

Recent advances in modeling and simulation of thermoelectric power generation

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Abstract: Thermoelectric power generation is a renewable energy conversion technology that can directly convert heat into electricity. In recent years, a great number of theoretical models have been established to predict and optimize the performance of both thermoelectric generators and thermoelectric generator systems. In this work, a comprehensive review of theoretical models is given with a specific focus on the different modeling approaches and different application scenarios. Firstly, the basic principles of theoretical models of the thermoelectric generator are presented, including the thermal resistance model, thermal-electric numerical model, and analogy model. Then, the theoretical models of the thermoelectric generator system are reviewed in detail, including the thermal resistance-based analytical model, computational fluid dynamics models, and fluid-thermal-electric multiphysics field coupled numerical model. The methods to improve the accuracy of theoretical models are also discussed. Furthermore, the transient thermal-electric numerical model of the thermoelectric generator and the transient fluid-thermal-electric multiphysics field coupled numerical model of the thermoelectric generator system are introduced, which can take into account the dynamic characteristics of the heat source, and may remain a hot research field in the upcoming years. Generally, thermal resistance models can quickly obtain the performance of the thermoelectric generator and thermoelectric generator system under different parameters, but suffer from relatively large errors; while it is the opposite for numerical models. To design a comprehensive thermoelectric generator system for practical application, it is suggested to combine the advantages of different models, to shorten the development time and ensure optimal performance at the same time.

Keywords: Thermoelectric generator; Theoretical model; Thermal resistance; Numerical model; Transient

| Nomenclature | | η | Conversion efficiency |
|----------------------|---|----------------------|------------------------------|
| <i>Symbols</i> | | ϕ | Electrical potential, V |
| A | Area, m ² | ρ | Density, kg·m ⁻³ |
| c | Specific heat, J·kg ⁻¹ ·K ⁻¹ | μ | Dynamic viscosity, Pa·s |
| \vec{E} | Electric field density vector, V·m ⁻² | δ | Thickness, m |
| H | Height, m | <i>Subscripts</i> | |
| h | Heat transfer coefficient, W·m ⁻² ·K ⁻¹ | c | Cold side |
| I | Current, A | ce | Ceramic plate |
| \vec{j} | Current density vector, A·m ⁻² | co | Copper electrode |
| \dot{m} | Mass flow rate, kg·s ⁻¹ | ex | Exhaust gas |
| N | Number | ext | External environment |
| Nu | Nusselt number | h | Hot side |
| P | Power, W | hp | Heat pipe |
| Pr | Prandtl number | in | Internal resistance |
| Q | Heat, W | L | Load resistance |
| \dot{q} | Heat flux, W·m ⁻² | leg | thermoelectric leg |
| R | Resistance, Ω or K·W ⁻¹ | m | Material name |
| Re | Reynolds number | n | n-type thermoelectric leg |
| T | Temperature, K | p | p-type thermoelectric leg |
| t | Time, s | pn | Thermoelectric couple |
| U | Voltage, V | sink | Heat sink |
| v | Velocity, m·s ⁻¹ | wa | Water |
| \vec{v} | Velocity vector, m·s ⁻¹ | <i>Abbreviations</i> | |
| x | x-dimension | CFD | Computational fluid dynamics |
| <i>Greek symbols</i> | | FDM | Finite difference method |
| α | Seebeck coefficient, V·K ⁻¹ | FEM | Finite element method |
| λ | Thermal conductivity, W·m ⁻¹ ·K ⁻¹ | FVM | Finite volume method |
| σ | Electrical conductivity, S·m ⁻¹ | TEG | Thermoelectric generator |
| | | UDF | User defined function |

1. Introduction

Due to the tremendous use of fossil fuels, energy shortage and environmentally harmful emissions have become global problems in recent years, and many countries have issued policies to reduce the use of fossil energy and promote the development of green alternative energy techniques. One feasible way is to convert the kinetic energy or potential energy produced in nature into electrical energy, such as hydropower, wind power, and tidal power stations, which usually need to convert the energy into mechanical energy and then drive the generator to produce electricity. Another way is to convert solar energy or thermal energy directly into electricity by using some particular semiconductors, such as photovoltaic and thermoelectric power generation, which do not need any intermediate energy

1 conversion unit. All the green alternative energy technologies mentioned, except for thermoelectric
2 technology, are more or less weather dependent. Besides, thermoelectric power generation was
3 regarded as a promising alternative energy conversion technology, owing to its unparalleled merits of
4 no moving parts, no pollution, silent operation, no maintenance costs, and long service life [1-3].

5 In practical application, a thermoelectric generator (TEG) module is used as the basic power
6 generation unit, which combines heat source, cooling source, and heat exchanger devices into a TEG
7 system, and then generates electricity to supply power for electronic devices. According to the different
8 heat sources, the TEG system can be classified into two types: the TEG system for fluid waste heat
9 recovery and the TEG system directly contacted with a heat source. The TEG system for fluid waste
10 heat recovery is generally used to recover the waste heat contained in thermal fluids, like automobile
11 exhaust waste heat and industrial waste heat. The corresponding automotive TEG system [4, 5] and
12 industry waste-heat-recovery TEG system [6, 7] prototypes have been developed to recycle the waste
13 heat and reduce energy consumption. As for the TEG system directly contacted with a heat source, the
14 heat source directly provides a high temperature or heat flux to the hot side of the TEG modules,
15 without the need for the heat exchanger to collect heat from thermal fluids. Using the decay energy of
16 radioactive elements as a heat source, the radioisotope TEG system [8, 9] has been widely used in the
17 spacecraft power supply. Due to the low requirement of power intensity, thermoelectric generators can
18 also be used to harvest body heat and supply power for wearable devices [10]. In off-grid areas and
19 emergencies, the stove-powered TEG system was an effective approach to obtaining electricity [11,
20 12]. Unlike TEG systems applied in fluid waste heat recovery, the heat source of these TEG systems
21 is directly imposed on the hot side surfaces of the TEG module or the plates contacted with the TEG
22 module.

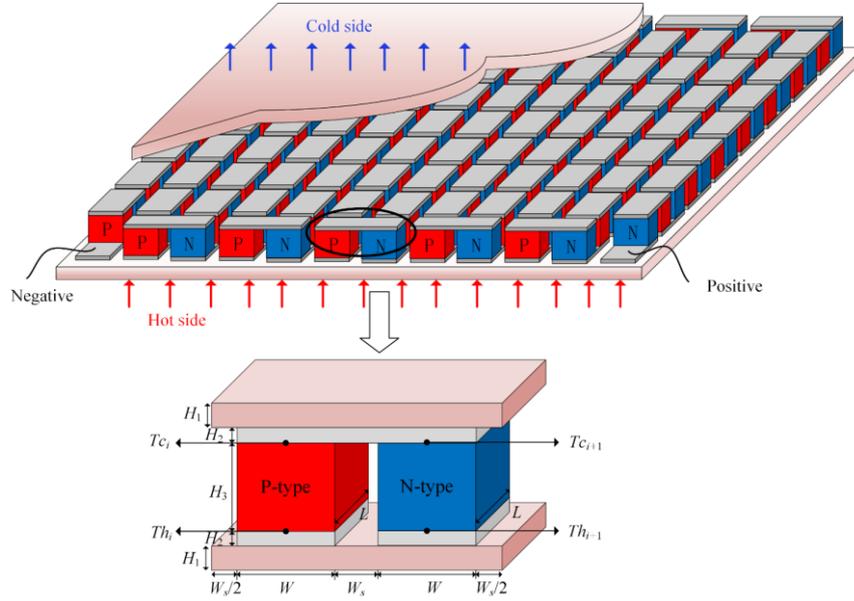
23 The behavior of TEG systems is generally evaluated by the output characteristic parameters of output
24 power and conversion efficiency, and great progress in the performance of TEG systems has been
25 made in recent years. However, the wide commercialization of TEG technology is still limited by the
26 low conversion efficiency of TEG systems. To further improve the heat-to-electricity conversion
27 efficiency, both the advancement of thermoelectric materials and the optimization of thermoelectric
28 devices need to be conducted. At present, the figure of merit (ZT) of most thermoelectric materials
29 ranges from 1 to 1.6, while the potential commercial application of waste heat recovery needs ZT to
30 reach 2.0 [13]. The threshold of $ZT = 2.0$ may be broken through shortly, thanks to the development
31 of modern synthesis and characteristic technologies, like nanostructured thermoelectric materials [14].
32 Besides the exploration of high-performance thermoelectric materials, the structural optimization

1 approaches of both TEGs and TEG systems can also improve the output power and conversion
2 efficiency. For the scenario of TEGs, segmented thermoelectric unicouples [15, 16], two-stage design
3 [17], and asymmetric thermoelectric devices [18] were commonly used optimization methods to
4 improve the efficiency and reduce the parasitic power losses. For the scenario of the TEG system
5 applied in fluid waste heat recovery, an additional heat exchanger was required to deliver heat from
6 thermal fluids to TEGs, and thus, many researchers [19, 20] have made great efforts to optimize the
7 heat transfer performance of heat exchanger.

8 Theoretical models are the premise to predict the performance and conduct the structure
9 optimizations of TEGs and TEG systems. Compared with experimental methods, model predictions
10 can save a lot of time and money, especially when several parameters need to be optimized.
11 Consequently, reasonable models need to be developed to predict the performance of TEGs and TEG
12 systems. As the heat flows through the TEG, the temperature difference will drive holes in p-type
13 thermoelectric materials and electrons in n-type thermoelectric materials moving from hot side to cold
14 side, so that a Seebeck voltage is generated, as shown in Fig. 1 (a). At the same time, the cold side
15 interface of carrier accumulation will release heat, and the hot side interface of carrier dissipation will
16 absorb heat, as a result of the Peltier effect; Because of the temperature gradient of thermoelectric
17 semiconductors, it will be accompanied by the generation of Thomson heat; As the electric current
18 flows through thermoelectric semiconductors, metal electrodes, and load resistance, it will be
19 accompanied by the generation of Joule heat. Based on these fundamental principles, various TEG
20 models [21, 22] have been proposed to evaluate the performance of a specific TEG design and optimize
21 its structure.

22 When TEGs are adopted in a specific field to recover waste heat or supply power, a more complex
23 heat transfer process is involved. Compared with TEGs, a Fourier heat conduction process from the
24 heat source to TEGs was involved in the TEG system directly contacted with a heat source. And the
25 performance of this TEG system can be predicted by adding additional heat transfer conservation
26 equations into the theoretical models of TEG. However, the situation of the TEG system for fluid waste
27 heat recovery is quite different and more complex. Taking the waste heat recovery from exhaust gases
28 as an example, the heat is first absorbed by the heat exchanger in the form of conjugate heat transfer,
29 then transferred from the heat exchanger to TEGs and heat sink, and finally taken away by the coolant,
30 as shown in Fig. 1(b). The intricate fluid flow and heat transfer process complicate the modeling of
31 TEG systems applied in fluid waste heat recovery [23]. Researchers [24, 25] have been trying to
32 establish a comprehensive model to accurately predict the performance of fluid-based TEG systems.

1 take a single TEG unit as the research object to establish the theoretical model of TEGs and analyze
 2 their performance. In this section, the fundamental principles of TEGs are introduced firstly, and then
 3 the recent development of TEG theoretical models is reviewed from one dimension to three
 4 dimensions, from TEG unit to TEG module, and from a steady state to a transient state. Finally, the
 5 comparative analysis and comment on different models are provided in Section 2.5.



6
 7 Fig. 2. Topological relationship between TEG module and TEG unit [26].

