-type and p-type legs. Peak ZT value of different Bi_2Te_3 alloys are usually in the range of 0.8 to 1.1 [21]. Peak ZT of different Bi_2Te_3 can be achieved at different temperatures by adjusting the carrier concentration, enabling the tuning of TE material for a specific application [24].

For middle temperatures (500–900 K), the TE materials are usually developed based on group-IV tellurides, such as PbTe , GeTe or SnTe [25, 26]. N-type middle temperature TE materials have been reported to reach Peak $ZT > 1$. P-type middle temperature TE materials have been reported to reach Peak $ZT > 1.2$ [21].

For high temperature TE materials (>900 K), silicon-germanium (SiGe) based alloys are usually used for both n-type and p-type legs. However, the ZT value of high temperature TE material is relatively low due to the high lattice thermal conductivity [21]. Basu et al. [27] reported a ZT of 1.8 at 800 °C for $\text{Si}_{80}\text{Ge}_{20}$. Wang et al. [28] reported a ZT of 0.67 at 727°C for $\text{Si}_{80}\text{Ge}_{18}\text{B}_2$.

The efficiency of a TEM is denoted by η , and defined as:

$$\eta = \frac{\text{maximum energy to the load}}{\text{absorbed heat at hot junction}} \quad (2.8)$$

The maximum efficiency for a given temperature difference could be written as (the detailed derivation is elaborated in Appendix A):

$$\eta = \frac{T_H - T_C}{T_H} \frac{\sqrt{1 + ZT} - 1}{\sqrt{1 + ZT} + T_C / T_H} \quad (2.9)$$

where T_H is the hot side temperature, T_C is the cold side temperature, ZT is the figure of merit.

Another parameter called power factor is defined as $\alpha^2\sigma$, where σ is the electrical conductivity given by $1/\rho$, ρ being the resistivity of the material.

Based on this definition, the material efficiencies of some common materials have been reported. For a low temperature material, an efficiency up to 8.5% has been achieved for $MgAg_{0.965}Ni_{0.005}Sb_{0.99}$ [29]. For a middle temperature material, based on a ZT value of 1.4 [30] and Eq. (2.8), the theoretical material efficiency would be around 17%, at $T_H = 500^\circ\text{C}$ and $T_C = 30^\circ\text{C}$.

Although the current development of TE material is promising, the TEM and HEX designs are still important limiting factors. The efficiency calculated by Eq. (2.8) is the material efficiency, and the overall efficiency can be much lower compared with the material efficiency, as shown in Figure 2.3. The system efficiency is 32%, 33%, and 59% lower than material conversion efficiency for the water heater, automotive exhaust, and industrial furnace applications, respectively [20]. Therefore, there is an urgent need to develop high efficiency TEM and TEG systems. The current research and development status of TEM and TEG are discussed in the following sections.

Figure 2.3 Thermoelectric material efficiency compared to generator system efficiency simulated for three potential applications

2.3 State of art of thermoelectric module development

A lot of work has been devoted to the development of TEM and TEG. The most common design of a commercial TEM is a “ π ” shape configuration as shown in Figure 2.4 [18]. One TE couple is composed by two separate semiconductor legs, p-type and n-type. In actual applications, lots of TE couples are connected electrically in series and thermally in parallel, forming a TEM. The ceramic layer is acting as electrical insulator and thermal conductor and the copper layer serves as electrical interconnector.

Figure 2.4 Diagram of a single TE couple [28]

Lots of off-the-self TEM products are made based on this “ π ” shape configuration. Several representative products have been summarized in Table 2.1. As shown in this table, the output power based on the same material can vary from 7 watts to 21.6 watts, which indicates the importance of proper TEM optimization and design.

Table 2.1 List of commercially available TEMs

Product name	Manufacturer	Dimensions (mm*mm)	Materials	Hot temperature	Output power
TEG1-12611-6.0	TECTEG MFR.	56*56	Bi_2Te_3	573 K	14.6 W
TEHP1-24156-1.2	Thermonamic	56*56	Bi_2Te_3	652 K	21.6 W
PowerCard- γ^{TM}	Alphabet Energy	NA	NA	773 K	9.2 W
TGPR-22W-7V	TEGpro	56*56	Bi_2Te_3	652 K	21.6 W
TEG1-PB	TECTEG MFR.	56*56	$PbTe$	623K	21.7 W
TEG1-4199-5.3	TECTEG MFR.	40*40	Bi_2Te_3	573 K	7.5 W

The first step in the TEM design is building an efficient and accurate TEM model and selecting the appropriate TEM geometry parameters. A lot of research has been devoted to developing TEM modeling and design. In 2013 G. Min et al. [31] investigated the effect of TEM length on the output performance under constant heat flux. As shown in Figure 2.5, the output power monotonically increases with the increase of TE element length. However, this conclusion only applies to certain conditions (material properties and temperature range).

Figure 2.5 output power of the TEG as function of TE element length under different ratio of cross-sectional area to thermoelements length [31]

In another study by Meng et al. [32], it is found that the power firstly increases and then decreases as the TE element height increases, as indicated in Figure 2.6. These controversial results show a need for systematic investigation of TEM design parameters at different conditions.

Figure 2.6 TEG output power for various leg lengths at different currents [32]

Besides the TE element length, the A_n/A_p ratio, which is the ratio of cross-section area of the n-type element respect to the p-type element, is also a critical parameter to consider to optimize the output performance. Although most commercial TEMs have equal size p-type and n-type legs, they are not necessarily identical. Actually, there exists an optimal ratio of p-type leg area to n-type leg area that maximizes the output performance [33]. Rezanian et al. [33] built a simulation model in ANSYS and studied the effect of A_n/A_p ratio on the output power and found that for n-type material, $Mg_2Si_{1-x}Sn_x$ and p-type material, Zn_4Sb_3 , the output power is maximized when $A_n/A_p < 1$.

Besides the conventional “ π ” shape TEM configuration, there is some research devoted to innovative device designs, which are reported to be more suitable under certain circumstances. Ibrahim et al. [34] investigated different shapes of TEMs, as shown in Figure 2.7, and conducted optimization on some parameters including: cross section area of TEM leg, height of TE leg, and shape factor, and found that the optimal design is not uniform width.

Figure 2.7 Nontraditional TEM design [34]

Although lots of efforts have been put on TEM development and optimization, most of these investigations are relatively preliminar, and the design parameters need to

be explored further in a systematical way.

2.4 State of art of thermoelectric generator system development

Besides the development of high efficiency TE materials and TEM, the TEG system design is also critical to the overall output performance. Lots of commercial activities and academic investigations have addressed the development of TEG systems.

Most research activities and development projects on TEG are developed by automotive manufacturers, such as Ford, BMW, GM, Volkswagen, which have developed TEG systems to improve the fuel economy of their automobiles. The reported output powers are in the range of a few hundreds of watts to one kilowatt [35]. Besides automotive companies, some start-up companies are also working on TEGs for various applications, such as Alphabet Energy (USA), Gentherm Inc. (USA), II-VI Inc. (USA), Ferrotec Corporation (Japan), Laird Plc. (UK), and Komatsu Limited (Japan). However, in order to further improve the efficiency, there are still many challenges that need to be solved regarding the use of certain materials in the devices. Several representative activities in TEG system development are listed in Table 2.2.

Table 2.2 Selected commercial activities on TEG

Company or institute	Application	Material	Efficiency /Power	Commercially available
Gentherm [36]	Automotive thermal management, power generation	Bi_2Te_3	550W	Yes

Evident (GMZ Energy)	Power generation,	High T: Half Heusler (ZT:1.0) Medium T: Skutterudite (ZT:1.0) Low T: Bi ₂ Te ₃ (ZT:1.0)	1-5% fuel economy	Yes
Fujifilm [37]	Human body	PEDOT [38]	NA	No
Alphabet Energy [17]	Mining and industry operation	Silicon-based materials	5% fuel economy	Yes
Panasonic [39]	Geothermal and waste heat	Bi ₂ Te ₃	0.4W/cm	No
Crane (BSST) [40]	3L BMW engine	Segmented TEM, half-Heusler and Bi ₂ Te ₃	125W	No
Kim et al. [41]	Radiator of 2L engine SUV	72 Bi ₂ Te ₃ TEMs	75W	No
Perpetua Power [42]	Wireless sensors	Thin-film Bi ₂ Te ₃	N/A	Yes

Alphabet Energy [17] is a leading company in TEG power generation with products ranging from small TEMs to TEG systems for industrial WHR. They claim their TEG system product E1 can achieve 5% fuel economy and generate the highest output power compared with other TEG products in the marker. The Evident [43] (former GMZ energy), has developed both TEMs and TEG systems. Rather than the waste heat recovery application, they tested their TEG for solar thermal application.

Panasonic [39] have developed a tubular shape TEG, which is designed for extracting geothermal, waste heat, or other thermal energy in contained liquid, as shown in Figure 2.8. A 10-cm long of this kind of TEG tube can produce about 4.7 W of electricity with 90°C hot water inside and 10°C cold water outside. Research activity is still undergoing on system design, optimization in manufacturing and feasibility studies.

Figure 2.8 Diagram of Panasonic's TEG tube [44]

Besides the industry sector, there have also been numerous contributions to the TEG simulation and design in academia. Several representative works have been summarized in Table 2.3. As shown in this table, current efficiencies of TEG systems are all below 5%. These efficiencies are calculated by comparing electrical output power to the heat input to the hot side. If the efficiency is calculated by comparing the electrical output power to the whole thermal energy contained in the exhaust gas, the efficiency is even lower, as the heat exchanger efficiency is way below 100% [45].

Research related to TEG system integration in academia has focused on different HEX design and TEM packaging. Liu et al. [12] compared the design of different HEXs and found that the HEX design has a significant influence on the output power. Sumeet et al. [43] compared the effect of different HEX topologies and concluded that the transverse design can achieve the maximum output power, 729.8 W, which is 95 W higher than the hexagonal design. Chen et al. [46] optimized the

design parameters of heat sink for TEM, and found that the heat sink length is the most important geometric design parameter as compared with the length and width of the heat sink, height and thickness of the fins. Zhang et al. [47] investigated design parameters such as height of TE couples in each section and area ratio of n-type material to p-type material, assuming fixed temperatures T_H and T_C (refer to Fig. 1) as boundary conditions; they compared different configuration on simulation and found that the module can achieve a record-high efficiency up to 12.0% by the optimal design. Chen et al. [48] investigated the effect of design parameters like the number of TE couples on output power and efficiency of a two-stage TEM, assuming a fixed temperature boundary condition, and found that the optimal TE couple number of the high temperature stage should always be smaller than that of the low temperature stage.

Table 2.3 Investigation on TEG development in academia sector

Year	Affiliation	Heat source	Output power	Efficiency	Method
2010	LPMCN, France [49]	11.0 L diesel engine	800-1000W	Not available	Simulation
2011	Clarkson University [50]	GM sports utility vehicle (SUV) engine exhaust	100-450W	1.25% fuel economy	Simulation
2012	Department of energy, USA [51]	BMW X6	480W	3.45% fuel economy	Experiments and simulation

2013	Purdue University [52]	GM engine	553W	3.33%	Simulation
2015	Wuhan University of Technology [16]	Truck engine 20-40KW	944W	1.85%	Experiments and simulation
2016	Industrial Technology Research Institute of Taiwan	Industrial Boiler	1kW	Not available	Experiments

Besides the conventional TEGs which recover energy from waste heat, original TEGs to harvest energy from other sources also have been proposed. Chen et al. [53] developed a novel solar TEG system. The diagram of this system is shown in Figure 2.9. This system combines both a solar system and the TE device. The low material cost makes this system competitive. Compared with PV, much less semiconductor material is needed as the absorber is metal, which is much cheaper than semiconductor. This system could generate hot water during the day and produce electricity at night, functioning similar to a heat storage system. Experimental testing shows that the efficiency of such a system is around 4% at a solar radiation flux of 1.0 kW/m^2 [54].

Figure 2.9 Solar-TEG system [53]

As shown above, the efficiencies of the mentioned TEG systems are all below 5% [16, 53], and a proper TEG topology design and parametric study can have significant influence on the output power and efficiency performance. In order to build an efficient TEG system, the first step is to build an accurate and efficient simulation tool. Lots of numerical models have been proposed to simulated TEG, from simplified analytical models [55] to complex 3-D FEM models [56].

G. Fraisse et al. [57] reviewed different TEG models, including simplified model, improved simplified model, analytical model, electrical analogy model and ANSYS (FEM) model, and compared their computational complexity and accuracy. Due to their simplicity and reasonable accuracy, the simplified and improved models are most widely adopted at system level simulation and preliminary design of TEG [52, 58, 59]. ANSYS (FEM) is a more accurate but more time-consuming method, therefore it is usually used for small scale simulation and design, like single TE couple or single TEM [33, 60, 61].

Another challenge in modeling TEGs is specifying the appropriate thermal boundary condition. Many established studies assume a constant temperature at the boundary of TE legs [59, 62]. Gao et al. [31] claim that in some circumstances, for example, in the case of radioisotope or solar TEG, compared with constant temperature boundary condition, a fixed heat input boundary condition is more

applicable for the TEG system modeling and design. While in other circumstances, temperature and heat flux at TE leg boundaries both vary with different designs and operating conditions. Take for instance the situation that the engine exhaust gas flow through the exhaust pipe with TEG on the pipe wall, the temperature and heat flux at TEM boundaries both changes with different module designs.

2.5 Summary

In this chapter, the current status of TEGs has been reviewed, including: TE material, TEM device development, and TEG. The emphasis is placed on the related topics of TEM, TEG designs and integration. Existing works have provided valuable insights into these topics. However, more research should be done to make further improvements, especially for improving the efficiency and accuracy of the simulation model, and the effect of different design parameters. Moreover, the effect of different boundary condition assumption on the design of TEGs has not been adequately investigated. Driven by the high demand of waste heat recovery, this thesis aims to build an accurate and efficient simulation model and provide guidance on the design and optimization of TEGs.

CHAPTER 3 Thermoelectric Element and Thermoelectric Module Model Development

3.1 Introduction

As defined in Section 2.1, the TEM is an essential part defined in the whole TEG system. The reliable estimation of TEG output power highly depends on the accuracy and efficiency of TEM modeling. Despite this, there are still research gap in the modeling of TEMs. Many existing numerical models for TEM performance prediction, design and optimization assume that the material properties are constant from the hot-end to the cold-end [63-67], and the variation of material properties with temperature along the TE element, electrical and thermal contact losses at the junctions [68] are usually neglected.

ANSYS (FEM) is more accurate but the most time consuming method, therefore it is usually used for small scale simulation and design, like single TE couple or single TEM consisted of several TE couples [33, 60, 61]. Due to simplicity and reasonable accuracy, the simplified analytical model and improved simplified model [52, 58, 59] are most widely adopted in system level simulation and preliminary design of TEG. G. Minet et al. [31] developed a simplified 1-D model and used it for the parametric study of TE element height. Rowe et al. [63] developed a TEG model which considers all thermal and electrical resistances, and the effect of contact resistances is also discussed. However, this model neglects the Peltier and Thomson effects. Circuit equivalent models [69], which consider the TEM similar as an electrical circuit, were also developed for simulation and design. However, this study [69] assume the inner TEM electrical resistance equal to the external load resistance, limiting the model applicability. All aforementioned models neglect the Thomson effect, and assume a symmetric distribution of the Joule heat.

An efficient TEM model with enough accuracy is needed. In this chapter, the basic transportations [10] are solved to develop an 1-D analytical model, simulating the energy transform inside TEM. Based on these basic equations, a simplified

analytical model is built to predict the output power and heat flux at both hot and cold side of the TEM. Experiments are conducted on a lab-scale TEM to verify the proposed analytical model, and an ANSYS model is also developed to evaluate the accuracy of the proposed analytical model. After that, a methodology to calculate the TEM key design parameters, Seebeck coefficient, thermal conductance and electrical resistance is developed.

The rest of the chapter is organized as follows. Section 3.2 introduces the basic transportation and energy conservation equations, which constitute the governing equations of TEM. Section 3.3 proposes an analytical TEM model. Section 3.4 describes the experimental setup and procedures for TEM model validation. Section 3.5 presents the ANSYS model development and validation, while Section 3.6 draws the key conclusions

3.2 Governing equations and boundary conditions for thermoelectric elements

The physical phenomena inside TE material can be described at two different levels: quantum mechanical and macroscopic level using transportation equations [70]. Quantum mechanical model by Boltzmann equation is the most fundamental and accurate method to simulate the basic material properties. However, the quantum mechanical model is too complex for engineering problems. On the other hand, the numerical model at macroscopic level is more practical and with enough accuracy.

In this study, a macroscopic level model is proposed using transportation equations, and solved by an iterative method. This model is more accurate compared with the previous simplified model, as it considers the temperature dependent material properties: Seebeck, Thompson effect, thermal conductivity, electrical conductivity, etc.

In the TE material part, the governing equations are derived with respect to the multi-physical phenomena: Seebeck effect, Peltier effect, Joule heating and Thomson effect. The heat flux conservation and electrical charge conservation

equation are shown below:

$$\frac{\partial \mathbf{q}}{\partial x} + \rho c \frac{\partial T}{\partial t} = \mathbf{j} \cdot \mathbf{E} \quad (3.1)$$

$$\frac{\partial j}{\partial x} + \frac{\partial \rho_e}{\partial t} = 0 \quad (3.2)$$

where $\mathbf{j}$ is the electrical current density vector and $\mathbf{E}$ is the electrical field vector, t is the time, ρ_e is the carrier density.

Besides the conservation equations, based on Onsager-Callen theory on irreversible thermodynamics [71, 72], electrical current and heat flux are coupled together as described by the following TE constitutive equations:

$$\mathbf{q} = \mathbf{j}\pi - \kappa \frac{\partial T}{\partial x} \quad (W / m^2) \quad (3.3)$$

$$\mathbf{j} = \sigma \mathbf{E} - \sigma \alpha \frac{\partial T}{\partial x} \quad (A / m^2) \quad (3.4)$$

where π is the Peltier coefficient, κ is the thermal conductivity, σ is the electrical conductivity, and α is the Seebeck coefficient.

In Eq. (3.3), the first term on the right-hand side is the heat flux induced by Peltier effect, from which it can be seen that an electrical current can cause a heat flux even if there is no temperature gradient. The second term on the right-hand side is the heat flux induced by heat conduction.

In Eq. (3.4), the second term on the right-hand side is induced by Seebeck effect, from which it can be seen that temperature gradient can cause an electrical field in the absence of electrical current.

Substituting Eq. (3.3) and Eq. (3.4) to Eq. (3.1) and Eq. (3.2), the transient TE equation is obtained as:

$$\rho c \frac{\partial T}{\partial t} = \frac{j^2}{\sigma} + \frac{\partial}{\partial x} \left(\kappa \frac{\partial T}{\partial x} \right) - T \mathbf{j} \frac{\partial \alpha}{\partial x} - T \alpha \frac{\partial \mathbf{j}}{\partial x} \quad (3.5)$$

3.3 An improved analytical model regarding the thermoelectric elements

3.3.1 Prediction of the output performance

The objective of this section is to build a numerical model to predict the output power of a TEM under a Dirichlet boundary condition, i.e. a specified temperature boundary condition. As stated in Eq. (2.1), the open circuit voltage is proportional to the temperature difference.

Figure 3.1 TE element with a simple Dirichlet boundary condition

Therefore, if a temperature difference is applied to a TE element, as shown in Figure 3.1, the voltage generated by the Seebeck is usually calculated as:

$$E = \alpha(T_H - T_C) \quad (3.6)$$

However, the Seebeck coefficient is a temperature dependent property [10]. Therefore, it is more accurate to calculate the voltage as:

$$E = \int \alpha(T) dT \quad (3.7)$$

The open circuit voltage given by Eq. (3.7) could be calculated by discretization. As shown in Figure 3.2, the TE element is discretized into n small zones:

Figure 3.2 Discretization of TE element to find the open circuit voltage

The open circuit voltage can be calculated by adding the voltages in each zone, as shown in Eq. (3.8):

$$E = \sum_1^n (\alpha_n \Delta T_n) \quad (3.8)$$

The first step is to find the temperature profile $T(x)$, which can be calculated by solving Eq. (3.5), the TE governing equation under transient state.

The following paragraphs will focus on solving the temperature profile $T(x)$. Assume the charge density does not change, as shown in Eq. (3.9):

$$\frac{\partial j}{\partial x} = 0 \quad (3.9)$$

Then Eq. (3.5) is reduced to:

$$\rho c \frac{\partial T}{\partial t} = \frac{j^2}{\sigma} + \frac{\partial}{\partial x} \left(\kappa \frac{\partial T}{\partial x} \right) - T \mathbf{j} \frac{\partial \alpha}{\partial x} \quad (3.10)$$

This equation could be explained in a more straightforward way, which enables the later simplification based on its physical meaning. A small section with infinite small height dx in the TE material is shown in Figure 3.3.

Figure 3.3 Energy balance in TE elements

According to Fourier's law, heat flux entering the control volume through the bottom face through to heat conduction is:

$$q_{cb} = -\kappa A \frac{\partial T}{\partial x} \quad (3.11)$$

Similarly, heat leaving the control volume through the top face by heat conduction is:

$$q_{ct} = \frac{\partial}{\partial x} \left(-\kappa A \frac{\partial T}{\partial x} \right) dx - \kappa A \frac{\partial T}{\partial x} \quad (3.12)$$

Thus, the net heat flow into this control volume dx by heat conduction is:

$$q_c = \kappa A \frac{\partial^2 T}{\partial x^2} dx + A \frac{\partial \kappa}{\partial x} \left(\frac{\partial T}{\partial x} \right)^2 dx \quad (3.13)$$

The heat generated in this control volume due to Joule heating is:

$$q_j = \frac{I^2}{A^2} \rho_e A dx \quad (3.14)$$

where ρ_e is the electrical resistivity, which is the reciprocal of electrical conductivity.

Based on Eq. (2.6), the third term on the right-hand-side of Eq. (3.10), could be considered as heat generated due to Thomson effect in this control volume:

$$q_t = -\tau I \frac{\partial T}{\partial x} dx \quad (3.15)$$

According to the energy balance, the inner energy change is equal to the net heat flow, which is given as:

$$\rho c A \frac{\partial T}{\partial t} dx = q_l + q_t + q_c = \frac{I^2}{A^2} \rho_e A dx - \tau I \frac{\partial T}{\partial x} dx + \kappa A \frac{\partial^2 T}{\partial x^2} dx + A \frac{\partial \kappa}{\partial x} \left(\frac{\partial T}{\partial x} \right)^2 dx \quad (3.16)$$

Further simplifying Eq. (3.16) to steady state, the governing equation then becomes:

$$\frac{I^2}{A^2} \rho_e - \tau \frac{I}{A} \frac{dT}{dx} + \kappa \frac{d^2 T}{dx^2} + \frac{d\kappa}{dx} \left(\frac{dT}{dx} \right)^2 = 0 \quad (3.17)$$

The boundary condition is at $x=0$, $T(0) = T_C$; $x=l$, $T(l)=T_H$.

By using a polynomial method, the solution to Eq. (7) is found as [73] [74]:

$$\theta = \xi^2 + a\xi(1 - \xi) + e^{b\xi} (C_1 \cos(d\xi) + C_2 \sin(d\xi)) + \sum_{r=0}^M w_r \xi^r \quad (3.18)$$

where θ is a dimensionless temperature, defined as:

$$\theta = \frac{T - T_c}{T_H - T_c} \quad (3.19)$$

ξ is a dimensionless distance, defined as:

$$\xi = \frac{x}{L} \quad (3.20)$$

and a , b , d , and w_r are parameters that depend on θ , as shown in Appendix B.

Further simplification could be made by neglecting the Thomson heat effect, which is considered negligible in most of the cases [15] because its contribution to the total heat input and output power is relatively small. As the Thomson term is $\tau I \Delta T$, with $\tau = T \frac{d\alpha}{dT}$, this term is negligible if the Seebeck coefficient does not have large gradient or the temperature difference across the device is small. It is reported that the Thomson heat term could be 150 times smaller compared with the Joule heating [75]. Therefore, it is a reasonable assumption to neglect the Thomson term. Then the temperature profile is:

$$T = (T_H - \frac{x}{l} \Delta T) + \frac{I^2 \rho}{2\kappa} x(l - x) \quad (3.21)$$

The model developed above can be implemented by using discretization. Although it is accurate, it could be computationally complex in some cases. Therefore, a lumped parameter model is also introduced in this section, for preliminary design where high processing speed is required but there is no need for high accuracy.