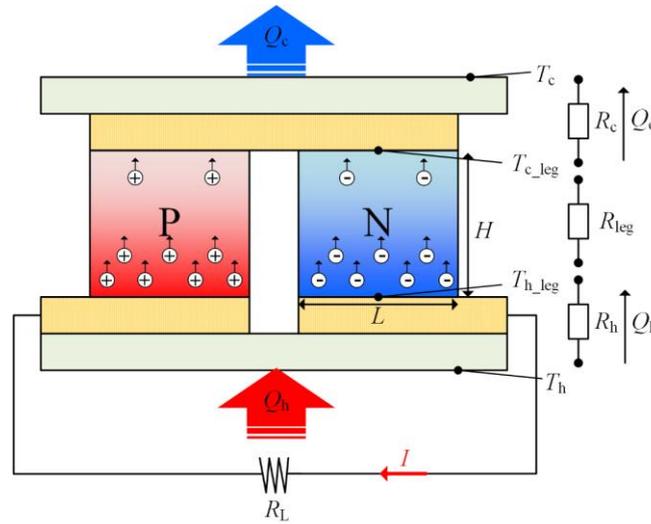
8 *2.1 Fundamental principles of thermoelectric generators*

9 The thermoelectric coupling effect includes the Seebeck effect, Peltier effect, and Thomson effect.
 10 Based on the Seebeck effect, the Seebeck voltage is determined, which equals the product of the
 11 Seebeck coefficient (α) and temperature difference (ΔT). Due to the Peltier effect, when the carriers
 12 of thermoelectric materials are transferred from the hot end to the cold end, the side of carrier
 13 accumulation will release heat, while the side of carrier dissipation will absorb heat. This endothermic
 14 and exothermic heat is called hot side Peltier heat and cold side Peltier heat respectively, which is
 15 equal to the product of Seebeck coefficient (α), current (I), and absolute temperature (T). Due to the
 16 Thomson effect, when the current direction is consistent with the temperature gradient direction,
 17 thermoelectric semiconductors will release heat, and vice versa. In addition to these three
 18 thermoelectric coupling effects, the Fourier heat conduction effect and Joule effect also occur. The
 19 amount of heat transfer from the hot end to the cold end is equal to Fourier heat. Joule heat is generated
 20 when the current passes through the thermoelectric semiconductor. Generally, the Fourier heat is the
 21 highest, followed by the hot side Peltier heat, cold side Peltier heat, Joule heat, and Thomson heat.

1 Furthermore, thermoelectric material properties are the necessary data to predict the TEG
 2 performance, including Seebeck coefficient (α), thermal conductivity (λ), and electric conductivity
 3 (σ). The thermoelectric properties establish the figure of merit (ZT), $ZT = \alpha^2 \sigma T / \lambda$, which
 4 characterizes the performance of thermoelectric material. In essence, the high Seebeck coefficient (α)
 5 helps to maximize the heat-to-electric conversion efficiency, the high electric conductivity (σ) can
 6 minimize the internal resistance and reduce the Joule heat, and the low thermal conductivity (λ) helps
 7 to maintain a high-temperature difference (ΔT) on both ends of thermoelectric semiconductors [27].
 8 Besides, thermoelectric properties are highly temperature-dependent. Chen et al. [28] conducted a
 9 comprehensive analysis of the TEG performance with constant and temperature-dependent properties
 10 and reported that the consideration of temperature dependence of thermoelectric materials can provide
 11 more realistic predictions. Consequently, the temperature-dependent material properties should be
 12 considered in the modeling process.

13 Based on the above basic principles, a reasonable theoretical TEG model can be established. At
 14 present, there are three main modeling methods, including the thermal resistance model, numerical
 15 model, and analogy model. In the following sections, recent developments of the three models are
 16 reviewed respectively.

17 2.2 Thermal resistance models



18
 19 Fig. 3. Schematic diagram of the thermal resistance model of the TEG unit.

20 The thermal resistance model is based on a global energy balance, assuming that Thomson heat and
 21 ambient convection heat transfer are negligible, and Joule heat is uniformly heated at both ends of
 22 TEG. The TEG output power is considered as the difference between the hot end heat flux and the cold

end heat flux. The schematic diagram of the thermal resistance model is shown in Fig. 3. The average temperature of different cross sections is taken as the actual working temperature to carry out the calculation of TEG output performance. However, the thermal resistance model can only consider the heat transfer from the hot side to the cold side, so it is a one-dimensional model and can not be extended to higher dimensions.

2.2.1 The simplified model

In the simplified thermal resistance models [29, 30], the temperature of the hot side ceramic plate (T_h) and the temperature of the cold side ceramic plate (T_c) are respectively used as the hot side and cold side working temperatures of p-type and n-type thermoelectric legs. Furthermore, the hot side flux can be expressed as:

$$Q_h = \alpha_{pn}IT_h + \frac{T_h - T_c}{R_{leg}} - \frac{1}{2}I^2R_{in} \quad (1)$$

where, I is the electric current, R_{leg} is the thermal resistance of thermoelectric legs, and R_{in} is the internal resistance of thermoelectric legs.

Also, the cold side flux can be written as:

$$Q_c = \alpha_{pn}IT_c + \frac{T_h - T_c}{R_{leg}} + \frac{1}{2}I^2R_{in} \quad (2)$$

with

$$\alpha_{pn} = \alpha_p - \alpha_n \quad (3)$$

$$R_{leg} = \frac{H_{leg}}{(\lambda_p + \lambda_n)A_{leg}} \quad (4)$$

$$R_{in} = (\sigma_p^{-1} + \sigma_n^{-1}) \frac{H_{leg}}{A_{leg}} \quad (5)$$

in which, H_{leg} and A_{leg} are the height and cross-sectional area of thermoelectric legs, respectively. Here, the size of the p-type thermoelectric leg is assumed to be equal to that of the n-type thermoelectric leg. σ^{-1} is the electric resistivity. Subscripts p and n denote p-type and n-type thermoelectric legs, respectively.

The output power of the TEG unit is obtained by subtracting Eq. (1) from Eq. (2):

$$P = Q_h - Q_c = \alpha_{pn}I(T_h - T_c) - I^2R_{in} \quad (6)$$

The electric current can be expressed as:

$$I = \frac{(T_h - T_c)\alpha_{pn}}{R_{in} + R_L} \quad (7)$$

where R_L is the external resistance.

Combining Eqs (1)-(2) and (6)-(7), there are four equations with four unknowns of P , Q_h , Q_c , and I , and finally, the output power (P) is obtained under the given thermoelectric material properties, geometrical features of thermoelectric legs, and load resistance. Besides, the conversion efficiency of the TEG unit is defined as:

$$\eta = \frac{P}{Q_h} \quad (8)$$

Furthermore, the thermal resistance model is easy to be extended from TEG unit to TEG module, by replacing Eqs (3)-(5) with

$$\alpha_{pn} = N(\alpha_p - \alpha_n) \quad (9)$$

$$R_{leg} = \frac{H_{leg}}{N(\lambda_p + \lambda_n)A_{leg}} \quad (10)$$

$$R_{in} = N(\sigma_p^{-1} + \sigma_n^{-1})\frac{H_{leg}}{A_{leg}} \quad (11)$$

where N is the number of TEG units. In essence, the Seebeck voltage of the TEG module is equivalent to the sum of Seebeck voltages of several TEG units, and TEG units are connected in parallel thermally and in series electrically.

Based on this model, Hsu et al. [30] proposed an effective Seebeck coefficient for the TEG module. According to the experimental results, the output power (P) is taken as the known variable and the Seebeck coefficient (α_{pn}) as the unknown variable, and the Seebeck coefficient (α_{pn}) under different working temperatures is obtained. The manufacturers of TEG modules usually do not provide customers with material properties or overestimate the given data. Their research provides an effective way for engineers to obtain material data by themselves. The authors in [31, 32] extended the model from a conventional TEG module to a two-stage TEG design and optimized the performance of the two-stage TEG module by using the simplified thermal resistance model.

2.2.2 The improved thermal resistance model

In practical situations, the temperature of the hot junction of thermoelectric legs is lower than the heat source temperature, and the temperature of the cold junction of thermoelectric legs is higher than the cooling source temperature, rendering the overestimation of temperature difference in the

1 simplified thermal resistance model. Consequently, the simplified thermal resistance model may
 2 overestimate the TEG output performance. Besides, the Seebeck coefficient, thermal conductivity, and
 3 electric resistivity of thermoelectric materials are highly temperature-dependent, and ignoring the
 4 temperature dependence may lead to additional errors. Considering these factors, an improved thermal
 5 resistance model was proposed in [25, 33], in which, the hot side and cold side heat flux were defined
 6 as:

$$7 \quad Q_h = \bar{\alpha}_{pn} I T_{h_leg} + \frac{T_{h_leg} - T_{c_leg}}{\bar{R}_{leg}} - \frac{1}{2} I^2 \bar{R}_{in} \quad (12)$$

$$8 \quad Q_c = \bar{\alpha}_{pn} I T_{c_leg} + \frac{T_{h_leg} - T_{c_leg}}{\bar{R}_{leg}} + \frac{1}{2} I^2 \bar{R}_{in} \quad (13)$$

9 where, T_{h_leg} and T_{c_leg} are the hot junction and cold junction temperature of thermoelectric legs,
 10 respectively; $\bar{\alpha}_{pn}$, \bar{R}_{leg} , and \bar{R}_{in} are the average Seebeck coefficient, the average thermal resistance,
 11 and the average internal resistance of the TEG unit, respectively.

12 When the heat is transferred from the heat source to the hot junction of thermoelectric legs and from
 13 the cold junction of thermoelectric legs to the cooling source, Q_h and Q_c can also be expressed as:

$$14 \quad Q_h = \frac{T_h - T_{h_leg}}{R_h} \quad (14)$$

$$15 \quad Q_c = \frac{T_{c_leg} - T_c}{R_c} \quad (15)$$

16 where R_h and R_c are the overall thermal resistance of the hot side and the cold side, respectively. R_h
 17 and R_c are defined as:

$$18 \quad R_h = R_c = R_{ce} + R_{co} \quad (16)$$

19 with

$$20 \quad R_{ce/co} = \frac{H_{ce/co}}{\lambda_{ce/co} A_{ce/co}} \quad (17)$$

21 where, R_{ce} (R_{co}), H_{ce} (H_{co}), λ_{ce} (λ_{co}), and A_{ce} (A_{co}) are the conductive thermal resistance, height, thermal
 22 conductivity, and cross-sectional area of ceramic plate (copper electrodes), respectively.

23 The output power of the TEG unit can be derived by:

$$24 \quad P = Q_h - Q_c = \bar{\alpha}_{pn} I (T_{h_leg} - T_{c_leg}) - I^2 \bar{R}_{in} \quad (18)$$

25 where

$$I = \frac{(T_{h_leg} - T_{c_leg}) \bar{\alpha}_{pn}}{\bar{R}_{in} + R_L} \quad (19)$$

The average Seebeck coefficient ($\bar{\alpha}_{pn}$), average thermal resistance (\bar{R}_{leg}), and average internal resistance (\bar{R}_{in}) of TEG unit can be expressed as:

$$\bar{\alpha}_{pn} = \bar{\alpha}_p - \bar{\alpha}_n \quad (20)$$

$$\bar{R}_{leg} = \frac{H_{leg}}{(\bar{\lambda}_p + \bar{\lambda}_n) A_{leg}} \quad (21)$$

$$\bar{R}_{in} = (\bar{\sigma}_p^{-1} + \bar{\sigma}_n^{-1}) \frac{H_{leg}}{A_{leg}} \quad (22)$$

with

$$T_{ave} = \frac{T_{h_leg} + T_{c_leg}}{2} \quad (23)$$

$$\bar{\alpha}_{p/n} = \frac{\alpha_{p/n}(T_{h_leg}) + \alpha_{p/n}(T_{c_leg}) + 2\alpha_{p/n}(T_{ave})}{4} \quad (24)$$

$$\bar{\lambda}_{p/n} = \frac{\lambda_{p/n}(T_{h_leg}) + \lambda_{p/n}(T_{c_leg}) + 2\lambda_{p/n}(T_{ave})}{4} \quad (25)$$

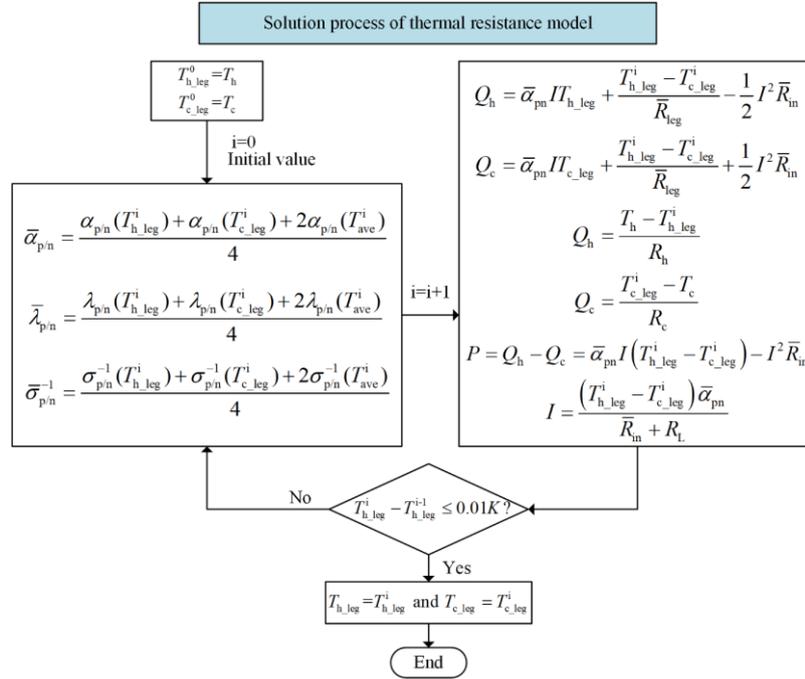
$$\bar{\sigma}_{p/n}^{-1} = \frac{\sigma_{p/n}^{-1}(T_{h_leg}) + \sigma_{p/n}^{-1}(T_{c_leg}) + 2\sigma_{p/n}^{-1}(T_{ave})}{4} \quad (26)$$

where $\alpha_{p/n}(T)$, $\lambda_{p/n}(T)$, and $\sigma_{p/n}^{-1}(T)$ are the temperature-dependent Seebeck coefficient, thermal conductivity, and electric resistivity of p/n-type thermoelectric materials.

Combining Eqs (12)-(15) and (18)-(19), there are six equations with six unknowns of Q_h , Q_c , T_{h_leg} , T_{c_leg} , P , and I . However, the $\bar{\alpha}_{pn}$, \bar{R}_{leg} , and \bar{R}_{in} are unknown in advance with the unknowns of T_{h_leg} and T_{c_leg} . The authors in Refs [25, 33] proposed an iterative calculation method to solve this problem, as shown in Fig. 4. The heat source temperature (T_h) and the cooling source temperature (T_c) are used as the initial values of T_{h_leg} and T_{c_leg} , and then the updated values are put back into the calculation until tolerance is satisfied.

Similarly, the improved thermal resistance model can be extended from the TEG unit to the TEG module by using the substitution method like from Eqs (3)-(5) to Eqs (9)-(11). Based on the improved thermal resistance model, Fan et al. [33] conducted a comprehensive optimization of the ratio of the thermoelectric leg length and cross-sectional area of the TEG unit; The effect of leg length and cross-sectional area on the maximum output power and maximum power density was also studied in their

1 research. Ignoring the temperature dependence, the authors in Ref. [34] proposed some optimal design
 2 methods for the TEG module by analyzing the η - R_{leg}^{-1} characteristic curves under different conditions.
 3 For the special structures of TEG devices, Liang et al. [35] and Zhang et al. [16] respectively utilized
 4 the improved thermal resistance model to predict the performance of the two-stage TEG module and
 5 the segmented TEG unit, and studied the influence of different structural parameters on the output
 6 power and conversion efficiency; The basic optimization design principles of these two structures can
 7 be found in their researches.



8
 9 Fig. 4. Solution process of the improved thermal resistance model [25].

10 As for the transient modeling, few researchers use the thermal resistance model to predict the
 11 dynamic performance of TEG, because the transient heat transfer involves the transient change of
 12 internal energy, which can not be expressed by thermal resistance. Under the dynamic temperature
 13 inputs of T_h and T_c , the corresponding dynamic output power and conversion efficiency of TEG can
 14 be predicted based on the temperature data of different discrete time points. However, in practical
 15 situations, the temperature change is continuous. Accordingly, the dynamic performance prediction
 16 through a thermal resistance model will further amplify the model error.

17 2.3 Numerical models

18 The numerical model is based on the partial differential equations of energy conservation and electric
 19 field conservation. Combined with boundary conditions, the partial differential equations can be solved

1 via numerical methods, and the finite difference method (FDM), finite element method (FEM), and
 2 finite volume method (FVM) are commonly used numerical approaches. For this reason, numerical
 3 analysis software programs such as ANSYS [36, 37] and COMSOL Multiphysics [38, 39] have been
 4 widely used to conduct numerical simulations of TEG devices. Generally, the numerical model can
 5 take into account all the factors in the actual situation, including the Seebeck effect, Peltier effect,
 6 Thomson effect, Joule effect, Fourier heat conduction, electric current flow, heat loss, etc., which is
 7 the most reasonable theoretical model to predict the performance of TEG devices. In addition,
 8 considering the change of transient internal energy, the numerical model can be extended from a steady
 9 state to a transient state.

10 2.3.1 One-dimensional steady-state numerical model

11 The governing equations of the TEG numerical model can be divided into three parts: p/n-type
 12 thermoelectric legs, copper electrodes, and ceramic plates. In a one-dimensional steady-state numerical
 13 model [40-42], the energy conservation of p/n-type thermoelectric legs can be described as:

$$14 \quad \lambda_p(T) \frac{d^2T}{dx^2} = -\sigma_p^{-1}(T) \bar{J}^2 + \alpha_p(T) \bar{J} \frac{dT}{dx} \quad (27)$$

$$15 \quad \lambda_n(T) \frac{d^2T}{dx^2} = -\sigma_n^{-1}(T) \bar{J}^2 + \alpha_n(T) \bar{J} \frac{dT}{dx} \quad (28)$$

16 where, x represents the direction of heat transfer, dx is the infinitesimal element, and \bar{J} is the current
 17 density vector. The first term on the left hand denotes the Fourier heat conduction, the first term on the
 18 right hand represents the Joule heat, and the second term on the right hand represents the Thomson
 19 heat along thermoelectric legs or Peltier heat on junctions.

20 In the regions of copper electrodes or solder layers, the energy conservation equation can be
 21 expressed as:

$$22 \quad \lambda_{co} \frac{d^2T}{dx^2} = -\sigma_{co}^{-1} \bar{J}^2 \quad (29)$$

23 Compared with Eqs (27)-(28), the term related to the Seebeck coefficient is absent. In the regions of
 24 ceramic plates, energy conservation is defined as:

$$25 \quad \lambda_{ce} \frac{d^2T}{dx^2} = 0 \quad (30)$$

26 In addition to the energy conservation equations of the thermal field, the thermoelectric legs and
 27 copper electrodes also follow the conservation equations of the electric field. The current density
 28 vector in Eqs (27)-(29) is defined as:

$$\vec{J} = \sigma \vec{E} \quad (31)$$

with

$$\vec{E} = -\frac{d\phi}{dx} + \alpha_{p/n}(T) \frac{dT}{dx} \quad (32)$$

where, \vec{E} is the electric field density vector, and ϕ is the electric potential.

Also, the electric current through thermoelectric legs and copper electrodes is continuous, which is defined by:

$$\frac{d\vec{J}}{dx} = 0 \quad (33)$$

Eqs (27)-(33) constitute the partial differential equations of the one-dimensional numerical model of TEG. Combined with the thermal field boundary conditions and the electric field boundary conditions, the equations can be solved via numerical methods, such as applying high temperature and low temperature respectively at the hot end and cold end of TEG; setting the sides of TEG exposed to the external environment as heat insulation; setting one terminal of TEG as grounding and another as an input current. The authors in Ref. [41] solved the above equations by using the MATLAB integrated development environment and performed the geometric optimization of the TEG unit. However, in the one-dimensional numerical model, the TEG unit needs to be simplified to a one-dimensional geometry structure, which will lead to an inevitable error. Due to the complexity of the three-dimensional structure of the TEG module, the one-dimensional model can not be used to predict its performance, and it is necessary to extend the numerical model from one dimension to three dimensions.

2.3.2 Three-dimensional steady-state numerical model

The three-dimensional numerical model is more accurate than the one-dimensional numerical model [43] because the directions of electric current and heat flux are not parallel in TEG units and TEG modules. In practical application, an energy recovery circuit is connected with TEG modules to recover the generated electricity. Therefore, the impedance matching characteristics should be considered when studying the output performance of TEG. The transport equations of the three-dimensional steady-state numerical model are consistent with those of the one-dimensional numerical model. For p/n-type thermoelectric legs, the energy conservation is defined as:

$$\nabla \cdot (\lambda_p(T) \nabla T) = -\sigma_p^{-1}(T) \vec{J}^2 + T \vec{J} \cdot \nabla \alpha_p(T) + \frac{\partial \alpha_p(T)}{\partial T} T \vec{J} \cdot \nabla T \quad (34)$$

$$\nabla \cdot (\lambda_n(T) \nabla T) = -\sigma_n^{-1}(T) \vec{J}^2 + T \vec{J} \cdot \nabla \alpha_n(T) + \frac{\partial \alpha_n(T)}{\partial T} T \vec{J} \cdot \nabla T \quad (35)$$

1 With the consideration of impedance matching, the energy conservation of load resistance should
 2 also be included in the numerical model, and it is the same as that of copper electrodes, that is:

$$3 \quad \nabla \cdot (\lambda_m \nabla T) = -\sigma_m^{-1} \vec{J}^2 \quad (36)$$

4 where, the subscript m represents the material regions involved in Fourier heat conduction and electric
 5 current flow, co for the copper electrodes, lo for the load resistance, respectively.

6 For the electrically insulated ceramic plates, Eq. (30) can be extended to Eq. (37), as follows:

$$7 \quad \nabla \cdot (\lambda_{ce} \nabla T) = 0 \quad (37)$$

8 Similarly, the electric field transport equation of the three-dimensional numerical model of TEG
 9 includes:

$$10 \quad \vec{J} = \sigma \vec{E} \quad (38)$$

$$11 \quad \vec{E} = -\nabla \phi + \alpha_{p/n}(T) \nabla T \quad (39)$$

$$12 \quad \nabla \cdot \vec{J} = 0 \quad (40)$$

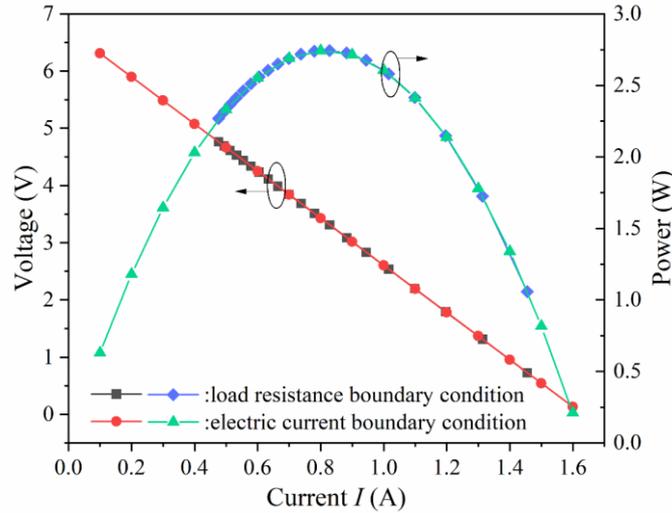
13 Besides, the thermal field boundary conditions of the three-dimensional numerical model consist of
 14 the first type boundary condition (temperature boundary), the second type boundary condition (heat
 15 flux boundary), and the third type boundary condition (convective heat transfer boundary, as defined
 16 by Eq. (41)). In most researches [44, 45], the first type boundary condition is applied on both ends of
 17 TEG, and the third type boundary condition is applied on the surfaces of TEG exposed to the external
 18 environment.

$$19 \quad -\lambda \frac{\partial T}{\partial n} = h_{\text{ext}} (T - T_{\text{ext}}) \quad (41)$$

20 where, h_{ext} and T_{ext} represent the external convective heat transfer coefficient and external temperature,
 21 respectively.