In this lumped parameter model, the TE element is considered as a box with uniform thermal and electrical properties. With this assumption, the heat flux and

output power become [10]:

$$\begin{aligned} Q_H &= \alpha_H IT_H + K\Delta T - \frac{1}{2} RI^2 \\ Q_C &= \alpha_C IT_C + K\Delta T + \frac{1}{2} RI^2 \end{aligned} \quad (3.22)$$

where K is the thermal conductance and R is the electrical resistance.

With respect to energy balance, the work generated by TEM is simply heat inflow minus heat outflow. Therefore, the output power is given by:

$$P = (\alpha_H T_H - \alpha_C T_C)I - RI^2 \quad (3.23)$$

The efficiency η is defined as:

$$\eta = \frac{P}{Q_H} = \frac{(\alpha_H T_H - \alpha_C T_C)I - RI^2}{\alpha_H IT_H + K\Delta T - \frac{1}{2} RI^2} \quad (3.24)$$

In this section, two analytical models have been developed to predict the TE element performance. This first model is a discretization model, which considers the temperature dependent material properties. The second model is a lumped parameter model which considers the TE element as a block with uniform material properties.

3.3.2 Thermal resistance network of a TEM

A power prediction model for a single TE element has been developed in previous subsection. As introduced in Chapter 2.1, a typical TEM usually consists of more than just TE elements. There are also other components like ceramic plate and copper stripes, which all induce thermal or electrical resistances. Those thermal and electrical resistances are listed in the thermal resistance network in Figure 3.4. Therefore, rather than the actual TE material properties, the equivalent parameters of TEM need to be adopted when solving the lumped parameter TEM model. The method of obtaining those equivalent parameters is introduced in following section.

Figure 3.4 Thermal resistance network of a TEM

3.3.3 Finding TEG key parameters from various data sources

The performance of TEG is characterized by three key parameters: Seebeck coefficient (α), thermal resistance (R_{th}), and the electrical resistance (R_e). Providing these three parameters, plus the operating conditions, the output power could be found by Eq. (3.6), Eq (3.18), or by Eq (3.23). However, those parameters are always unknown in engineering problems, and need to be calculated or estimated based on limited information. Three methods are introduced below for calculation of these parameters in different actual problems. The appropriate method may be selected based on available information.

(a) Finding key parameters based on TEM parameters

If the key parameters of a single TE couple are known, then the TEM parameters can be estimated by this method. Similarly, if the key parameters of a single TEM are known, the key parameters of the TEG system can be estimated by the same

method. The following equations show the process of finding key parameters of TEG by known TEM parameters.

Figure 3.5 Modules contained in calculation sections

The equivalent parameters of a TEG calculated from parameters of TEMs are given as:

$$\begin{aligned}\alpha &= \alpha_m Num_{TEM} \\ R_e &= R_{e,m} Num_{TEM} \\ R_{th} &= \frac{R_{th,m}}{Num_{TEM}}\end{aligned}\quad (3.25)$$

where α_m , $R_{th,m}$, $R_{e,m}$ are Seebeck coefficient, thermal and electrical resistances, respectively, for single module.

(b) Finding parameters from manufacturer data

When purchasing TEM from TEG manufacturers, the following parameters are commonly provided: open circuit voltage (V_{oc}) under specific temperature condition (T_H , T_C), corresponding heat flux (q_H) at given temperature, electrical resistance (R_e) and match load current (I_{load}). Then the equivalent TEG parameters are calculated as:

$$\alpha = \frac{V_{oc}}{T_h - T_c} \quad (3.26)$$

$$R_{th} = \frac{T_h - T_c}{q_h - \alpha I_{load} T_h + \frac{1}{2} I_{load}^2 R_e} \quad (3.27)$$

(c) Calculation from TE leg geometries and material properties

In this subsection, a method of calculating key parameters based on material properties is introduced, which can be adopted to simulate the system with custom made TEMs.

Commonly, after building the material, thermal conductivity (λ) and electric resistance (ρ) are measured, together with geometry factors and other easily measured values. TEM key parameters ($\alpha_{p,n}$, R_{th} , R_e) can be calculated [76], then these parameters can be expanded to TEG level using Eq. (3.25).

First, the calculation of Seebeck coefficient is introduced from the energy balance equation at hot side:

$$\begin{aligned} q_p &= (\alpha_p - \alpha^*) I T_h - \lambda_p A_p \frac{dT_p}{dx} \\ q_n &= -(\alpha_n - \alpha^*) I T_h - \lambda_n A_n \frac{dT_n}{dx} \end{aligned} \quad (3.28)$$

where subscripts n and p represent the positive and negative semiconductor, respectively, q is heat flow into the semiconductor at the hot side, and α^* is the relative Seebeck coefficient. In order to find the Seebeck coefficient, the differential term should be removed, which is achieved through the heat conduction equation in each leg:

$$\begin{aligned} -\lambda_p A_p \frac{d^2 T}{dx^2} &= \frac{I^2 \rho_p}{A_p} \\ -\lambda_n A_n \frac{d^2 T}{dx^2} &= \frac{I^2 \rho_n}{A_n} \end{aligned} \quad (3.29)$$

where ρ is the electrical resistivity. In this equation, only Joule heating is

considered. Boundary conditions of Eq. (3.29) are defined as: $x=0$, $T=T_H$; $x=l$, and $T=T_C$.

From Eq. (3.29), one can obtain the temperature gradient:

$$\frac{dT_p}{dx} = -\frac{I^2 \rho_p}{\lambda_p A_p^2} x + \frac{T_c - T_h}{l} + \frac{I^2 \rho_p l}{2 \lambda_p A_p^2} \quad (3.30)$$

Temperature distribution in n-type leg is the identical expression as above.

The energy balance equations at hot side where $x=0$ becomes:

$$q_p = (\alpha_p - \alpha^*) I T_h - \frac{\lambda_p A_p (T_c - T_h)}{l} - \frac{I^2 \rho_p l}{2 A_p} \quad (3.31)$$

$$q_n = -(\alpha_n - \alpha^*) I T_h - \frac{\lambda_n A_n (T_c - T_h)}{l} - \frac{I^2 \rho_n l}{2 A_n} \quad (3.32)$$

Since q_n , q_p are heat flow in n-type and p-type legs, respectively, the total heat flow in the TE pair is adding them together:

$$q_h = (\alpha_p - \alpha_n) I T_h - (T_c - T_h) \left(\frac{\lambda_p A_p}{l} + \frac{\lambda_n A_n}{l} \right) - \frac{I^2}{2} \left(\frac{\rho_p l}{A_p} + \frac{\rho_n l}{A_n} \right) \quad (3.33)$$

Therefore, the Seebeck coefficient of TE couple is:

$$\alpha = \alpha_p - \alpha_n = \frac{q_h}{I T_h} - \frac{(T_h - T_c)}{I T_h} \left(\frac{\lambda_p A_p}{l} + \frac{\lambda_n A_n}{l} \right) + \frac{I^2}{2 I T_h} \left(\frac{\rho_p l}{A_p} + \frac{\rho_n l}{A_n} \right) \quad (3.34)$$

The thermal resistance of the TE couple is:

$$R_{th} = \frac{1}{\frac{\lambda_p A_p}{l} + \frac{\lambda_n A_n}{l}} \quad (3.35)$$

and the electrical resistance is:

$$R_e = \frac{\rho_p l}{A_p} + \frac{\rho_n l}{A_n} \quad (3.36)$$

3.4 Experimental validation of analytical model

To verify the simulation model developed in Section 3.3.1, an experimental setup was built. The TEM used in this experiment is a commercial available product TEG1-12611-6.0. The TE material used in this TEM is Bi_2Te_3 . The outward appearance of the module in use and the inward arrangement of the TEM are shown in Figure 3.6 and Figure 3.7, respectively. Inside this type of TEM, there are 127 TE couples connected in series; each of these TE couples are made of two 2.5 x 2.5 x 1.5 mm small cube, with ceramic substrate on up and bottom.

The experimental testing setup is shown in Figure 3.8. The top metal block is the cooling block where the cooling water flows through, acting as the cold side of TEMs. The bottom is a hot plate, acting as the hot side. The TEMs are placed in the middle of these two parts so there will be a temperature difference across the two sides of TEMs, from which the voltage and output power are generated.

Figure 3.6 Outward appearance of TEM adopted in the experiments

Figure 3.7 Inward arrangement of the TEM adopted in the experiments. A total 127 TE couples of identical size of $2.5 \times 2.5 \times 1.5$ mm, where 1.5 mm is the vertical length, integrate the module.

Figure 3.8 Experimental setup for TEM level testing.

Figure 3.9 Comparison of simulation and experiments at TEM level.

A sweep of different temperature boundary condition is conducted to verify the

TEM model under different conditions. The comparison between simulation results and measured data in terms matched load power is plotted in Figure 3.9. It is shown that the simulation value is still slightly higher compared with the measured value provided in the datasheet. This over-estimation value is partially attributed to the thermal radiation loss and contact resistance. The radiation loss between TE legs is not considered in this simulation.

The discrepancy between simulation and experiments may also be due to the temperature dependent contact resistance in experiments, since the contact resistance used in the model is based on empirical values [77, 78], which is assumed to be constant. The contact resistance value is highly dependent on each specific application. Therefore, this discrepancy does not influence the applicability of the proposed model if the contact resistance is properly estimated when applying the model.

3.5 3-D model development in ANSYS and comparison with improved analytical TEM model

Although the analytical model has been verified by experiments, many parameters in the experiments are unknown due to technical limitations, e.g., the heat flux at hot and cold side and the exact temperature at two sides of TE elements. Therefore, the analytical model is also compared with commercial CFD software, whose accuracy has been well validated in existing literature [79, 80].

A 3-D simulation model is built, which simultaneously considers all coupled-field phenomena such as heat conduction and Joule heating as well as Seebeck, Peltier and Thomson effects. Figure 3.10 and Figure 3.11 show the temperature field and electrical potential field calculated by ANSYS mechanical at the boundary condition and material properties are same as in the analytical model.

Figure 3.10 Temperature field calculated by ANSYS Mechanical. At hot side temperature of 750K, cold side temperature of 400K.

Figure 3.11 Electrical potential field calculated by ANSYS Mechanical. At hot side temperature of 750K, cold side temperature of 400K.

The material properties used in this model are based on Table 3.1.

Table 3.1 TE material properties used for ANSYS validation of the improved TEM analytical model.

	$\rho (\Omega \cdot \mu)$	$\alpha (V/K)$	$\kappa (W/m \cdot K)$
N-type	$\rho_n = \frac{0.001746}{T - 310}$	$(0.268T - 329) \cdot 10^{-6}$	5400/T
P-type	4×10^{-4}	$(0.150T + 211) \cdot 10^{-6}$	319.4/T

The results obtained by the improved analytical model developed in this chapter matches with the results obtained by ANSYS Mechanical. The heat flux absorbed at hot side of TEM and open circuit voltage generated are compared with these two models under four different boundary conditions. As shown in Table 3.2, the errors are within 5 % under different scenarios. Therefore, the accuracy of this improved analytical model is well validated by ANSYS model.

Table 3.2 Comparison between results obtained by ANSYS Mechanical and by 1D analytical model.

Hot-cold side temperature (K)	Open circuit voltage-Proposed model(V)	Open circuit Voltage-ANSYS(V)	Error	Proposed model Q_h (W)	ANSYS Q_h (W)	Error
850-400	0.21	0.22V	4.5%	78.1	80.07	2.3%
400-750	0.169	0.174	2.9%	70.23	73.46	4.4%
400-650	0.12	0.125	4%	54.3	57	4.7%

400-550	0.073	0.0752	2.9%	35.4	36.6	3.3%
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3.6 Summary

This chapter proposes an analytical TEM model by solving the multi-physics governing equations. The temperature dependent material properties, Seebeck coefficient, thermal conductivity, electrical conductivity, are considered in this analytical model. The model also considers the Seebeck, Peltier, Thomson effects and Joule heating. A discretization scheme has been developed to solve the temperature profile for the output power and efficiency prediction.

An experimental setup has been built to validate the analytical model. The output power predicted by the analytical model matches well the experiments.