22 There are two kinds of electric field boundary conditions: load resistance boundary condition and
 23 the electric current boundary condition. When considering the topological connection of load
 24 resistance, one side of the terminals of TEG and load resistance is set to be grounded ($U = 0$ V), and
 25 another side is set to be connected to each other. When replacing the load resistance with an input
 26 current, the geometry of load resistance is absent, and one terminal of the TEG is set as the input
 27 current boundary, while another terminal is set to be grounded. The direction of the input current is the
 28 same as the moving direction of holes in p-type thermoelectric legs, but opposite to the moving
 29 direction of electrons in n-type thermoelectric legs. Fig. 5 shows the comparison of numerical results
 30 between these two kinds of electric field boundary conditions. Here, the TEG device in Ref. [37] was

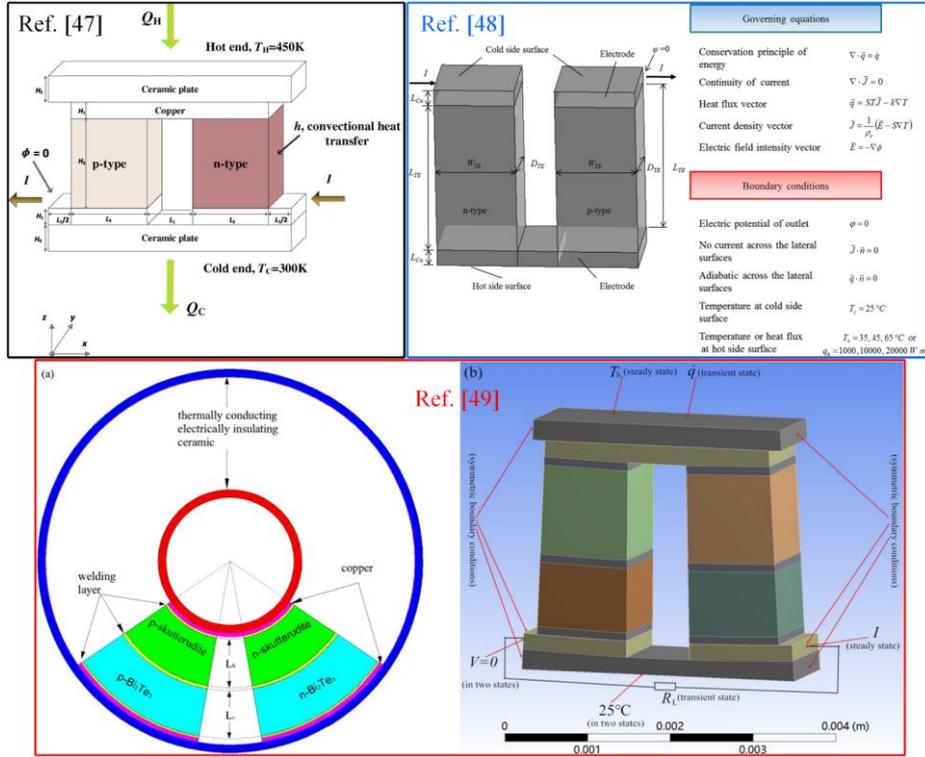
1 chosen for the numerical simulation, and other boundary conditions were set as $T_h = 450$ K, $T_c = 310$
 2 K, and $h_{ext} = 10$ W/(m·K). Under the load resistance boundary condition, the load resistance changes
 3 from 0.5Ω to 10Ω at a rate of 0.5Ω , while under the electric current boundary condition, the input
 4 current changes from 0.1 A to 1.6 A at a rate of 0.1 A. The results indicated that both output voltage
 5 and output power predicted by using load resistance boundary conditions are consistent with those
 6 predicted by using electric current boundary conditions. Therefore, both can be used to conduct the
 7 numerical simulation of TEG devices.



8
 9 Fig. 5. Comparison of numerical results between load resistance boundary condition and electric current boundary
 10 condition.

11 Chen et al. [46] established a three-dimensional numerical model of the TEG unit by using the user-
 12 defined function (UDF) of Fluent, and the model was solved by the FVM computational fluid dynamics
 13 (CFD) software package. In their research, the load resistance was incorporated into the input current
 14 boundary to handle the field-electric interface, and the distribution characteristics of temperature,
 15 Seebeck potential, and heat flux of TEG were successfully obtained, which provides a new modeling
 16 approach for predicting the performance of TEG devices. The authors in Ref. [47] investigated the
 17 effects of variable material properties and convective heat losses on the performance of the TEG unit
 18 using the three-dimensional numerical model. The results indicated that the assumption of constant
 19 material properties will underestimate the internal resistance, and the heat loss will slightly enlarge the
 20 output power, but significantly lower the conversion efficiency. Based on the three-dimensional
 21 numerical model, a multi-objective genetic algorithm was proposed to optimize the geometric structure
 22 of TEG element, and the optimal structural design of TEG unit under the first and second type thermal
 23 field boundary conditions was studied by Chen et al. [48]. They reported that a smaller leg height

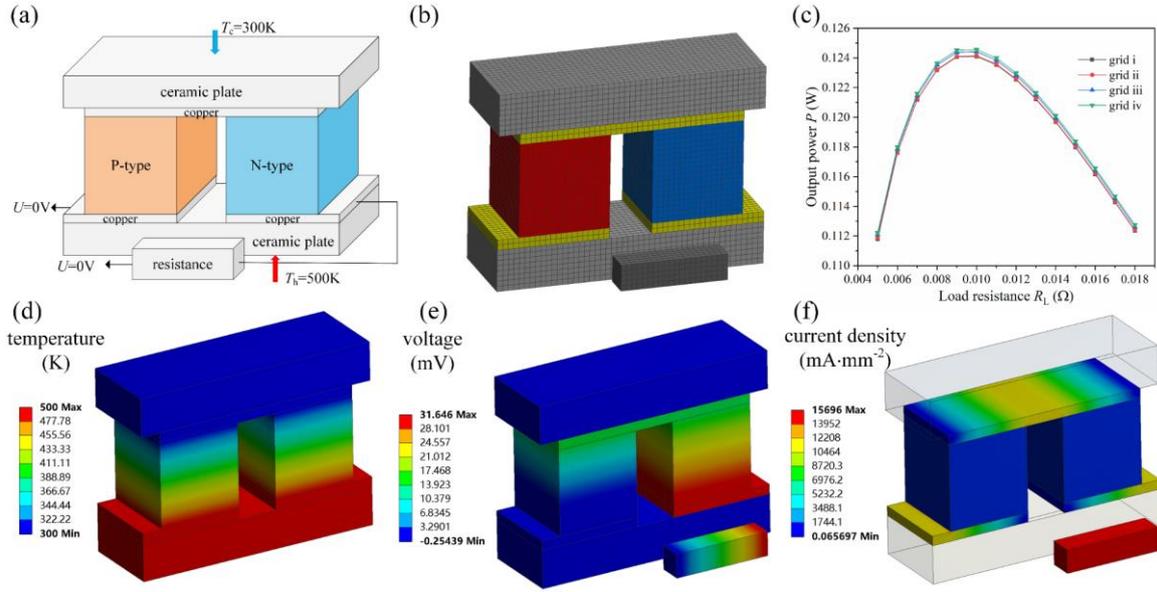
1 enables greater output power under a fixed temperature difference, whereas a larger leg height enables
 2 greater output power and conversion efficiency based on a fixed heat flux on the hot end. Fan and Gao
 3 [49] proposed a segmented annular TEG unit and utilized the three-dimensional numerical model to
 4 analyze its performance. The output power of the segmented annular TEG unit was 18.3% higher than
 5 that of the single-Skutterudite annular TEG unit. As can be seen, the three-dimensional numerical
 6 model has been widely used to study and optimize the performance of TEG devices because of its high
 7 precision.



8
 9 Fig. 6. Schematic of the three-dimensional numerical model and boundary conditions of TEG unit in Refs [47-49].

10 In the above research [46-49], the electric current boundary condition is used to replace the load
 11 resistance to form the circuit loop. Fig. 6 shows the details of the three-dimensional numerical model
 12 and boundary conditions in Refs [47-49], in which the numerical simulation is carried out by ANSYS.
 13 In practice, TEG is usually connected to an energy recovery circuit, and the electric current is generated
 14 naturally under the effect of the temperature difference and thermoelectric coupling effect, therefore,
 15 no input current is required, and the load resistance boundary condition is closer to the practical
 16 situation than the electric current boundary condition. Besides, the electric field distribution
 17 characteristics of load resistance can directly reflect the output performance of TEG. Taking the
 18 asymmetric TEG device as the research objective, Luo et al. [50] established a three-dimensional
 19 numerical model of the TEG unit considering the topological connection of load resistance, and

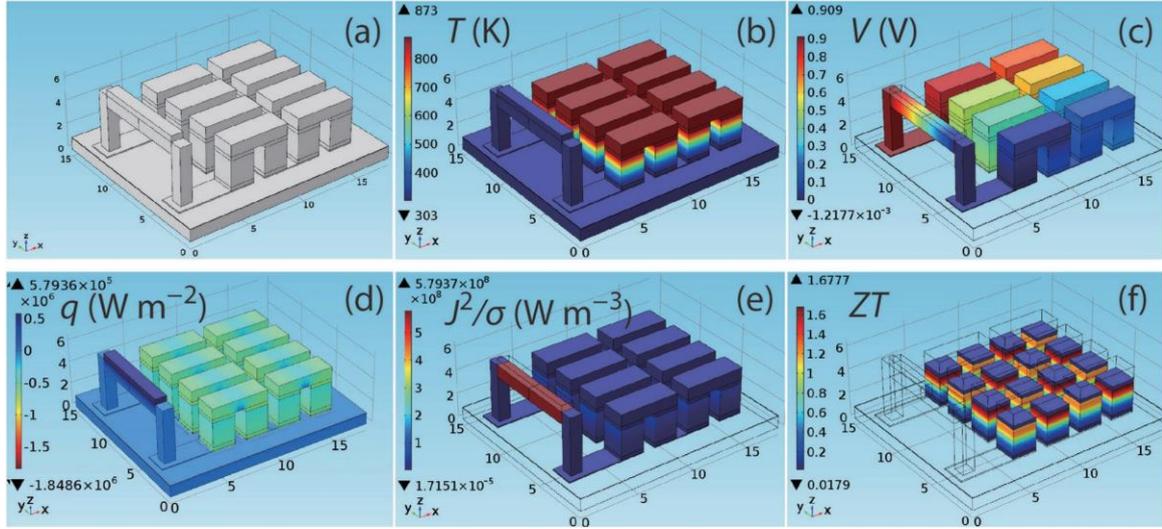
1 investigated the influence of the cross-sectional area ratio of the p-type leg and n-type leg on TEG
 2 performance. The schematic diagram and numerical results of the TEG unit were shown in Fig. 7, in
 3 which the load resistance was electrically connected with the TEG unit, and the numerical simulation
 4 was completed by using ANSYS/Thermal-Electric package. According to the numerical results, the
 5 optimal cross-sectional area ratio of p-type leg and n-type leg mainly depends on the asymmetric
 6 thermoelectric material properties.



7
 8 Fig. 7. Schematic of the TEG unit and its numerical results at $T_h = 500$ K, $T_c = 300$ K, and $h_{ext} = 0$ [50]. (a) Boundary
 9 conditions. (b) Three-dimensional finite element model. (c) Grid independence examination. (d) Temperature distributions.
 10 (e) Voltage distributions. (f) Current density distributions.

11 Furthermore, the three-dimensional numerical model can be extended from the TEG unit to the TEG
 12 module by establishing the three-dimensional CAD geometry of the TEG module and considering the
 13 topological relationship among TEG units. Based on simulation platforms of ANSYS and
 14 ANSYS/Thermal-Electric respectively, Ming et al. [51] and Luo et al. [37] have carried out numerical
 15 simulations on the TEG module and studied the influence of structural parameters on the performance
 16 of the TEG module. Also, COMSOL Multiphysics is a powerful tool to simulate the multiphysics
 17 coupling phenomena, and more and more researchers use it to predict the performance of TEG devices
 18 [52]. Hu et al. [53] used COMSOL to calculate the three-dimensional numerical model and predict the
 19 behavior of a nanostructured PbTe-based TEG module, as shown in Fig. 8. In the study, only the
 20 grounding boundary condition needs to be defined to compute the electric field governing equations,
 21 and the load resistance was set to be in electrical and thermal contact with TEG module. Through finite
 22 element simulations, the physical field distribution characteristics of the whole geometry were

1 obtained, including temperature, voltage, heat flux, Joule heat, and ZT values. Compared with the
 2 ANSYS/Thermal-Electric simulation platform [37, 50], the load resistance in COMSOL follows the
 3 governing equations of Eqs (36) and (38)-(40), while in ANSYS/Thermal-Electric, the load resistance
 4 only involves the calculation of electric field governing equations of Eqs (38)-(40). The difference in
 5 numerical results between these two solvers can be ignored because the Fourier heat conduction of
 6 load resistance has an insignificant influence on the temperature distributions of the whole TEG
 7 module [54].



8
 9 Fig. 8. Numerical results of a TEG module predicted by COMSOL Multiphysics [53]. (a) Three-dimensional geometry.
 10 (b) Temperature distributions. (c) Voltage distributions. (d) Heat flux distributions. (e) Joule heat density distributions. (f)
 11 ZT values of thermoelectric materials.

12 2.3.3 Transient numerical model

13 Compared with the thermal resistance model, the numerical model can not only predict more
 14 reasonable results but also can be used to predict the transient performance of TEG. In some
 15 applications, the heat source is time-dependent, for example, the automotive exhaust temperature
 16 changes with the vehicle speed; the flame temperature of the stove-powered TEG system is not static;
 17 the TEG will show dynamic characteristics during the start-up or shut-down stages. Consequently, it
 18 is necessary to build a transient numerical model to predict the dynamic response characteristics of
 19 TEG devices. In order to extend the numerical model from a steady state to a transient state, the term
 20 concerning the transient internal energy change should be included in the energy conservation
 21 equations. The thermal field transport equations of the transient numerical model are as follows:

$$22 \quad (\rho c)_p \frac{\partial T}{\partial t} = \nabla \cdot (\lambda_p(T) \nabla T) + \sigma_p^{-1}(T) \bar{J}^2 - T \bar{J} \cdot \nabla \alpha_p(T) - \frac{\partial \alpha_p(T)}{\partial T} T \bar{J} \cdot \nabla T \quad (42)$$

$$(\rho c)_n \frac{\partial T}{\partial t} = \nabla \cdot (\lambda_n(T) \nabla T) + \sigma_n^{-1}(T) \bar{J}^2 - T \bar{J} \cdot \nabla \alpha_n(T) - \frac{\partial \alpha_n(T)}{\partial T} T \bar{J} \cdot \nabla T \quad (43)$$

$$(\rho c)_m \frac{\partial T}{\partial t} = \nabla \cdot (\lambda_m \nabla T) + \sigma_m^{-1} \bar{J}^2 \quad (44)$$

$$(\rho c)_{ce} \frac{\partial T}{\partial t} = \nabla \cdot (\lambda_{ce} \nabla T) \quad (45)$$

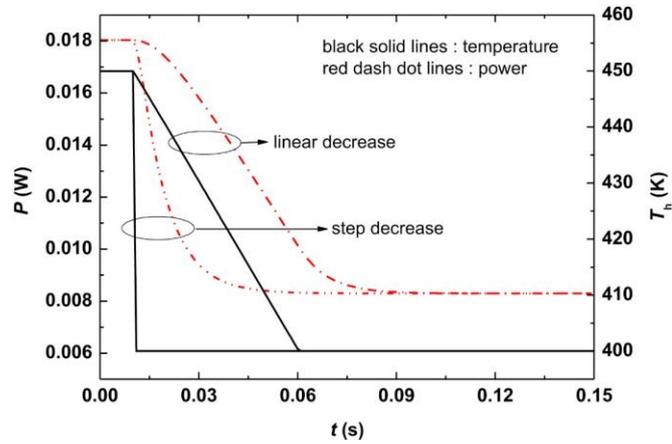
where, ρ is the density, c is the specific heat, and t is the time. Other symbols and subscripts have the same meaning as those of the steady-state numerical model. The term on the left hand of Eqs (42)-(45) represents the transient internal energy change.

As for the electric field, the governing equations of the transient numerical model are the same as Eqs (38)-(40) in the steady-state numerical model, and the only difference is that all variables in the transient numerical model are time-dependent.

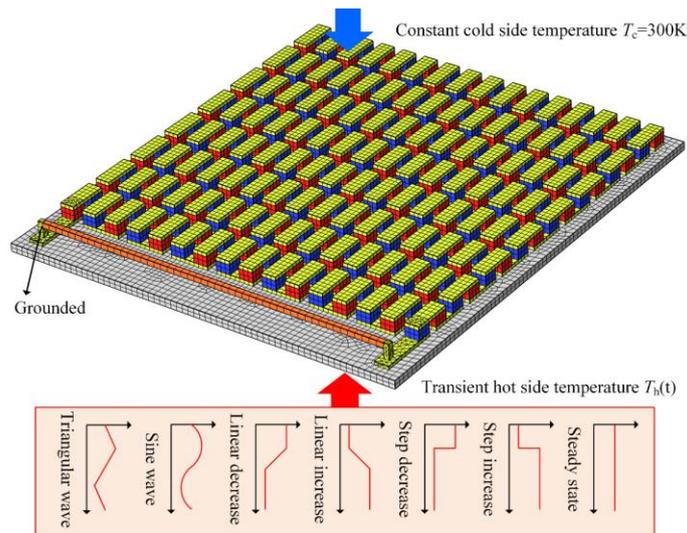
Combined with the transient boundary conditions, the transport equations (Eqs (38)-(40) and (42)-(45)) of the transient numerical model can be worked out by using numerical analysis tools. Transient boundary conditions generally refer to the transient input of heat source, including the first type transient boundary condition of temperature $T_h(t)$ and the second type transient boundary condition of heat flux $\dot{q}(t)$. The cold side thermal field boundary conditions and ambient convection heat transfer boundary conditions can be set as steady state or transient state according to actual situations. However, the boundary conditions of the electric field are all steady state, because the dynamic electric field parameters respond correspondingly with the transient change of temperature.

Yan and Malen [55] simplified the transient numerical model from three-dimensional to one-dimensional, and solved the one-dimensional transient numerical model by a central difference approximation and explicit time matching method. When applying a periodic heat flux on the hot end and adopting the current boundary condition to replace the load resistance, the numerical results indicated that the periodic heat source can amplify the heat-to-electric conversion efficiency of TEG. Based on the previous steady-state works, Meng et al. [56] further proposed a transient numerical model of the TEG unit to deeply investigate its dynamic response characteristics under transient boundary conditions (including variations of hot side temperature, cold side temperature, and load current). Some useful results were obtained by their research, such as the response hysteresis of output power was founded due to the delay of thermal diffusion, as shown in Fig .9. However, the research on the temperature-dependent properties of thermoelectric materials and geometric dimensions of TEG unit is still insufficient in their study. For this reason, Jia et al. [57] developed a two-dimensional transient numerical model considering the temperature-dependent thermoelectric material properties,

1 and utilized the model to investigate the transient behavior of a linear-shaped TEG unit under different
 2 thermal load and geometric dimensions of legs. The numerical simulation was carried out by ANSYS,
 3 and the results contributed to further understanding the transient behavior of TEG. But the transient
 4 numerical model used by the authors is two-dimensional.



5
 6 Fig. 9. Dynamic output power variations under step and linear decrease in hot side temperature [56].



7
 8 Fig. 10. Finite element features and boundary conditions of the transient numerical model of TEG module [58].

9 To be more accurate, a complete three-dimensional transient numerical model considering the
 10 temperature-dependent properties and the topological connection of load resistance was proposed by
 11 Luo et al. [58]. Also, the authors extended the transient numerical model from a TEG unit to a TEG
 12 module, and the finite element simulations were conducted via COMSOL. Fig. 10 shows the finite
 13 element features and boundary conditions of the transient numerical model of the TEG module. By
 14 comparing the numerical results under different transient temperature excitations, they reported that
 15 the time delay of the output response of the TEG module is contingent on the rate of temperature

change, the dynamic response characteristic of conversion efficiency is synchronous with that of output power, and the periodic temperature excitation may amplify the output power, but does not affect the conversion efficiency. The findings are helpful to deeply understanding the dynamic response characteristics and the causes, and the developed transient numerical model of the TEG module can be further extended to the whole TEG system.

2.4 Analogy models

Based on the analogy between thermal and electrical variables, the thermal resistance model can be equivalent to an electrical circuit model [59]. In an electrothermal analogy, heat flow is expressed as current, the temperature is expressed as voltage, and thermal resistance is expressed as electrical resistance. The heat and cooling source can be represented as the ideal voltage source, and the zero temperature is the electrical ground. The supplemented current sources can represent the internal heat sources like Peltier heat, Joule heat, and so on [60]. Through the electrothermal analogy, the thermal resistance model mentioned in Section 2.2 can be worked out by an equivalent circuit. On the platform of the SPICE simulation program, the equivalent circuit model considering the temperature dependence of material properties was established by Mitrani et al. [61], in which the equivalent electrical circuit represented by thermal variables is connected with a pure load circuit. The model results were in good agreement with those predicted by a one-dimensional numerical model.

In addition, the equivalent electrical circuit model facilitates the transient simulation by applying transient temperature (voltage) inputs on both ends (two terminals of the equivalent circuit) of TEG. The one-dimensional transient differential governing equation of thermoelectric legs is [60]:

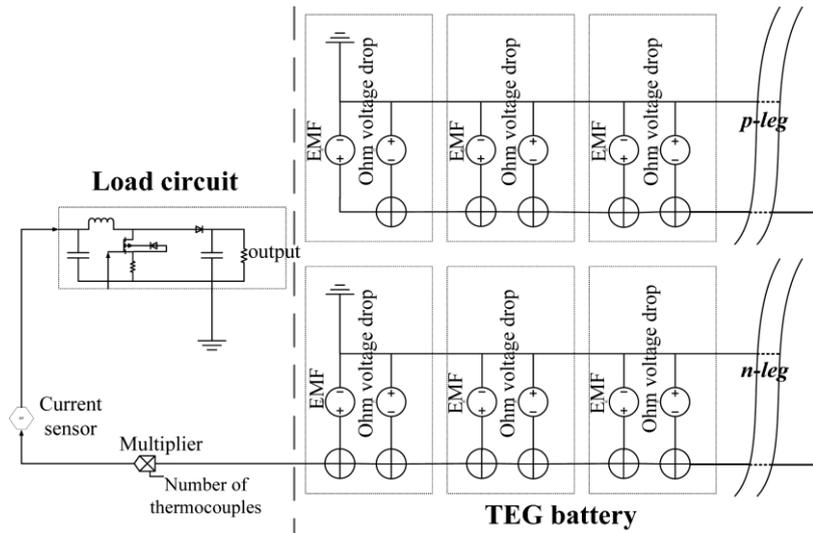
$$\begin{aligned} dQ_{p/n} &= Q_{p/n}(x+dx) - Q_{p/n}(x) \\ &= c_{p/n} m_{p/n} \frac{dT_{p/n}(x)}{dt} + I^2 \frac{\sigma_{p/n}^{-1}(T_{p/n}(x))}{A_{p/n}} dx + d\alpha_{p/n}(T_{p/n}(x)) T_{p/n}(x) I \end{aligned} \quad (46)$$

where, $c_{p/n}$ and $m_{p/n}$ are respectively the specific heat and mass of p-type and n-type legs. The first term is the transient term, which can be represented by paralleling an electrical capacitor C_e in the equivalent circuit. Also, the transient heat transfer term can be modeled by an electrical analogy of a capacitor, which is:

$$I_e = C_e \frac{dV_e}{dt} \quad (47)$$

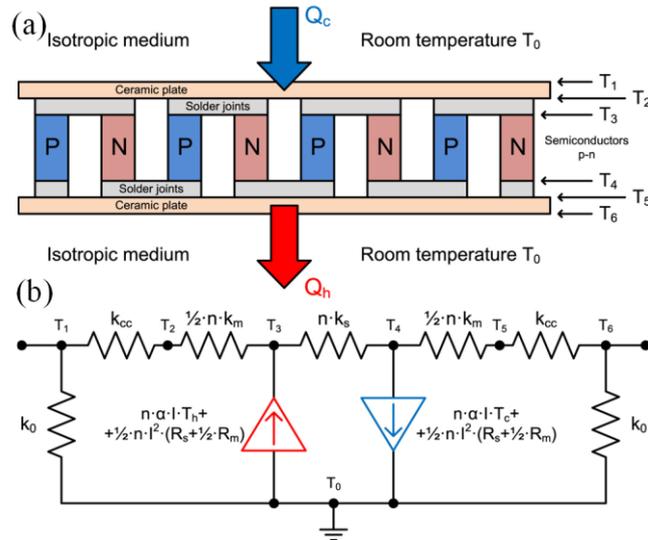
where, C_e is taken as $c_{p/n} m_{p/n}$, and V_e is the equivalent voltage of temperature $T_{p/n}(x)$. Consequently, the transient term can be considered as an analogy of supplemented current source I_e .