CHAPTER 4 Integrated Heat Exchanger and Thermoelectric Model Development

4.1 Introduction

As introduced in Section 2.1, TEMs are usually integrated with HEXs when applied to waste heat recovery applications for better heat transfer efficiency. A typical TEG WHR system is presented in Figure 4.1. A TEG system usually contains an engine, HEX (HEX), TEG and pump, which is used for circulating the cooling water. The optimization of TEM highly depends on the thermal boundary condition. Besides, during the optimization of HEX, the trade-off between heat transfer ability and pressure drop is a critical issue to consider [81]. This trade-off also depends highly on the TEM design; therefore, an integrated HEX and TEM model is needed.

Figure 4.1 Diagram of TEG system

In this chapter, an integrated TEM and HEX model is proposed for performance prediction and preliminary design of TEG systems. The proposed HEX model considers both the heat transfer efficiency and pressure drop properties of HEX. The solution of the entire calculation domain is achieved by discretization.

Figure 4.2 shows a diagram for the calculation of the integrated TEG model. The calculation zone is discretized into many small zones, and the TEM model and HEX mode are both solved at each small zone. Unlike other traditional TEM models, this integrated model enables simultaneous simulation and optimization of TEM and HEX.

Figure 4.2 Diagram of a TEM and HEX system

The rest of the chapter is organized as follows. Section 4.2 presents the development of HEX numerical model. Section 4.3 discusses the integration of TEM model and HEX model into an integrated TEG model. Section 4.4 describes the experimental validation of this integrated TEG model. In Section 4.5, some parametric studies are conducted to test the TEG performance under various input conditions and different designs.

4.2 Development of heat exchanger model

HEX is a device for increasing the heat transfer between TEM and exhaust gas and cooling water. In this section, empirical correlations are employed to investigate the heat transfer and pressure drop characteristics of straight fin heat exchanger. The 3-D straight fin HEX geometry is shown in Figure 4.3.

Figure 4.3 Straight fin HEX

Building an accurate HEX model is very crucial for predicting the output power of a TEG system, since the heat transfer coefficient calculation determines the boundary conditions of the TE device temperature profile calculation. Accurate HEX modeling is crucial also because it is used for calculation of the associated power requirement like pumping power and backpressure to the engine.

The heat transfer coefficient calculation depends on the inlet fluid parameters and flow geometry. There are hot and cold sides of HEX, as shown in Figure 4.2. On both sides of the HEX, HEX geometry has a significant influence on the flow pattern, which strongly affects the heat transfer rate. For example, the fin geometry would create complex vortex structures and wakes behind fins, and turbulence in the flow. These phenomena induce non-uniform local heat transfer rates and complex temperature fields. Moreover, if boiling phenomena happens, the computational cost will increase significantly as latent heat and two-phase flow unhomogeneous distribution need to be considered. The governing equations can be formulated, which are known as Navier Stokes equation [82].

At the hot side and cold side fluids, the fluid motion and temperature profile are described by Navier-Stokes and energy equations combined with the continuity

equations[82].

Continuity equation:

$$\nabla \bullet (\rho \mathbf{u}) + \frac{\partial \rho}{\partial t} = 0 \quad (4.1)$$

Momentum Conservation equation (Navier-Stokes equation)

x-momentum:

$$\frac{\partial(\rho u)}{\partial t} + \text{div}(\rho u \mathbf{u}) = -\frac{\partial p}{\partial x} - \text{div}(\mu \text{ grad } u) + S_{Mx} \quad (4.2)$$

y-momentum:

$$\frac{\partial(\rho v)}{\partial t} + \text{div}(\rho v \mathbf{u}) = -\frac{\partial p}{\partial y} - \text{div}(\mu \text{ grad } v) + S_{My} \quad (4.3)$$

z-momentum:

$$\frac{\partial(\rho w)}{\partial t} + \text{div}(\rho w \mathbf{u}) = -\frac{\partial p}{\partial w} - \text{div}(\mu \text{ grad } w) + S_{Mw} \quad (4.4)$$

Energy equation:

$$\frac{\partial(\rho i)}{\partial t} + \nabla(\rho \mathbf{u} i) = -p \text{div} \mathbf{u} + \text{div}(k \text{ grad } T) + \Phi + S_i \quad (4.5)$$

However, analytical solutions to these non-linear PDE equations can only be found in very limited circumstances. In most cases, they are solved numerically. Commercial CFD (computational fluid dynamics) software packages have been developed to find numerical solutions to heat transfer and fluid dynamics problems. Popular commercial software packages include ANSYS-FLUENT and COMSOL. However, calculation using CFD software can be significantly expensive and time consuming, which is not suitable for preliminary design and optimization. In this study, empirical solutions to these equations under specific circumstances are

adopted to describe the heat transfer and fluid mechanic phenomena within HEX. Fluid flow inside a duct can be classified as turbulent flow and laminar flow [83], which is characterized by the Reynold number (Re):

$$Re = \frac{\rho v D}{\mu} \quad (4.6)$$

where D is the diameter of the flow channel, μ is the dynamic viscosity of the fluid ($Pa \cdot s$ or $N \cdot s/m^2$ or $kg/m \cdot s$), v is the velocity of the fluid with respect to the object (m/s), and ρ is the density of the fluid (kg/m^3). A turbulent flow usually has better heat transfer characteristics than laminar flow, and the heat transfer coefficient calculation is different in turbulent flow than in laminar flow.

For rectangular flow channel, the hydraulic diameter is given by [83]:

$$D = \frac{4A}{P} \quad (4.7)$$

where A is the cross-sectional area and P is the wetted perimeter [83].

Generally, when the Re number is less than 2300, the flow is considered as laminar flow. The flow is considered as turbulent when the Re larger than 3000. In this section, we consider this flow of exhaust gas as turbulent, since in most regions except a small part in the entrance region, the flow follows a turbulent pattern.

Another dimensionless parameter of fluid, Prandtl number (Pr) is also needed to calculate the heat transfer coefficient. The Pr is calculated as the ratio of momentum diffusivity to thermal diffusivity:

$$Pr = \frac{\text{viscous diffusion rate}}{\text{thermal diffusion rate}} = \frac{c_p \mu}{\kappa} \quad (4.8)$$

where c_p is the specific heat ($J/kg \cdot K$).

In order to calculate the heat transfer coefficient (h), the first step is to calculate the

Nusselt number (Nu), the relationship between Nu and h is given by:

$$Nu = \frac{hl}{k} \quad (4.9)$$

Nu is calculated by empirical equations consisting Re and Pr . There are lots of correlations for calculating the Nusselt number using Re and Pr under different conditions: different fluid, temperature difference, flow channel geometry, etc. On the hot side of HEX, where the exhaust gas flow through, the Re number is around 80000~100000, which is considered as fully developed turbulent flow. Gnielinski correlation is adopted in this case:

$$Nu = \frac{(f/8)(Re-1000)Pr}{1+12.7(f/8)^{1/2}(Pr^{2/3}-1)} \quad (4.10)$$

where f is the Darcy friction factor. The Gnielinski correlation is one of the most accurate empirical equations for calculating Nu . Among 800 experiments, 90% of the data are within 20% error, and most of them are within 10% error. It is valid for:

$$2000 > Pr > 0.6, 5 \times 10^6 > Re > 3000 \quad (4.11)$$

The Darcy friction factor can be found by Moody Chart or calculated by empirical equations [83]. In this study, the Darcy friction factor is obtained by Filonenko equation for its accuracy in a wide range [83]:

$$f = (1.82 \lg Re - 1.64)^{-2} \quad (4.12)$$

The heat transfer coefficient is used to characterize the heat transfer ability, whilst the other character of HEX, pressure drop, has to be calculated in order to find the backpressure to the engine or pumping loss.

The pressure drop is induced by friction loss. In this study, empirical correlations are adopted to calculate the friction loss in HEX. Darcy–Weisbach equation is selected in this study to calculate the friction loss because of its wide applicability [83].

Firstly, the head loss is calculated:

$$h_f = f \frac{L}{D} \frac{V^2}{2g} \quad (4.13)$$

where:

h_f is the head loss due to friction (m)

L is the length of flow channel (m)

D is hydraulic diameter of flow channel (m)

V is volumetric flow rate (m^3/s)

Based on the head loss calculated in the above equation, the pressure drop is calculated:

$$\Delta p = \rho g h_f \quad (4.14)$$

On the exhaust gas side, pressure drop causes backpressure to the engine. Therefore, the engine needs to produce extra power to pump exhaust gas. This power (P_b) is calculated as:

$$P_b = V \Delta p \quad (4.15)$$

For water flow in the duct, the flow could be either laminar or turbulent under different conditions. In turbulent flow region, Nu number, heat transfer coefficient and pressure drop are calculated by Gnielinski correlation. In the laminar region, Nu is usually constant for certain geometry and is available in the literature. For the rectangular duct, Nu number is given in Table 4.1 [84]:

Table 4.1 Calculation of Nu and f for laminar flow in a duct

Rectangular duct	$Nu = \frac{hl}{k}$		f
	Constant heat flux	Constant temperature	
$b/a=2$	4.12	3.39	62
$b/a=3$	4.79	3.96	69
$b/a=4$	5.33	4.44	73
$b/a=8$	6.49	5.60	82
$b/a=\text{infinite}$	8.23	7.54	96

The pumping power is then calculated as:

$$P'_{\text{pump}} = V \Delta P \quad (4.16)$$

Assume the pump efficiency is η , the pumping power is given as:

$$P_{\text{pump}} = \frac{V \Delta P}{\eta} \quad (4.17)$$

The pressure drop calculations are with respect to the loss along the flow channel inside the HEX. Besides the pressure drop along the flow channel, there are also pressure losses due to the sudden change of cross-section area at the junctions, i.e. at entry and exit region of HEX, as shown in Figure 4.4.

Figure 4.4 Sudden expansion and contraction of flow channel

The pressure losses at sudden expansion and contraction are calculated by empirical correlations. Those correlations are in the form as below[85]:

$$\Delta h = K \frac{V^2}{2g} \quad (4.18)$$

where K is the resistance coefficient at sudden expansion and contraction, usually given by empirical correlations.

At the sudden contraction circumstance, there are usually two cases, i.e. the square expansion and tapered contraction, as shown Figure 4.5.

Figure 4.5 Sudden contraction of flow channel: (a) square reduction; (b) tapered reduction

For square contraction, the K -value is given by [85]:

$$K = (1.2 + \frac{160}{Re_1})[(\frac{D_1}{D_2})^4 - 1]; \text{ for } Re_1 < 2500 \quad (4.19)$$

$$K = (0.6 + 0.48f_1)\left(\frac{D_1}{D_2}\right)^2\left[\left(\frac{D_1}{D_2}\right)^2 - 1\right]; \text{ for } Re_1 > 2500 \quad (4.20)$$

For tapered contraction, the K -value is calculated as [85]:

For $45^\circ < \theta < 180^\circ$, multiply K value of square contraction by $\sqrt{\sin(\frac{\theta}{2})}$,

For $\theta < 45^\circ$, multiply K value of square contraction by $1.6\sin(\frac{\theta}{2})$.

For expansion circumstance, as shown in Figure 4.6, the K -value for squared expansion is calculated as:

$$K = 2\left[1 - \left(\frac{D_1}{D_2}\right)^4\right]; \text{ for } Re_1 < 4000 \quad (4.21)$$

$$K = (1 + 0.8f_1)\left[1 - \left(\frac{D_1}{D_2}\right)^2\right]^2; \text{ for } Re_1 > 4000 \quad (4.22)$$

For tapered expansion, the K -value is calculated as [85]:

For $45^\circ < \theta < 180^\circ$, the K value is the same as in squared expansion

For $\theta < 45^\circ$, multiply the K value of square expansion by $2.6\sin(\frac{\theta}{2})$.

Figure 4.6 Sudden expansion of flow channel: (a) square expansion; (b) tapered expansion

Fin is adopted in HEX as heat transfer enhancement method, which increases heat transfer area and induces turbulence. Heat transfer coefficient calculated in the previous section using Nu , Pr , Re is for duct without fin. Therefore, fin efficiency should be adjusted as surface area exposed to fluid is increased compared with bare

duct. Single fin efficiency η_f is calculated first, and then the overall fin efficiency:

For the adiabatic fin tip condition, the fin efficiency is calculated as [83]:

$$\eta_f = \frac{\tanh mL}{mL} \quad (4.23)$$

where L is the length of the fin, and m is a parameter defined as:

$$m = \sqrt{\frac{hP}{kA}} \quad (4.24)$$

where P and L are cross-section perimeter and area of the fin, respectively.