1 An accurate TEG analogy model was proposed and implemented in a SPICE environment by Chen
 2 et al. [60], as shown in Fig. 11. The model took into account all temperature-dependent characteristics
 3 of thermoelectric materials and all heat source terms, and it was validated with one-dimensional
 4 numerical simulation results from ANSYS and experimental data from an actual TEG module,
 5 respectively. Their research provides useful guidance for the electrothermal modeling of TEG devices.
 6 However, the thermal resistances from ceramic plates to thermoelectric legs are omitted, and the heat
 7 source temperature and cooling source temperature of the TEG module are directly used as the working
 8 temperatures of legs in their study. Fisac et al. [62] proposed an improved analogy model considering
 9 the thermal resistances from ceramic plates to legs, as shown in Fig. 12. The model was used to study
 10 the transient response characteristics of the TEG module under conditions of smaller thermal inertia,
 11 and the results indicated that the response time of TEG module depends on the structural
 12 characteristics.



13
 14 Fig. 11. Equivalent circuit of the thermoelectric battery model [60].

15 The analogy model is derived from the equations of the thermal resistance model, therefore, it can
 16 only deal with a one-dimensional thermoelectric phenomenon, and can not consider the ambient
 17 convection heat loss. In previous research [63, 64], the software of SPICE was commonly used to
 18 establish and solve the equivalent circuit model. Compared with the thermal resistance model, the
 19 analogy model has advantages in predicting the dynamic performance of the TEG module, because the
 20 transient heat transfer term can be represented as a supplementary current source in the equivalent
 21 circuit. The transient characteristics of the TEG module can be obtained under the condition of pulse
 22 input. The analogy model also facilitates the simulation of a TEG module and its interconnections with
 23 electronic control circuits, such as the maximum power point tracking circuit.



1

2 Fig. 12. Schematic diagram of TEG module with different temperatures (a) and the equivalent electrical circuit model (b)
 3 [62].

4 *2.5 Comparison of different models*

5 In recent years, great progress has been made in the theoretical models of TEG devices. From TEG
 6 unit to TEG module, from one-dimensional to three-dimensional, from steady-state to transient state,
 7 more and more complete theoretical models have been proposed by researchers. In general, theoretical
 8 models can be classified into three categories: thermal resistance model, numerical model, and analogy
 9 model. Taking a thermoelectric element as the research objective, Fraisse et al. [22] compared the
 10 prediction results of one-dimensional models, including the thermal resistance model, analogy model,
 11 and numerical model. The numerical simulation was performed by the finite element method of
 12 ANSYS. According to their research, the results predicted by the numerical model are consistent with
 13 those predicted by the analogy model, but the thermal resistance model may overestimate the output
 14 voltage and power. By comparing the simplified thermal resistance model with the three-dimensional
 15 numerical model, the same conclusions were obtained by Meng et al [47].

16 In summary, the numerical model can take into account various factors in the actual situation, such
 17 as the temperature dependence of thermoelectric materials, three-dimensional geometry, transient
 18 response characteristics, and so on, which is the most reasonable theoretical model. But the numerical
 19 model suffers from a relatively long computation time. The thermal resistance model has the
 20 advantages of short calculation time and no complicated modeling process, but the model error is larger
 21 than the numerical model. The analogy model can be used to study the dynamic response
 22 characteristics of TEG devices under pulse input, also, it facilitates the joint simulation with electronic
 23 control circuits. However, the analogy model is derived from the basic equations of the thermal

1 resistance model, rendering inevitable errors. Due to the advantages of the high accuracy and the
 2 visualization of physical field distribution characteristics, the numerical model has become the most
 3 commonly used model to predict the performance of TEG devices.

4 In Table 1, recent works on the theoretical model of TEG devices are presented. As can be seen, the
 5 development of theoretical models for predicting the performance of TEG devices has been mature. In
 6 practical application, TEG modules are usually placed between the heat collector and the radiator as
 7 the power supply. However, the working temperature of TEG modules is unknown and difficult to be
 8 measured directly, which leads to the theoretical models of TEG devices being unable to be solved.
 9 The data that can be measured directly include the parameter characteristics of the heat source or
 10 cooling source. Therefore, it is necessary to establish some comprehensive models of the TEG system
 11 to predict its performance, taking into account the heat transfer process from heat/cooling sources to
 12 hot/cold sides of TEG modules.

13 Table 1. Summary of theoretical models of TEG devices.

| Model | Dimensions | Using simplified temperatures | Considering temperature-dependent properties | Steady/transient state | TEG unit/module | Sources |
|--------------------------|------------|-------------------------------|--|------------------------|-----------------|-------------------------|
| Thermal resistance model | 1-D | yes | no | steady state | TEG unit | [22, 30, 47] |
| | | yes | no | | TEG module | [31, 32] |
| | | no | no | | TEG unit | [65, 66] |
| | | no | no | | TEG module | [34, 35] |
| | | no | yes | | TEG unit | [16, 33] |
| | | no | yes | | TEG module | [25] |
| Numerical model | 1-D | no | yes | steady state | TEG unit | [22, 40-42] |
| | 3-D | | no | steady state | TEG unit | [21, 43, 49] |
| | 3-D | | no | steady state | TEG module | [21, 67] |
| | 3-D | | yes | steady state | TEG unit | [36, 38, 44-48, 50] |
| | 3-D | | yes | steady state | TEG module | [37, 39, 51-53, 68, 69] |
| | 1-D | | no | transient state | TEG unit | [55] |
| | 3-D | | no | transient state | TEG unit | [56] |
| | 3-D | | yes | transient state | TEG module | [58] |
| Analogy model | 1-D | no | yes | steady state | TEG unit | [22] |
| | | no | yes | steady state | TEG module | [61] |
| | | yes | no | transient state | TEG module | [70] |
| | | yes | yes | transient state | TEG module | [60] |
| | | no | no | transient state | TEG module | [62] |
| | | no | yes | transient state | TEG module | [63, 64] |

14 3. Theoretical models of thermoelectric generator systems

15 Due to the advantages of no moving parts, no pollution, and long service life, a large number of TEG
 16 systems have been developed to harvest thermal energy and generate electricity. The condition where

1 the TEG module is used and the nature of the heat source are two classification criteria for TEG
2 systems [71]. According to the condition where the TEG is used, TEG systems can be grouped into
3 six categories:

4 i) radioisotope TEG systems: the natural radioactive decay energy of radioactive elements is used as
5 the heat source to produce electricity for electronics, such as power supply in the field of space
6 exploration;

7 ii) solar-based TEG systems: the solar energy is used as a heat source;

8 iii) stove-powered TEG systems: the source of energy is from burning solid fuels, such as power
9 supply in the field of combined heat and power generation system;

10 iv) wearable TEG systems: the source of energy comes from the heat of the human body;

11 v) micro-generation for sensors and microelectronics: the power level is very low and all sources of
12 heat are feasible;

13 vi) waste heat recovery: the TEG system is used to recover the waste heat contained in thermal fluids,
14 such as exhaust waste heat from automobiles, aircraft and helicopters, ships, and industries.

15 To predict the performance of the above TEG systems, several theoretical models for the
16 corresponding TEG systems are proposed, such as FEM/FVM-based numerical models and thermal
17 resistance-based analytical models. According to the different physical fields involved, the
18 FEM/FVM-based numerical models are classified into three groups: thermal-electric numerical
19 models, fluid-thermal numerical models, and fluid-thermal-electric numerical models. The
20 performance of different TEG systems can be estimated by the same theoretical model, for example,
21 the thermal-electric numerical model can predict the output performance of radioisotope, solar-based,
22 stove-powered, and wearable TEG systems by setting different boundary conditions. Consequently,
23 the condition where the TEG is used can not be used as the classification criteria for the theoretical
24 models of the TEG system. Based on the nature of the heat source, the theoretical models of the TEG
25 system are grouped into two categories in this chapter: TEG systems directly contacted with the heat
26 source and TEG systems for fluid waste heat recovery.

27 *3.1 Thermoelectric generator systems directly contacted with the heat source*

28 In radioisotope, solar-based, stove-powered, and wearable TEG systems, the heat source is directly
29 in contact with TEG modules or indirectly through a heat transfer unit. The thermal resistance model
30 in section 2.2 and the numerical model in section 2.3 can be used to predict their performance under
31 different heat sources. When a heat transfer unit is placed between the heat source and the TEG module,

the output performance of the TEG module can be estimated by adding parasitic thermal resistances to the thermal resistance model or adding an energy conservation differential equation to the numerical model. For the heat dissipation of TEG systems, there are two cooling modes: natural air cooling and water cooling, which can be characterized by the convective heat transfer analysis.

3.1.1 Thermal resistance-based analytical model

Using solar energy as a heat source, He et al. [72] reported a solar heat pipe TEG system comprising a TEG module, a finned heat pipe, and an evacuated double-skin glass tube. The system takes advantage of the heat pipe to convert the solar irradiation into a heat flux to meet the TEG working requirement. Also, water cooling is adopted in the system. The authors integrated Eqs (48)-(49) into the simplified thermal resistance model to calculate the output power and conversion efficiency of the system, and then studied the influence of solar irradiation, cooling water temperature, thermoelectric leg length and cross-sectional area, and the number of TEG units, etc. on the maximum power output and conversion efficiency of the TEG system. Some optimal structural parameters were obtained. In the subsequent work [73], the authors improved the model by considering the contact thermal resistance and conductive thermal resistance from the heat pipe and radiator to the hot and cold side of thermoelectric legs respectively. According to the improved model, the Peltier cooling and heating performance of the thermoelectric module was investigated. However, the thermoelectric material properties used in the model are constant. The accuracy of the model can be further improved by considering the temperature dependence of thermoelectric materials.

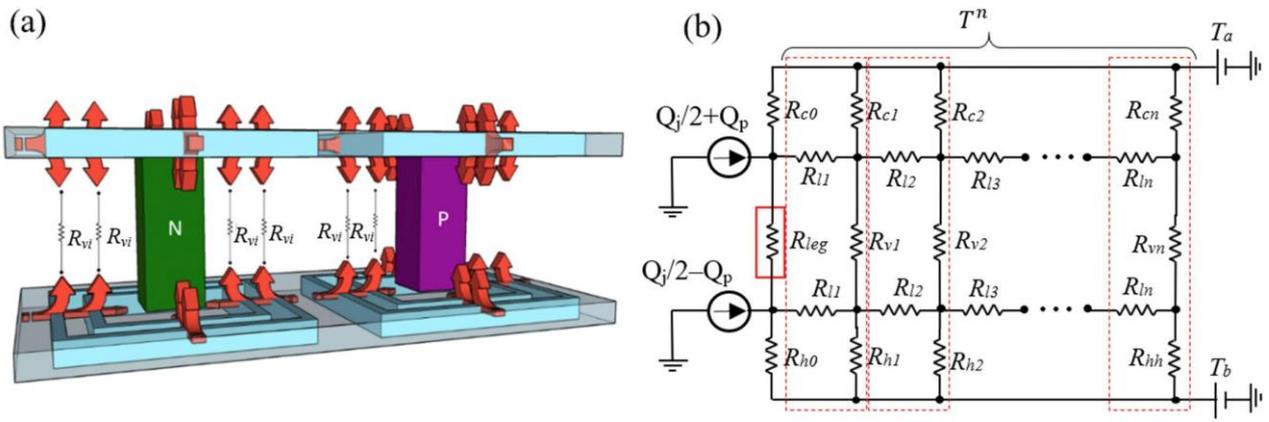
$$Q_h = h_{hp} A_{hp} (T_{hp} - T_h) = \alpha_{pn} IT_h + \frac{T_h - T_c}{R_{leg}} - \frac{1}{2} I^2 R_{in} \quad (48)$$

$$Q_c = h_{wa} A_{ce} (T_c - T_{wa}) = \alpha_{pn} IT_c + \frac{T_h - T_c}{R_{leg}} + \frac{1}{2} I^2 R_{in} \quad (49)$$

where, h_{hp} is the heat transfer coefficient between the heat pipe condenser and the ceramic plate of the TEG module, A_{hp} is the plate copper fin area, T_{hp} is the temperature of the heat pipe, h_{wa} is the effective heat transfer coefficient between the cooling water and the ceramic plate, A_{ce} is the area of ceramic plate, and T_{wa} is the temperature of cooling water.

Stove-powered TEG systems show great potential in developing countries, which can not only improve the air-fuel ratio by using an electric fan to realize complete combustion in the stoves but also meet the power supply requirements of low-power electronic products such as lights and phones [74]. The thermal resistance model is the most commonly used method to predict the performance of stove-powered TEG systems. Similarly, Champier et al. [74] established a theoretical model by integrating

1 the thermal resistance between the heat (cooling) source and TEG module into the simplified thermal
 2 resistance model in section 2.2.1. In their research, the average temperature $T_a = (T_h + T_c)/2$ was used
 3 to evaluate the thermoelectric material properties, and the temperature of the heat source and cooling
 4 source was measured by thermocouples. According to the temperature data at different time points,
 5 the output power of a stove-powered TEG system developed by the authors was analyzed and verified
 6 by experimental results. Considering the heat radiation of the hot source and cooling source, Najjar
 7 and Kseibi [75] carried out a comprehensive heat transfer and performance analysis of a multi-purpose
 8 stove-powered TEG system. The modeling process for all the subcomponents was described in detail,
 9 and the research results provided powerful guidance for further improving the thermal resistance-based
 10 analytical model of stove-powered TEG systems.



11
 12 Fig. 13. Schematic of the quasi three-dimensional thermal resistance model of wearable TEG module [76].

13 Wearable TEG systems can continuously convert body heat into electrical energy, attracting lots of
 14 interest in self-powered electronic devices. The performance of wearable TEG systems is limited by
 15 the large external thermal resistances, and it is desirable to design a TEG module with a substantially
 16 larger thermal resistance than the external thermal resistances. It seems that the thermoelectric leg
 17 should be designed with a high height-to-area ratio. However, due to body comfort and the increase in
 18 internal resistance, the leg height can not be increased indefinitely. Therefore, the parameters of TEG
 19 legs should be balanced between performance and wearability. Nozariasbmarz et al. [76, 77] proposed
 20 a quasi three-dimensional thermal resistance model to optimize the parameters of the TEG module, as
 21 shown in Fig. 13. In the model, according to the distance between the thermoelectric leg and the leg
 22 center, thermoelectric legs were divided into different rectangular rings and characterized by different
 23 thermal resistances. In addition, the contact thermal resistance from the skin to TEG module, and the
 24 convective thermal resistance from the heat sink to ambient were taken into account. Based on the
 25 developed model, the structural parameters of the wearable TEG system were optimized.

1 In the modeling of the radioisotope TEG system, few papers are using the thermal resistance model
2 to predict its performance, because the heat transfer from the radioisotope heat source to the hot side
3 of the TEG module can not be represented as thermal resistance. More importantly, the TEG modules
4 used in the system usually present a radial shape instead of the conventional π shape. The research
5 objective of the thermal resistance model is based on the TEG module with a π shape. Therefore,
6 researchers prefer to use a numerical model to predict the performance of radioisotope TEG systems,
7 because the numerical model is not limited to geometric shapes of TEG modules.

8 When using thermal resistance-based analytical models to predict the performance of solar-based,
9 stove-powered, and wearable TEG systems, it is recommended to consider the thermal resistance of
10 all components, including convective thermal resistance, contact thermal resistance, and conductive
11 thermal resistance. Besides, due to the high dependence of thermoelectric materials on temperature,
12 the assumption of constant Seebeck coefficient, thermal conductivity, and electric resistivity has a
13 great influence on the model accuracy. On the other hand, it is not accurate enough to use the average
14 temperature to evaluate the properties of thermoelectric materials due to the nonlinearity of
15 thermoelectric material properties. Therefore, appropriate methods should be adopted to deal with the
16 temperature dependence of the thermal resistance model, such as the iterative calculation method
17 described in Fig. 4. For the transient performance analysis of these TEG systems, the thermal
18 resistance-based analytical model suffers from the same problems as the thermal resistance model of
19 TEG module, as mentioned in the last paragraph of Section 2.2.

20 3.1.2 Thermal-electric numerical model

21 For TEG systems directly contacted with the heat source, the thermal-electric multiphysics coupled
22 numerical model has been widely used to simulate precisely the thermoelectric conversion process and
23 optimize the geometrical size of TEG systems. The TEG modules contained in the system can be
24 modeled by the transport equations in Section 2.3.2, and the heat transfer components placed on both
25 sides of TEG modules can be characterized by Eq. (37).

26 In the field of radioisotope TEG system, Liu et al. [78] utilized the thermal-electric numerical model
27 to optimize the structural size of a micro-radial milliwatt-power radioisotope TEG system. A solid heat
28 transfer unit was placed in the center of the system as the equivalent heat source of ^{241}Am isotope
29 element. During the numerical simulation, the solid heat transfer unit provided a constant heat source
30 temperature, which was set to contact with the hot side of the TEG legs, and was set to be grounded in
31 the current unit. Also, the TEG system was exposed to the indoor environment with an air convection
32 coefficient of $6 \text{ W}/(\text{m}^2\cdot\text{K})$. Ultimately, the temperature distributions and the open-circuit voltage of the

1 TEG system were obtained by numerical simulations in the platform of COMSOL. Through the
2 optimization, the open-circuit voltage of 605.84 mV and the maximum output power of 423.50 μ W
3 were obtained. Khajepour and Rahmani [79] proposed a multi-stage design method for the radioisotope
4 TEG system, in which COMSOL was used for thermal-electric numerical simulation to determine the
5 parameters of the TEG module, and ANSYS was used for thermal numerical simulation to determine
6 the parameters of isotope heat source and its accessories. However, the load response characteristics
7 were ignored in Refs [78, 79]. It is not accurate enough to use the open-circuit voltage to evaluate the
8 output performance of the TEG system, because the load resistance at the maximum output power is
9 higher than the internal resistance of the TEG module, which is different from the common circuit
10 [50].

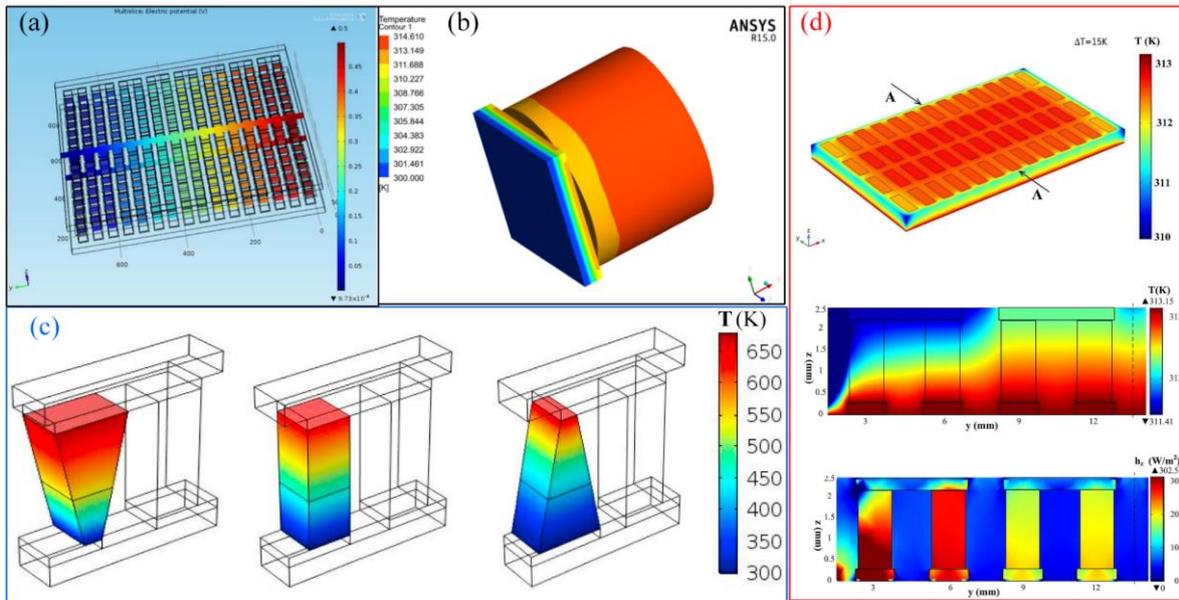
11 In the field of solar-based TEG systems, Liu et al. [80] proposed a novel solar TEG module design
12 to enhance the output power and conversion efficiency, which combines the asymmetric legs with the
13 variable cross-sectional area and segmented thermoelectric materials. The geometric parameters of the
14 legs were optimized by the thermal-electric numerical model, and the numerical simulation was carried
15 out by COMSOL software. In the model, a heat flux boundary condition was applied on the hot side
16 of the TEG module, a heat sink with a constant temperature of 300 K was applied on the cold side of
17 the TEG module, and a current input boundary condition was adopted to form a circuit. Here, the heat
18 flux absorbed from solar energy is defined by the following formula [81]:

$$19 \quad q = q_{\text{solar}} C_g A_{\text{ce}} \eta_{\text{opt}} a_{\text{ce}} \quad (50)$$

20 where q_{solar} is the solar irradiance. C_g is the concentration ratio, which is estimated by the area of the
21 lens divided by that of the collector. A_{ce} is the cross-sectional area of the collector and is usually equal
22 to the cross-sectional area of the ceramic plate. η_{opt} is the optical efficiency of the Fresnel lens. a_{ce}
23 is the absorptivity of the collector coating. Generally, parameters in Eq. (50) are given values in a specific
24 numerical simulation. Thus, the performance of a solar-based TEG system can be predicted under
25 specific solar energy input.