For non-adiabatic fin tip condition, the fin efficiency is calculated as [83]:

$$\eta_f = \frac{1}{mL} \frac{\sinh mL + (\frac{h}{mk}) \cosh(mL)}{\cosh(mL) + (\frac{h}{mk}) \sinh(mL)} \quad (4.25)$$

The relationship between single fin efficiency and overall fin efficiency is:

$$\eta = 1 - N \frac{A_f}{A_{tot}} (1 - \eta_f) \quad (4.26)$$

where N is the number of fins, A_f is the area of a single fin and A_{tot} is the total area of the fins and the open base.

4.3 Integration of thermoelectric generator model

After the HEX and TEM models are developed, the next step is the integration of these two models into an integrated TEG model. This integration is achieved by discretization and integration. In this section, the process of integration of TEM and HEX model developed in previous sections is presented. The parameter flow and its relationship in the integrated model is briefly illustrated in Figure 4.7.

Figure 4.7 Parameter relationship in the integrated TEG model

The HEX model simulates the thermal and fluid mechanics phenomena. From the HEX model, the temperature and pressure field are obtained, which are used for calculating TEG power and pressure loss. On the other hand, the TEM also has influence on the temperature field.

The system is divided into small zones, and the HEX and TEM models are solved in each zone. A diagram containing three zones is shown in Figure 4.8. For the TEM model, the lumped parameter model developed in Chapter 2 is adopted. In each zone, the output power and pressure drop are calculated, and the input parameters needed in the next zone are also calculated. This iteration process is shown in Figure 4.10.

The TEM and HEX models are solved in each cell by considering energy balance, as shown in Figure 4.9. The output power calculation is based on the lumped parameter TEM model, while the thermal resistance and pressure drop calculation is based on the HEX model. In order to calculate the energy balance in each cell, the thermal resistance is also calculated. The calculation of each thermal resistance shown in Figure 4.9 is as follows:

The total thermal resistance from exhaust gas to the hot side junction of TEMs $R_{comb,h}$ is given as:

$$R_{comb,h} = R_{fin,h} + R_{conduction,h} + R_{contact,h} = \frac{1}{h_h \eta A} + \frac{L}{k_h A} + \frac{1}{h_{contact} A} \quad (4.27)$$

$$R_{comb,c} = R_{fin,c} + R_{conduction,c} + R_{contact,c} = \frac{1}{h_c \eta A} + \frac{L}{k_c A} + \frac{1}{h_{contact} A} \quad (4.28)$$

The energy balance equations on the hot side of each cell are given as:

$$m_h C_{p,h} (T_{h,i} - T_{h,o}) = q_h + q_{ins} \quad (4.29)$$

where m_h is the hot side gas mass flow rate, $C_{p,h}$ is the heat capacity of the exhaust gas, $T_{h,i}$ is the temperature at which the exhaust gas flow into each cell, and $T_{h,o}$ is the temperature at which the exhaust gas flow out of each cell, q_h is the hot side heat flux at TEM surface, and q_{ins} is the heat flux through surrounding insulations.

Figure 4.8 Discretization of HEX flow channel after symmetric simplification

Figure 4.9 Energy flow in each zone

Figure 4.10 Flow chart of the integrated TEG model

Similarly, the energy balance equations on the cold side are given as:

$$m_c C_{p,c} (T_{c,o} - T_{c,i}) = q_c + q_{ins} \quad (4.30)$$

where m_c is the cold side cooling water flow rate, $C_{p,c}$ is the heat capacity of the cooling water, $T_{c,i}$ is the temperature at which the cooling water flow into each cell, and $T_{c,o}$ is the temperature at which the cooling water flow out of each cell, q_h is the cold side heat flux at TEM surface, and q_{ins} is the heat flux through surrounding insulations.

The heat transfer between hot side exhaust gas to hot side of TEM is described as:

$$q_{h,tot} = q_h + q_{ins} = \frac{T_{avg} - T_h}{R_{comb,h}} \quad (4.31)$$

where $R_{comb,h}$ is the thermal resistance from exhaust gas to hot side of TEM.

However, the temperature increase of hot side gas is always nonlinear, therefore using the average temperature leads to inaccuracy. In order to improve the accuracy, the mean temperature is transformed into log mean temperature difference (LMTD) [81], which is closer to a real situation in HEX:

$$\Delta T_{lm,h} = \frac{T_{h,i} - T_{h,o}}{\ln\left(\frac{T_{h,i} - T_h}{T_{h,o} - T_h}\right)} \quad (4.32)$$

where $\Delta T_{lm,h}$ is the hot side LMTD, and the cold side LMTD has the same expression.

4.4 Validation of integrated thermoelectric generator model

The integrated TEG model was compared with the experimental results from [86]. The input design and operating parameters are based on the exhaust system of a truck engine [86], as listed in Table 1. Fig. 4.11 shows the comparison results between simulation and experiment: the output power is plotted versus current where the curves were generated by varying the external load resistance. The

relative error of the simulated average power and peak power are 9.1% and 10.0%, respectively. It can be noticed that the power-current curve of the present simulation model does not exactly match with the power curve of the experimental results, which is asymmetrical. However, even though the simulation model over-predicts 9.1% of the output power, the difference in value is still well within the claimed possible error of 20% of Gnielinski correlation [22], which proves the simulation model predicts the output power of TEG well.

Table 4.2 Input parameters for integrated TEG model validation [86].

	Value	Unit
<u>Engine parameters</u>		
Engine power	108	<i>kW</i>
Engine revolution	3000	<i>r/min</i>
<u>Fluid parameters</u>		
Exhaust inlet temperature	350	$^{\circ}\text{C}$
Cooling water temperature	90	$^{\circ}\text{C}$
Exhaust flow speed	15.2	<i>m/s</i>
Flow rate of water	9.27	<i>L/min</i>
<u>HEX parameters</u>		
Hot side transfer coefficient h^*	15	$\text{W}/(\text{m}^2 \text{K})$
HEX material	Brass	-

HEX length	0.4	<i>m</i>
HEX width	0.29	<i>m</i>
HEX height	18	<i>mm</i>
<u>TEM parameters</u>		
Each module's area A	0.050 * 0.050	<i>m</i> ²
Module height	0.005	<i>m</i>
Module fill factor	0.032	-
Module number	60	-
PN couple number	127	-

Figure 4.11 Comparison of simulation and experiments

4.5 Parametric study on different input and design parameters

After the method is validated by experiments, a parametric study is conducted to investigate the performance of TEG under different input conditions. In this section, the parameters from the exhaust system of marine engine of 1.73 MW is adopted. 100 commercial TEMs are assumed to be placed on a plate-fin HEX. The detailed input parameters can be found in

Table 4.3.

Table 4.3 Integrated TEG model parameters and configuration

MODEL PARAMETER	VALUE	UNIT
Exhaust gas inlet temperature	693	K
Exhaust flow rate	5.8	m ³ /s
Cooling water inlet temperature	298	K
Cooling water flow rate	2.8	kg/s
HEX [length, width, height]	[1, 0.5, 0.2]	m
HEX material	Austenitic stainless steels	
TEMs [length, width, height]	[0.056, 0.056, 0.06]	m

The results generated by this integrated TEG model are listed in

Table 4.4.

The output power 9.97kW is nearly 1% of engine rated power, which means 1% fuel saving. At rated power, this could save the fuel at 0.2 Liter/min.

The temperature distribution of exhaust gas, TEG hot and cold surface, cooling water with respect to their axial location of the HEX are plotted in Figure 4.12. As shown in this figure, outlet temperature of exhaust gas does not change much, which shows there is still great potential to improve the ability of retrofitting energy from exhaust gas. Besides, there is significant temperature difference between the hot side of TEG and exhaust gas, which indicates potential of improving HEX

capability.

Table 4.4 Output performance predicted by the integrated TEG model

Output	Value
TEG electrical power	9.97 kW
Heat transferred from exhaust	56.79 kW
Coolant heat	46.83 kW
Pressure loss of exhaust	445 Pa
Exhaust outlet temperature	675 K
Cooling water outlet temperature	301.7 K

Figure 4.12 Temperature distribution of exhaust gas, TEG hot and cold surface, and

cooling water with respect to their axial location of the HEX

Beside the baseline model performance prediction, a parameter study is also conducted to find the performance of the TEG system under different inlet parameters. The effect of the cooling water flow rate is investigated, and the results are shown in Figure 4.13. As observed, there is a sudden increase of TEG power when water flow rate reaches around 2-3kg/s, this is because the flow pattern changes to turbulent flow in the empirical fluid mechanic equations.

Figure 4.13 Output power with various cooling water flow rates

4.6 Summary

The design and optimization of TEM and HEX have been correlated with each other in this chapter. An integrated TEG model is proposed, which consists HEX model and TEM model. The HEX model is built based on empirical equations, and LMTD method is adopted to improve the accuracy. A discretization scheme is proposed to integrate the TEM and HEX model into a TEG model, enabling simultaneous simulation of TEM and HEX. Experimental results show that the model is able to predict the TEG output power performance accurately. Additionally, the proposed

integrated TEG model is also used for conducting a parametric study and output performance under different operating conditions.

CHAPTER 5 Thermoelectric Module Design and Optimization

5.1 Introduction

As the most important part in the TEG system, a proper design of TEM is critical to the overall TEG performance. Numerous research efforts have been devoted to the design and optimization of the TEM [7-11]. Ugur et al. [87] studied the effect of TE leg dimension and spacing using FEM software, and this simulation work assumes a fixed temperature boundary condition. Gao et al. [88] optimized the TE elements height in terms of power-per-unit-area, cost-per-watt, and found that for most commercial TEM, the optimal height is around 1-2mm. Omer et al. [89] developed an improved model and analysed the optimum TE leg length based on maximum output power. This study considers the effect of thermal contact resistances at hot and cold junction. JW Stevens et al. [66] studied the effect TEM geometry design at a low temperature difference and concluded that the TEG should be designed in a way that TEM thermal resistance equals the external thermal resistance in order to achieve maximum output power. In these studies, the thermal boundary conditions are assumed to be at constant temperature on both hot heat source and cold heat sink. Rezania et al. [33] optimized the A_n/A_p ratio, which is the horizontal cross-section area ratio of n-type legs to p-type legs, and found that, for n-type material, $\text{Mg}_2\text{Si}_{1-x}\text{Sn}_x$ and p-type material, Zn_4Sb_3 , the output power is maximized when $A_n/A_p < 1$. The boundary condition assumption is fixed hot side temperature T_H .

Most of these investigations assume a fixed temperature boundary condition, i.e. the temperature at the end of the TEM stays constant despite of module design. However, under some engineering problems, this assumption cannot accurately capture the influence of temperature fluctuation under different TEM designs.

In this chapter, simulation and optimization are conducted to investigate the effect of a key design parameter on the output power, the TEM height. The effect of different boundary conditions on the optimization, namely the first type and second type boundary conditions are also investigated. The maximum output power is the main objective and the TEM height is the design parameter to maximize the output power. Unlike the existing approaches, optimization of TEM height is conducted under both the first and second type boundary conditions. Compared with the common approach of using simple boundary condition, the optimization approach provides more guidance on the design of TEMs under various conditions since it helps to find the effect of boundary condition on the optimal design corresponding to maximum output power.

The rest of the chapter is organized as follows. Section 5.2 details thermal boundary conditions and thermal resistance network. Section 5.3 conducts TEM simulations with the baseline model. Section 5.4 investigates the effect of different thermal boundary conditions at different values. The effect of multiple design parameters is investigated in Section 5.5. The conclusions are drawn in Section 5.6.

5.2 Thermal resistance network and boundary conditions

Figure 5.1 Thermal resistance network of TEM model

The thermal resistance network and equivalent circuit of a typical TEM is shown in Figure 5.1. The hot side of TEM is usually connected with hot source, like exhaust gas and waste hot water. The cold side is usually connected to water tank, or convective heat transfer mechanism to maintain a cold temperature.

A faithfully description of boundary conditions is critical to the heat transfer simulation and power prediction. Commonly, there are three types of boundary conditions in heat transfer problem [90]:

(1) Temperature boundary condition, also known as first kind boundary condition or Dirichlet condition, specifies a known value of temperature T at the boundary. This kind of boundary condition is usually applied to a large heat sink, like water tank. The Dirichlet condition can be expressed as:

$$t_w = f(\tau) \quad (5.1)$$

where the subscript w means the boundary, t_w is the temperature at the boundary and τ is the time.

(2) Heat flux boundary condition, also known as second kind boundary condition or Neumann boundary condition, specifies the known value of heat flux density across

the boundary. This boundary condition could be used for describing engineering application like joule heating from a metal with constant current. The Neumann condition can be expressed as:

$$-\lambda \left(\frac{\partial t}{\partial n} \right)_w = f(\tau) \quad (5.2)$$

where λ is the thermal conductivity and n is the normal direction.

(3) Convection boundary condition, also known as third kind boundary condition or Robin boundary condition, specifies the convective heat transfer coefficient h and the ambient temperature T_f :

$$-\lambda \left(\frac{\partial t}{\partial n} \right)_w = h(t_w - t_f) \quad (5.3)$$

where h is the heat transfer coefficient at the solid-fluid boundary, and t_f is the temperature of the fluid.

5.3 Parametric study of thermoelectric module height at original working condition

The original working condition comes from a commercial TEM TEG1-12611-6.0. The detailed data of this working condition is shown in Table 5.1. This working condition has been simulated by the numerical model developed in Chapter 3. In this section, the TEM height is changed in the range of 0.5mm-10mm, which is a reasonable range considering manufacturing limits and practical engineering applications.

Table 5.1 Input parameters for original working condition

Parameter	Value
Hot side temperature (T_H)	573K
Cold side temperature (T_C)	303K
Hot side heat flux (Q_H)	398W
TE leg width	2.5 mm

TE leg length	2.5 mm
TE leg height (H)	1.5 mm
Fill factor (FF)	50%
Seebeck coefficient	Temperature dependent, reference graph [91]
TE thermal conductivity (κ)	
TE electrical conductivity (σ)	
Ceramic plate thermal conductivity (κ_c)	35 W/(m·K)

Figure 5.2 shows the changes in the voltage, current and output power with the TEM height under the first type of boundary condition at hot side, i. e. fixed hot side temperature. As shown in Figure 5.2 (a), the electrical current generally decreases as the TEM height increases while the voltage continuously increases as the TEM height increases. Figure 5.2(b) shows the change in output power as the TEM height increases. Through a combined effect from changes in both the voltage and current, the output power first increases and then decreases, reaching a peak value at TEM height of about 1.9 mm. This feature of TEG output power can be explained by the variance of internal thermal resistance and electrical resistance. When TEM height increases, the internal thermal resistance (R_{TE}) and electrical resistance (R_e) both increase, which has positive and negative effects on the output power, respectively. The influence of thermal resistance is more significant when the TEM height is small. As shown in the thermal resistance network in Figure 5.1, increasing thermal resistance can significantly increase the temperature difference ($T_H - T_C$), which increases the output voltage by Seebeck effect, therefore the output power is increased. The electrical resistance has a relatively more significant effect when the TEM height is large, and the output power decreases as the internal electrical resistance (R_e) increases.

Figure 5.2(a) Voltage, current and (b) power changes with TE element height under fixed T_H , $T_H=573\text{K}$, $T_C=303\text{K}$.

Figure 5.3 shows the change in voltage, current and output power as a function of TEM height under second type thermal boundary condition at hot side, i.e. fixed Q_H . Unlike the first type of boundary condition, both voltage and current increase as TEM height increases when TEM height is small, while voltage keeps increasing with TEM height in the entire range. Output power continuously increases as the TEM height increases in the entire range. This feature of output power under fixed Q_H is significantly different from the performance under fixed T_H , which suggests that the optimal design may be far from the correct value if the boundary condition assumption used for optimization is inaccurate.

Figure 5.3 (a) Voltage, current and (b) power changes with TE element height under constant temperature boundary condition; $Q_H=398\text{W}$, $T_C=303\text{K}$

5.4 Parametric study of thermoelectric TEM design parameters under different boundary conditions

In this section, simulation is conducted with varied boundary condition values, i.e., different fixed Q_H and T_H values, to test whether the patterns found in the original working condition can be validated.

Figure 5.4 shows the change in electrical output power as the module height increases under the first type of boundary condition with different T_H . Same as the pattern shown in the original working conditions, there exists an optimal module height that produces maximum output power, and this height has almost no dependence on the hot side temperature T_H . The output power shows a linear increase with the hot side temperature. Therefore, the change in the hot side temperature has negligible effect on the optimal module design but has a strong effect on the output power.

Figure 5.4 Output power versus TE leg height under different fixed T_H , while $T_C=303\text{K}$

Figure 5.5 shows electrical output power change as the module height increases under second type boundary condition with different Q_H value. Like in the original working condition, the output power increases continuously with module height under all six Q_H values. However, at high heat flux, the slope is steeper, which suggests that with larger heat flux, larger module height is more influential in producing more electrical power.

Figure 5.5 Output power versus TE leg height under different fixed Q_H , while $T_C=303\text{K}$

5.5 Parametric study at different fill factor values

The fill factor (FF) value used in Sections 5.3 and 5.4 is 0.5. In this section, the effect of FF change on the output power is investigated by changing the FF in the range of 0.2 to 0.7.

Figure 5.6 shows the effect of the FF on module height optimization. First, as shown in Figure 5.6 (a) and (b), the output power increases as the module height increases, and this feature suggests that under the current working conditions, a larger FF is always preferred as long as it is feasible. Second, Figure 5.6(a) shows that under different FF s and fixed T_H and fixed T_C , the output power always exhibits the same pattern as in Sections IV.A and IV.B, that there exists an optimal module height that achieves maximum output power. The optimal module height changes under different FF s, and the optimal value increases from 1.5 mm to 2.1 mm as the FF increases from 0.2 to 0.7. Third, Figure 5.6 (b) shows that under fixed Q_H , the output power also increases with the module height, but increases less with the FF at larger FF values, exhibiting a demising margin effect.

Figure 5.6 Output power versus TE leg height under different FF . (a) Fixed T_H , and fixed T_C and (b) fixed Q_H and fixed T_C

5.6 Summary

The optimal TEM height corresponding to maximum output power has been investigated under both first type and second type boundary conditions, i.e. fixed hot side temperature and fixed hot side heat flux, respectively. Based on the results, geometry optimization may have distinct results under first type and second type of boundary conditions.

The output power is significantly affected by the TEM height under both first type and second type boundary conditions. Under the second type boundary condition, output power continuously increases with TEM height, suggesting that a larger TEM height is always preferred. However, under first type boundary condition of fixed hot side temperature at 573K, the output power first increases and then decreases with TEM height increase, reaching a maximum output power at TEM height of 1.9 mm. While the optimal TEM height does not change with different T_H values, it increases with the FF s, increasing from 1.5 mm to 2.1 mm as the FF increases from 0.2 to 0.7. Therefore, under the first type of boundary condition, the optimal TEM height needs to be carefully selected to reach the maximum output power. These results can be used as a reference for choosing appropriate boundary conditions.

CHAPTER 6 Co-Optimization of Thermoelectric and Heat Exchanger for Waste Heat Recovery

6.1 Introduction

Most of previous optimization studies on the TEM design parameters considered the TEM alone and assumed fixed temperature or fixed heat fluxes as boundary condition for the TEM. The effects of the hot and cold side HEX on the TEM design are neglected. However, in real applications the TEM boundary conditions vary due to the thermal resistance of the HEX; when the TEM design changes, the boundary conditions change. Stevens et al. [66] simulated the TEM as an external thermal resistance and found that the output power is maximized when the thermal resistance of the TEMs matches with the sum of the hot and cold side HEX thermal resistance. This is an interesting outcome which has not been further explored and it was only limited to small temperature differences.

In this section, a general framework to co-optimize the design parameters of TEM together with the design parameters of HEX based on the Taguchi statistical method is proposed. The Taguchi method has been widely used for design and analysis of HEXs and other energy systems, and it is demonstrated to be a powerful tool due to its simplicity and robustness [46, 92-94]. The Taguchi method is capable of identifying the important design parameters and determining the optimized design parameters in different conditions.

The Taguchi method is used to investigate the sensitivity and contribution of five design parameters on the output power recovered by the TEG; including the TEM height, TEM fill-ratio (ratio of cross-sectional area covered by TE material divided by total cross-sectional area), TEM A_n/A_p ratio (ratio of cross-sectional area of n-type material over p-type material), the HEX length, and the HEX material. Interaction effects between the design parameters are also studied. The exhaust gas flow rate and heat transfer conditions vary in different engineering applications. To investigate the difference in the effect of design parameters in different applications,

this co-optimization framework is applied to study the same five design parameters on two different applications: an automotive engine of 108kW and a marine engine of 3.2 MW. The effect of scale on the design of TEG is investigated.

The structure of the study is as follows. In Section 6.2, the Taguchi method is introduced. In Section 6.3, the Taguchi method is applied considering an automotive application. In Section 6.4, the Taguchi method is conducted in a marine application. The conclusions are drawn in Section 6.5.

6.2 Taguchi method

Compared with the full factorial design, the Taguchi method can obtain maximum information from the minimum number of experiments with the help of an orthogonal array. In the evaluation process, the Taguchi method employs signal-to-noise (S/N) ratio defined in terms of the mean value and variance of the response. There are three categories of S/N ratio in the analysis of objective functions, including “the larger the better”, “the smaller the better” and “the nominal the better”. In this paper, the objective is to maximize the output power, which is “the larger the better” situation. The larger the better S/N ratio is calculated using the following equation:

$$S/N \text{ ratio} = -10 \log_{10} \left(\frac{1}{n} \sum_{i=1}^n y_i^2 \right) \quad (6.1)$$

where y_i represents the value of TEG output power and n is the number of simulation runs.

The Taguchi method ensures that every level (= value) of all the factors (= design parameters) is equally considered. Although only a fraction of the full factorial design experiments is conducted, the factors can be evaluated independently from each other at a much lower computation cost. After the simulation tests are completed, the analysis of variance (ANOVA) is conducted to analyze the model results, which provides information about the influence and contribution of each

single factor. The ANOVA analyzes the mean S/N ratio under each factor level to determine the sensitivity of each design parameter and determine the contribution ratio of each factor to the overall response. The optimum combination of design parameters and the interaction effects between design parameters are also obtained by ANOVA.

6.3 Taguchi method on automotive application

6.3.1 Problem description

In this section, five design parameters that influence the TEG output power are evaluated. The input parameters for automotive application baseline model are the TEM height (A), TEM fill-ratio (B), TEM A_n/A_p ratio (C), HEX length (D), and HEX material (E). Three levels are evaluated for each set of design parameters. The selected factors and levels are shown in

Table 6.1. Considering five factors with three levels, the number of tests would be $3^5 = 243$ should each possible combination is considered by full factorial design. However, with the Taguchi method, a five-factor problem with three levels can be analyzed by the L_{27} orthogonal array, and the number of experiments is reduced from 243 to 27. Among those levels, level 2 is the original design parameter in the reference experiments [12], while level 1 and level 3 are the lower and upper bounds of design limits determined based on engineering feasibility. The TEM height is the height of the semiconductor leg within TEM. The fill ratio is the ratio of cross-sectional area covered by TE material divided by total cross-sectional area. The TEM A_n/A_p ratio is the ratio of cross-sectional area of n-type material divided by p-type material. The HEX length is the axial length of HEX. For the HEX material, Aluminun is Aluminun alloy 195, Brass is copper cartridge brass and Steel is steel AISI 347.

Table 6.1 Selected factors and levels for automotive application

Label	Factor	Level 1	Level 2	Level 3
A	TEM height [mm]	1	5	9
B	Fill-ratio	0.1	0.32	0.8
C	TEM A_n/A_p ratio	0.5	1	2
D	HEX length [m]	0.2	0.4	0.6
E	HEX material	Aluminum	Brass	Steel

6.3.2 Modeling results and SNR ratio

Twenty-seven simulation tests were conducted according to the L_{27} orthogonal array. The output power in each run of simulation results, together with corresponding S/N ratio are listed in

Table 6.2. As can be seen from the results, the largest power is obtained in run 23, reaching 167.5W, while the smallest power obtained in run 8 is 7.7 W, which is almost 22 times smaller than that in run 22. This result suggests that the output power is very sensitive to design parameters, indicating the selected parameters are critical to the TEG system design.

Table 6.2 Orthogonal array and simulation results in automotive application

Run	TEM height [mm]	fill- ratio	TEM A_n/A_p ratio	HEX length[m]	HEX material	Power [W]	S/N ratio
1	1	0.1	0.5	0.2	1	19.4	25.7
2	1	0.1	1	0.4	2	40.3	32.1
3	1	0.1	2	0.6	3	48.7	33.8
4	1	0.32	0.5	0.4	3	17.7	25.0
5	1	0.32	1	0.6	1	29.1	29.3
6	1	0.32	2	0.2	2	19.0	25.6
7	1	0.8	0.5	0.6	2	11.1	20.9
8	1	0.8	1	0.2	3	7.7	17.7
9	1	0.8	2	0.4	1	14.9	23.5
10	5	0.1	0.5	0.2	1	45.0	33.1
11	5	0.1	1	0.4	2	86.5	38.7
12	5	0.1	2	0.6	3	98.2	39.8
13	5	0.32	0.5	0.4	3	96.7	39.7
14	5	0.32	1	0.6	1	139.7	42.9

15	5	0.32	2	0.2	2	58.8	35.4
16	5	0.8	0.5	0.6	2	97.9	39.8
17	5	0.8	1	0.2	3	48.4	33.7
18	5	0.8	2	0.4	1	79.9	38.1
19	9	0.1	0.5	0.2	1	42.8	32.6
20	9	0.1	1	0.4	2	77.9	37.8
21	9	0.1	2	0.6	3	85.7	38.7
22	9	0.32	0.5	0.4	3	122.2	41.7
23	9	0.32	1	0.6	1	167.5	44.5
24	9	0.32	2	0.2	2	60.4	35.6
25	9	0.8	0.5	0.6	2	156.1	43.9
26	9	0.8	1	0.2	3	68.1	36.7
27	9	0.8	2	0.4	1	107.2	40.6

6.3.3 Analysis of variance

The modeling results were collected and analyzed using Minitab 17 software. The mean responses of S/N ratio at each level of five factors are listed in Table 6.3. To better illustrate how the mean S/N ratio changes, the mean S/N ratio at each level is plotted in Figure 6.1. It can be seen from Fig. 1 that all five factors have certain

influence on the S/N ratio, and a higher TEM height is preferred for larger S/N ratio. As shown in Eq. (11) and Eq. (12), increasing TEM height leads to a smaller thermal conductance and larger electrical resistance, which has positive and negative effects on the output power, respectively. Smaller thermal conductance leads to a larger temperature difference and therefore larger output power; on the other hand, higher electrical resistance leads to higher Joule heating loss and therefore lower output power. Which effect is greater depends on the relative significance between TEM thermal resistance and HEX thermal resistance [95]. When the thermal resistance of TEM is much smaller than that of HEX, the effect of reducing TEM thermal conductance is greater, and it is clear that the output power increases as the TEM height increases [96]. When the thermal resistance of TEM is much larger than that of HEX, the output power decreases as the TEM height increases. The results in Table 6.3 and Figure 6.1 suggest that in automotive applications, the thermal resistance of TEM is smaller than that of HEX, and a larger TEM height is preferred. Besides, as shown in Eq. (12), changing the fill ratio and A_n/A_p also changes the thermal resistance and electrical resistance. Therefore, the optimal fill ratio and A_n/A_p ratio also depends on the relative significance between TEM thermal resistance and HEX thermal resistance. In this case, both the fill ratio and A_n/A_p are preferred at level 2 for maximum output power.

For the HEX length, the larger the better. Larger HEX exchange length means larger heat transfer area, which causes the thermal resistance of HEX exchanger become smaller. The TEM and HEX are connected thermally in series. With the thermal resistance of TEM kept constant, smaller HEX thermal resistance means larger temperature difference between two sides of TEM, thus the output power becomes larger. For the HEX material, the output power under Aluminum alloy and copper cartridge brass generate nearly the same output power, both larger than the output power under steel. This result is mainly attributed to the higher thermal conductivity of Aluminum and brass.

The percentage contributions of different factors are plotted in Figure 6.2. As shown, the TEM height is the most important design parameter that influences the

output power, contributing 69.6% of all design parameters. The other two important parameters are HEX length and the interaction factor AB, contributing 14.18% and 11.23%, respectively. The other six parameters play insignificant roles in the design of TEG system, contributing 4.99% in total.

Table 6.3 Response table for S/N ratios in automotive application

Level	A	B	C	D	E
1	25.95	34.71	33.60	30.68	34.47
2	37.91	35.52	34.83	35.25	34.43
3	39.12	32.76	34.55	37.06	34.09
Delta	13.17	2.76	1.22	6.38	0.38
Rank	1	3	4	2	5

Figure 6.1 Mean S/N ratio analysis in automotive application

Figure 6.2 Contribution of selected factors to the S/N ratio in automotive application

Figure 6.3 Effect of interactions in automotive application

Figure 6.3 shows the interaction effect between any two factors. Generally, parallel plots denote no interaction effect between two factors while crossing plots denote significant interaction effect. Strong interaction between two design parameters indicates that the optimum value of one design parameter depends on the value of the other parameter. As can be seen, parameter B exhibits strongest effect to other factors, which means the optimal fill ratio value is highly dependent on other design parameters. The optimal TEM height is influenced by TEM fill ratio and A_n/A_p ratio, and independent to HEX length and HEX material. Besides, the HEX material selection also has significant influence on the design of other parameters.

6.3.4 Comparison of original experiment and optimized design

The optimum combination of the design parameters could be determined based on the results in Figure 6.1 by selecting parameters at level of the highest S/N ratio. The ideal combination of design parameters regarding the output power is A3-B2-C2-D3-E1. The comparison of output power under the original design and the optimum design is shown in Figure 6.4. The comparison is conducted under various exhaust gas flow rates. The range of exhaust gas flow rate in Figure 6.4 can represent exhaust gas flow rate from the small mini-car to large bus or truck. As can be seen, the optimized design obtained by Taguchi method can improve the output power significantly. However, it needs to be mentioned that some engineering difficulties are not fully considered in this optimization by Taguchi method. For example, the level 3 TEM height is 9 mm. Although TEM with 10 mm TEM height has been manufactured in some research groups, the height of commercial TEM usually ranges from 1 mm - 3 mm due to the challenge of mechanical strength.

Figure 6.4 Comparison of output power under the original and the optimal design parameters

6.4 Taguchi method on marine application

6.4.1 Problem description

To compare the applications of different scales, the effects of the same five design parameters are analyzed in large marine applications using Taguchi method. A medium size marine internal combustion engine and its exhaust system are selected as baseline model, and the input parameters are listed in Table 6.4. The exhaust gas flow rate $11 \text{ m}^3/\text{s}$ is 140 times higher than the exhaust gas flow rate in the baseline case of automotive application $0.0783 \text{ m}^3/\text{s}$.

Table 6.5 shows the selected factors and levels. To compare directly with the automotive application, TEM design parameters, TEM height, TEM fill ratio, TEM A_n/A_p ratio, and HEX materials are set the same as in the automotive application.

HEX length is larger for the larger size of marine exhaust pipeline system.

Table 6.4 Input parameters in marine application- baseline model

Parameters	Value	Unit
<u>Engine parameters</u>		
Model	M73 20V	
Fuel consumption	821	<i>L/h</i>
Rated power	3.2	<i>MW</i>
<u>Fluid parameters</u>		
Exhaust temperature	798	<i>K</i>
Exhaust flow rate	11.7	<i>m³ /s</i>
<u>HEX parameters</u>		
HEX [length, width, height]	[1.2, 0.5, 0.2]	<i>m</i>
HEX material	Copper brass	Cartridge -
<u>TEM parameters</u>		

TEM [length, width, height]	[50, 50, 5]	<i>mm</i>
TE legs in one TEM	127	-
TEM number	300	-
TE material	N type: $\text{Mg}_2\text{Sn}_{0.75}\text{Ge}_{0.25}$ P type: Cu_2Se , $\text{Cu}_{1.98}\text{Se}$	-
Ceramic Substrate	Al_2O_3	-

Table 6.5 Selected factors and levels in marine application

Label	Factor	Level 1	Level 2	Level 3
A	TEM height [mm]	1	5	9
B	Fill-ratio	0.1	0.32	0.8
C	TEM A_n/A_p ratio	0.5	1	2
D	HEX length	0.6	1.2	1.8
E	HEX material	Aluminum	Brass	Steel

6.4.2 Modeling results and SNR ratio

Table 6.6 shows the 27 runs generated by a L_{27} orthogonal array, same as in the automotive application. The largest power reaches 6058.6W in run 25, while the smallest power obtained in run 8 is 41 W, which is almost 147 times smaller than the largest power. Compared with the 22 times difference between bottom value and peak value in automotive application, the TEG system in marine application is even more sensitive to the selected design parameters.

Table 6.6 Orthogonal array and simulation results in marine application

Run	TEM height [mm]	fill-ratio	TEM A_n/A_p ratio	HEX length[m]	HEX material	Power [W]	S/N ratio
1	1	0.1	0.5	0.6	1	422.70	52.52
2	1	0.1	1	1.2	2	1051.84	60.44
3	1	0.1	2	1.8	3	495.96	53.91
4	1	0.32	0.5	1.2	3	120.00	41.58
5	1	0.32	1	1.8	1	1785.45	65.03
6	1	0.32	2	0.6	2	647.50	56.22
7	1	0.8	0.5	1.8	2	714.90	57.08
8	1	0.8	1	0.6	3	41.06	32.27
9	1	0.8	2	1.2	1	996.11	59.97

10	5	0.1	0.5	0.6	1	687.28	56.74
11	5	0.1	1	1.2	2	1619.36	64.19
12	5	0.1	2	1.8	3	1360.49	62.67
13	5	0.32	0.5	1.2	3	867.74	58.77
14	5	0.32	1	1.8	1	5007.98	73.99
15	5	0.32	2	0.6	2	1589.94	64.03
16	5	0.8	0.5	1.8	2	4460.30	72.99
17	5	0.8	1	0.6	3	355.53	51.02
18	5	0.8	2	1.2	1	4097.24	72.25
19	9	0.1	0.5	0.6	1	649.40	56.25
20	9	0.1	1	1.2	2	1428.84	63.10
21	9	0.1	2	1.8	3	1325.02	62.44
22	9	0.32	0.5	1.2	3	1259.77	62.01
23	9	0.32	1	1.8	1	5084.47	74.12
24	9	0.32	2	0.6	2	1500.86	63.53
25	9	0.8	0.5	1.8	2	6058.60	75.65
26	9	0.8	1	0.6	3	582.38	55.30

27	9	0.8	2	1.2	1	4641.66	73.33
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6.4.3 Analysis of variance

The mean responses of S/N ratio at each level of five factors are shown in Table 6.7. To better illustrate how the mean S/N ratio change with each level, the mean S/N ratio at each level and the rank of each factor in terms of significance is plotted in Figure 6.5. All five factors have certain influences on the S/N ratio. As can be seen, a higher TEM height is preferred for a larger S/N ratio. Same as in the automotive application, the mean S/N ratio is the highest when TEM height is level 3. This result suggests that in the marine application, the thermal resistance of TEM is also much smaller compared with that of HEX, and increasing the TEM height can significantly improve the output power. To generate the largest output power, the fill ratio should be set as level 2, same as in the case of automotive application. The A_n/A_p ratio optimal at level 3, which is different than in the case of automotive application. In the marine exhaust system, the exhaust gas flow rate and HEX size is bigger than those in the automotive application. Therefore, the Reynold number and heat transfer coefficient of the flow in HEX are different with those in the automotive application, and consequently the thermal resistance of HEX is different. Since the optimal A_n/A_p ratio also depends on the relative significance between TEM thermal resistance and HEX thermal resistance, the optimal A_n/A_p ratio varies when the HEX design changes. Similar to the case of automotive application, the HEX length is also expected to be larger in the marine application, mainly due to the decreased conductive thermal resistance of HEX. For the HEX material, the optimum material for maximum output power is Aluminum. In contrast to the automotive application, the S/N ratio changes more significantly with different material selections.

Table 6.7 Response table for S/N ratios in marine application

Level	A	B	C	D	E
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1	53.23	59.14	59.29	54.21	64.91
2	64.07	62.14	59.94	61.74	64.14
3	65.08	61.10	63.15	66.43	53.33
Delta	11.86	3.00	3.86	12.22	11.58
Rank	2	5	4	1	3

Signal-to-noise: Larger is better

Figure 6.5 Mean S/N ratio analysis in marine application

Figure 6.6 Contribution of selected factors to the S/N ratio in marine application

Figure 6.7 Effect of interactions in marine application

The percentage contributions of each factor are plotted in Figure 6.6. As shown, the most important design parameter that influences the output power is also TEM height, contributing 30.25% of all design parameters, which is only half as in the automotive application. The other two important parameters are HEX length and material, contributing 26.62% and 29.35%, respectively. In contrast to automotive application, the HEX design parameters are more important in marine application. Figure 6.7 shows the interaction effect between any two factors. It is found that significant interaction is found between TEM fill ratio, A_n/A_p ratio, HEX length and material. However, it is noted that the TEM height does not interact significantly with the other design parameters, and always the larger the better for the S/N ratio. This result suggests that in all scenarios, TEM thermal resistance is always smaller than HEX thermal resistance, and increasing TEM height always has a positive effect on the output power. From the above discussion, it can be concluded that the TEG design for different scales is similar. The TEM height is desired to be large in both applications. On the other hand, there exist differences in the design for different application scales, as some parameters have more significant effects in the marine application, and the parameter interaction effect is also different. Therefore, individualized TEM and HEX design is needed for different application scales.

6.5 Summary

In this chapter, a framework to co-optimize the TEM and HEX has been proposed to select the key design parameters of TEG for waste heat recovery. The proposed method adopts the Taguchi statistical method which analyzes the effect of each design parameters (namely TEM height (A), TEM fill-ratio (B), TEM A_n/A_p ratio (C), the HEX length (D) and the HEX material (E)). In the Taguchi analysis, an orthogonal array L_{27} with five design parameters at three levels has been considered in both the automotive and the marine application. The key findings have been summarized as follows:

For the smaller scale automotive application, the TEM height is the most critical design parameter, contributing 69.6% to the total S/N ratio variation. The other two

important design parameters are the HEX length and the interaction between the TEM height and TEM fill ratio. The optimal set of design parameters achieving the largest output power is A3-B2-C2-D3-E1, which outperforms the original design over a wide range of exhaust gas flow rate from 0.05 m³/s to 1.5 m³/s. For the larger scale marine application, the TEM height is still the most critical design parameter, contributing 30.25% to the overall response. The other two important design parameters are the HEX length and HEX material, contributing 26.62% and 29.35% to the total S/N ratio variation, respectively. The optimal set of design parameters is found to be A3-B2-C3-D3-E1 in the marine application. The TEM height is the most important design factor, which enables output power maximization as long as the mechanical strength can be tolerated.

CHAPTER 7 Conclusions and Future Research

7.1 Conclusion

The development of models and methodologies for the design and optimization of TEGs has been the focus of this thesis, aiming at improving efficiency and output power of TEGs. Numerical models of TEM and TEG have been proposed.

A numerical model of TEM based on discretization is built by numerically solving the multi-physics governing equations, considering Seebeck effect, Joule heating, Thompson effect, and Peltier effect. A discretization scheme is developed to solve the temperature profile in order to obtain output power and efficiency predictions. This model is validated against experiments and the results match well. A simplified lumped parameter TEM model is also built for quick power prediction.

Since the TEM design is highly dependent on the thermal boundary condition. An integrated TEM and HEX model is proposed. The HEX model is built based on empirical equations, and LMTD method is adopted to improve the accuracy. A discretization scheme is proposed to integrate the TEM and HEX model into a TEG model. Experimental results suggest that the model is able to predict the TEG output power performance accurately.

After the numerical model is developed and validated, parametric and optimization studies are conducted at TEM and TEG levels to improve the output power and efficiency. At the TEM level, the optimal TEM height corresponding to maximum output power has been investigated under both first type and second type boundary conditions, i.e. fixed hot side temperature and fixed hot side heat flux, respectively. It is shown in the simulation results that the output power is significantly affected by the TEM height under both first type and second type boundary conditions. However, geometry optimization may have distinct results under different types of boundary conditions. Under the second type boundary condition, the output power continuously increases with TEM height, suggesting that a larger TEM height is

always preferred. However, under first type boundary condition of fixed hot side temperature at 573K, the output power first increases and then decreases with increasing TEM height, reaching a maximum output power at TEM height of 1.9 mm.

For TEG level optimization, a framework based on Taguchi method to co-optimize the TEM and the HEX has been proposed. Five design parameters have been investigated, (namely TEM height (A), TEM fill-ratio (B), TEM A_n/A_p ratio (C), the HEX length (D) and the HEX material (E)). In the Taguchi analysis, the orthogonal array L_{27} with five design parameters at three levels has been considered in both automotive and the marine applications. It is found that the TEM height is the most critical design parameter, contributing 69.6% to the total S/N ratio variation in automotive application and 30.25% in marine application. The optimal parameter sets in both marine and automotive applications are found.

7.2 Recommendations for Future Works

Notwithstanding the progress made so far in this thesis, several other topics in the field of TEG simulation, more accurate CFD modeling, new experimental setup development, and some other relevant issues are worthy of pursuing for the future work.

7.2.1 Prototype development of TEG system

Throughout this thesis, TEM and TEG systems are designed and optimized by an analytical model. For the next step of work, TEMs with different sizes and TEG system with HEX could be manufactured to further verify the findings in this study. In Chapter 4, optimal TEM height is recommended in several different engineering circumstances. The testing of TEMs with different heights in different engineering applications will be an interesting topic that is worth investigating, which will provide guidance for commercial TEG activities.

7.2.2 Improve heat transfer by heat pipe or phase change material

The thesis emphasizes on developing a methodology to improve the TEG output power and efficiency. More detailed strategy to improve the TEG output power is to be identified and tested.

One existing challenge of current TEG system is relatively low heat transfer ability. A heat pipe employing phase change heat transfer can significantly improve heat transfer ability [97]. Another challenge in the practical application of TEG for waste heat recovery from exhaust gas is the temperature variation. The fluctuated temperature results in further losses, as the TE material may not work at its optimal temperature. One potential strategy would be adopting phase change material (PCM) as an intermediate layer between the heat source and hot side of TEM, to maintain a constant temperature at the hot side of TEM.

Appendix A: Derivation of efficiency and figure of merit

In this section, the maximum efficiency under certain temperature is derived. The efficiency of a TE generator is defined as:

$$\eta = \frac{\text{load output power}, P_{load}}{\text{heat input}, Q_{in}} \quad (7.1)$$

And can be found as:

$$\eta = \frac{T_H - T_C}{T_H} \frac{\sqrt{1 + ZT} - 1}{\sqrt{1 + ZT} + T_C / T_H} \quad (7.2)$$

Starting from the current equation:

$$\mathbf{J} = \sigma \mathbf{E} - \sigma \alpha \nabla T \quad (7.3)$$

When the device is in open circuit, the current $J = 0$, and the equation then becomes:

$$\mathbf{E} = \alpha \nabla T \quad (7.4)$$

In 1-D condition, integrating the above equation, the total open circuit voltage produced by Seebeck effect can be obtained:

$$V = \int_{T_L}^{T_H} \alpha_{pn} dT = (\alpha_{pn})(T_H - T_L) \quad (7.5)$$

where $\alpha_{p,n}$ is the Seebeck coefficient of TE couple considering both p-type and n-type leg.

If this TEG is then connected with an external load, the current is:

$$I = \frac{(\alpha_p - \alpha_n)(T_H - T_L)}{R + R_L} \quad (7.6)$$

,

The output power produced by the load is:

$$P = I^2 R_L \quad (7.7)$$

The efficiency is then

$$\eta = \frac{P}{Q_H} = \frac{I^2 R_L}{\pi_h - k_p(T_h)T'_p(0) - Ak_n(T_h)T'_n(0)} \quad (7.8)$$

According to Burshtein, when the thermal conductivity k and Thomson coefficient τ are independent of temperature and electric resistivity $\rho(T) = \rho_0 + \rho_1 T$, the temperature gradient at the hot surface $T'(0)$ is given by:

$$T'(0) = \frac{-\Delta T}{L} + \frac{J^2 L}{2k} [\rho_0 + \rho_1 \frac{2T_h + T_c}{3}] + \frac{\tau J}{2k} [\Delta T - \frac{J^2 L^2 (\rho_0 + \rho_1 T_1)}{6k} - \frac{\tau J L \Delta T}{6k}] + \dots \quad (7.9)$$

Substituting (7.7) into (7.6), then the efficiency can be written as:

$$\eta = \frac{I^2 R}{\alpha_{pn} T_h I + \Delta T L^{-1} (k_p + Ak_n) - \frac{I^2 L (\rho_p + \rho_n A^{-1})}{2}} \quad (7.10)$$

In order to find the maximum efficiency, the derivative is made zero

$$\frac{d\eta}{dm} = 0 \quad (7.11)$$

Obtaining:

$$m = \sqrt{1 + Z \frac{T_c + T_h}{2}} \quad (7.12)$$

where Z is given as:

$$Z = \frac{\alpha^2}{\rho\kappa} \quad (7.13)$$

Substituting in the efficiency equation (7.1), one obtains:

$$\eta = \frac{T_H - T_C}{T_H} \frac{\sqrt{1 + ZT} - 1}{\sqrt{1 + ZT} + T_C / T_H} \quad (7.14)$$

Appendix B: Solution of temperature field inside TE element

As introduced in Chapter 3.3, the solution of temperature field is expressed in a dimensionless form. The coefficient in the temperature field solution is introduced as follows [98].

The Seebeck coefficient (α), thermal conductivity (κ), electrical resistivity (ρ) are approximated by third order polynomials:

$$\alpha(T) = \sum_{i=0}^3 a_i T^i, k(T) = \sum_{i=0}^3 k_i T^i, \rho(T) = \sum_{i=0}^3 \rho_i T^i \quad (7.15)$$

and the a , b , d , and w_r are functions of θ , as follows:

$$\begin{aligned} f(\theta) &= \sum_{j=0}^3 f_j \theta^j, g(\theta) = \sum_{j=0}^3 g_j \theta^j, h(\theta) = \sum_{j=0}^3 h_j \theta^j, \\ q(\theta) &= \sum_{j=0}^3 q_j \theta^j, \end{aligned} \quad (7.16)$$

where the coefficients are given by:

$$f_0 = A(T_H - T_C)^3 (3k_3 T_C^2 + 2k_2 T_C + k_1) / L^2 \quad (7.17)$$

$$f_1 = 2A(T_H - T_C)^4 (k_2 + 3k_3 T_C) / L^2 \quad (7.18)$$

$$f_2 = 3A(T_H - T_C)^5 k_3 / L^2 \quad (7.19)$$

$$g_0 = A(T_H - T_C) (k_0 T_C + k_1 T_C + k_2 T_C^2 + k_3 T_C^3) / L^2 \quad (7.20)$$

$$g_1 = A(T_H - T_C)^3 (3k_3 T_C^2 + 2k_2 T_C + k_1) / L^2 \quad (7.21)$$

$$g_2 = A(T_H - T_C)^4 (k_2 + 3k_3 T_C) / L^2 \quad (7.22)$$

$$g_3 = A(T_H - T_C)^4 k_3 / L^2 \quad (7.23)$$

$$h_0 = I(T_H - T_C) (3a_3 T_C^3 + 2a_2 T_C^2 + a_1 T_C) / L \quad (7.24)$$

$$h_1 = I(T_H - T_C)^2 (9a_3 T_C^3 + 4a_2 T_C + a_1) / L \quad (7.25)$$

$$h_2 = I(T_H - T_C)^3 (9a_3 T_C + 2a_2) / L \quad (7.26)$$

$$h_3 = 3I(T_H - T_C)^4 a_3 / L \quad (7.27)$$

$$q_0 = I^2 (r_0 + r_1 T_C + r_2 T_C^2 + r_3 T_C^3) / A \quad (7.28)$$

$$q_1 = I^2 (T_H - T_C) (r_1 + 2r_2 T_C + 3r_3 T_C^2) / A \quad (7.29)$$

$$q_2 = I^2 (T_H - T_C)^2 (r_2 + 3r_3 T_C) / A \quad (7.30)$$

$$q_3 = I^2 (T_H - T_C)^3 r_3 / A \quad (7.31)$$

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