26 For the application of thermoelectric power generation in the field of self-powered wearable devices,
27 the TEG module usually works under a small temperature gradient, such as the temperature difference
28 between body temperature and ambient temperature. To maintain the wearability and flexibility of
29 devices, Francioso et al. [82] fabricated a flexible heat sink-free wearable TEG system, in which two
30 metal layers were screen-printed on both ends of the TEG module. The hot side metal layer was to
31 enhance the thermal contact with the skin, and the cold side one was to enhance the heat dissipation
32 and lower the thermal resistance of ambient air. As already discussed, the leg height, as well as the

1 height of the metal layer, have opposite effects on the output performance and wearability. For this
 2 reason, the thermal-electric numerical model was adopted to determine the optimal ones. Under the
 3 boundary conditions of constant heat flux at the hot end and natural convection on the cold end, the
 4 numerical simulations were performed by using COMSOL software. The results indicated that the
 5 optimal leg height and Ag metal layer height are 2 mm and 500 μm respectively. However, the
 6 thermoelectric material properties were assumed to be constant in their study. The use of flexible
 7 encapsulation is an effective approach to maintain flexibility and protect the TEG legs against
 8 mechanical vibration and reduce stress. Based on the thermal-electric numerical model, Liu et al. [83]
 9 conducted a comprehensive performance evaluation for a wearable TEG module with flexible
 10 encapsulation. In the modeling, the practical boundary conditions have been completely considered,
 11 including the temperature-dependent thermoelectric material properties, the natural convection heat
 12 transfer, and the topological connection of load resistance. The results showed that the average
 13 performance deviation between the model results and the experimental data was 4.2%. Under the fixed
 14 temperature difference of 15 K, the maximum output power of the optimized wearable TEG module
 15 is 598.1% higher than that of the original design. Some useful results were obtained in their study.



16
 17 Fig. 14. Numerical results of TEG systems directly contacted with the heat source reproduced from Refs [79, 80, 83]. (a)
 18 Open-circuit voltage distribution of a radioisotope TEG module obtained by COMSOL [79]; (b) Temperature distributions
 19 of a radioisotope TEG module and its heat source obtained by ANSYS [79]; (c) Temperature profile of a solar-based TEG
 20 unit obtained by COMSOL [80]; (d) Temperature and heat flux profiles of a wearable TEG module obtained by COMSOL
 21 [83].

22 It can be seen that numerical modeling plays a significant role in predicting and optimizing the

1 performance of TEG systems. Fig. 14 shows the numerical results of radioisotope, solar-based, and
2 wearable TEG systems in Refs [79, 80, 83], respectively. The thermal-electric numerical model of the
3 TEG module has been widely adopted to study its characteristics in these application scenarios, in
4 which the heat transfer components on both sides of the TEG module were omitted by setting
5 appropriate thermal boundary conditions. Compared with the thermal resistance-based analytical
6 model, the thermal-electric numerical model can consider all the actual boundary conditions and
7 predict more reasonable results. However, there were few reports on numerical modeling of the stove-
8 powered TEG system, and researchers mainly used the thermal resistance-based analytical model to
9 study its performance. Numerical investigation on the stove-powered TEG system may grow up in
10 future works.

11 Another unparalleled advantage of the numerical model is that it is capable of predicting the transient
12 behavior of TEG systems directly contacted with the heat source. By extending the transient numerical
13 model in Section 2.3.3 from the TEG module to the TEG system and combining it with transient hot
14 side temperature input, the transient performance prediction can be completed by using numerical
15 analysis software (e.g. COMSOL Multiphysics). The transient temperature variation of the heat source
16 can be obtained through experimental measurement. At present, most researches focus on steady-state
17 performance analysis. In practical application, the heat source is not static. It is more meaningful to
18 study the dynamic response characteristics of the TEG system.

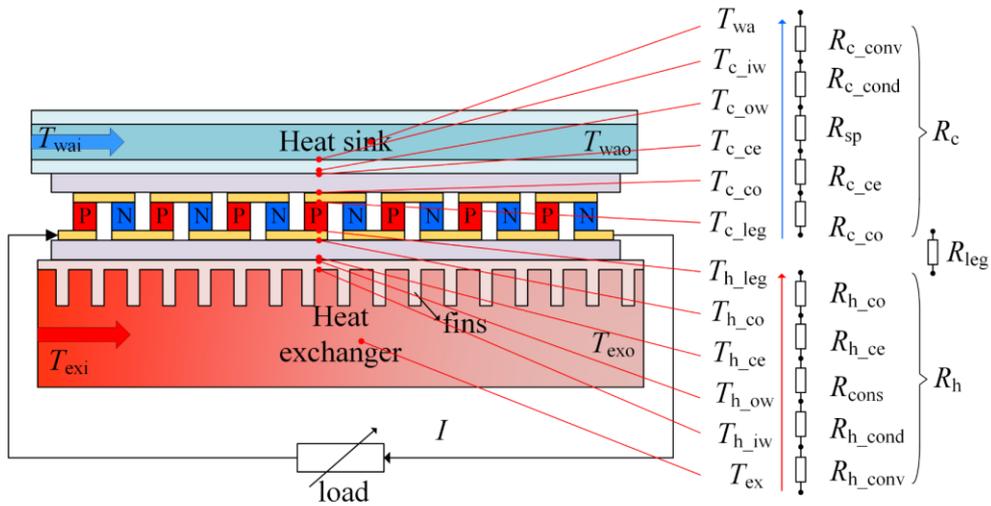
19 *3.2 Thermoelectric generator systems for fluid waste heat recovery*

20 In recent decades, thermoelectric power generation technology has aroused great interest in the field
21 of fluid waste heat recovery, such as automobile exhaust waste heat recovery, industrial waste heat
22 recovery, ship exhaust waste heat recovery, and so on, among which the automobile exhaust waste
23 heat recovery is the most popular research object. For automobile engines, about one-third of the heat
24 generated by burning fossil fuels is directly discharged into the environment in the form of exhaust
25 gases, causing serious energy shortage and environmental pollution [84]. Thermoelectric power
26 generation is an effective manner to recover the heat energy from exhaust gases, and the electricity
27 generated by the TEG system can be used for the power supply of vehicle electronics or stored in a
28 battery. A great number of automotive TEG system prototypes have been developed by researchers
29 [85, 86]. The results showed that the maximum output power of the automotive TEG system can reach
30 500-1000 W, which exhibits a good application prospect.

31 In order to predict and optimize the performance of automotive TEG systems, several theoretical

1 models have been proposed in previous studies. According to different principles, theoretical models
 2 can be grouped into three categories: thermal resistance-based analytical model, computational fluid
 3 dynamics (CFD) model, and fluid-thermal-electric multiphysics field coupled numerical model.
 4 Compared with TEG systems directly contacted with the heat source, the automotive TEG system
 5 involves complex fluid flow, which brings great difficulties to the modeling process. In addition, the
 6 theoretical model of the automotive TEG system can be used to predict the characteristics of the TEG
 7 system in other fluid waste heat recovery applications, because they follow the same governing
 8 equations.

9 3.2.1 Thermal resistance-based analytical models



10
 11 Fig. 15. Schematic diagram of the thermal resistance network of the water-cooled automotive TEG system.

12 In order to effectively dissipate heat and reduce the cold side working temperature of the TEG
 13 module, the water cooling mode is a more attractive method than the air cooling mode. Besides, the
 14 heat transfer process of water cooling is more complex than that of air cooling, because air cooling can
 15 be estimated by a convective thermal resistance. Therefore, the water-cooled automotive TEG system
 16 is taken as the objective to elucidate the thermal resistance-based analytical model in this section. Fig.
 17 15 shows the schematic diagram of the thermal resistance network of the water-cooled automotive
 18 TEG system. In most cases, the known parameters of the automotive TEG system only include given
 19 temperature data, fluid parameters of exhaust gases and cooling water, geometrical features, and
 20 material properties of the TEG system. According to these known parameters, it is required to calculate
 21 the output parameters of the TEG system, such as output power and conversion efficiency.

22 The given temperature data include the inlet exhaust temperature (T_{exi}), inlet water temperature
 23 (T_{wai}), outlet exhaust temperature (T_{exo}), and outlet water temperature (T_{wao}), which can be measured

1 by using thermocouples. However, in the case of theoretical analysis, it is usually necessary to predict
 2 the performance of the automotive TEG system under the given inlet air temperature (T_{exi}) and inlet
 3 water temperature (T_{wai}), while the outlet exhaust temperature (T_{exo}) and outlet water temperature
 4 (T_{wao}) can not be known. The modeling approaches of these two cases are described respectively as
 5 follows:

6 Under the given T_{exi} , T_{wai} , T_{exo} , and T_{wao} , the amount of heat transfer between exhaust gases and heat
 7 exchanger, and between cooling water and heat sink can be expressed by Eq. (51) and Eq. (52),
 8 respectively.

$$9 \quad Q_h = h_{\text{ex}} A_{\text{eff}} (T_{\text{ex}} - T_{\text{h_iw}}) \quad (51)$$

$$10 \quad Q_c = h_{\text{wa}} A_{\text{sink}} (T_{\text{c_iw}} - T_{\text{wa}}) \quad (52)$$

11 with

$$12 \quad T_{\text{ex}} = \frac{T_{\text{exi}} + T_{\text{exo}}}{2} \quad (53)$$

$$13 \quad T_{\text{wa}} = \frac{T_{\text{wai}} + T_{\text{wao}}}{2} \quad (54)$$

14 where, h_{ex} and h_{wa} are the convective heat transfer coefficients of exhaust gases and water respectively.
 15 A_{eff} is the effective contact area between exhaust gases and the heat exchanger. A_{sink} is the contact area
 16 between cooling water and heat sink. $T_{\text{h_iw}}$ is the inner wall temperature of the heat exchanger. $T_{\text{c_iw}}$ is
 17 the inner wall temperature of the heat sink.

18 To compute convective heat transfer coefficients of h_{ex} and h_{wa} , empirical formulas are commonly
 19 used. Considering the different flow patterns of exhaust gases and cooling water, different empirical
 20 formulas can be used to minimize the error [87]. For exhaust gases, the mean Nusselt number can be
 21 estimated by the Gnielinski correlation, which is:

$$22 \quad \text{Nu} = \frac{(f/8)(\text{Re}-1000)\text{Pr}}{1+12.7\sqrt{f/8}(\text{Pr}^{2/3}-1)} \quad (55)$$

23 with

$$24 \quad f = (1.82 \lg \text{Re} - 1.64)^{-2} \quad (56)$$

25 For cooling water, its mean Nusselt number can be obtained by the Dittus-Boelter correlation, which
 26 is:

$$27 \quad \text{Nu} = 0.023 \text{Re}^{0.8} \text{Pr}^{0.4} \quad (57)$$

28 In Eqs (55), (56) and (57), the Reynold number (Re) and Prandtl number (Pr) can be expressed as:

$$\text{Re} = \frac{\rho v D}{\mu} \quad (58)$$

$$\text{Pr} = \frac{\mu c}{\lambda} \quad (59)$$

with

$$v = \frac{\dot{m}}{\rho A} \quad (60)$$

$$D = \frac{4A}{L} \quad (61)$$

where, ρ is the fluid density, v is the fluid velocity, D is the hydraulic diameter, μ is the dynamic viscosity of fluids, c is the specific heat of fluids, λ is the thermal conductivity of fluids, \dot{m} is the mass flow rate of fluids, A is the cross-sectional area, and L is the wetted perimeter over the cross section.

Under the given mass flow rates of exhaust gases and cooling water, their Nusselt numbers can be calculated. And then, the convective heat transfer coefficient can be computed by:

$$h = \lambda \frac{\text{Nu}}{D} \quad (62)$$

And then, the convective thermal resistances of exhaust gases (R_{h_conv}) and cooling water (R_{c_conv}) can be estimated by:

$$R_{h_conv} = \frac{1}{h_{ex} A_{eff}} \quad (63)$$

$$R_{c_conv} = \frac{1}{h_{wa} A_{sink}} \quad (64)$$

In which, A_{sink} can be directly obtained by the geometrical sizes of the heat sink. However, the situation of the heat exchanger is quite different. To effectively enhance the convective heat transfer between exhaust gases and the heat exchanger and improve the working temperature of the hot side of the TEG module, a fin structure is usually used in the heat exchanger to increase the contact area of convective heat transfer. The effective contact area is defined by:

$$A_{eff} = A_b + \eta_{fin} A_{fin} \quad (65)$$

with

$$\eta_{fin} = \frac{\tanh(mH_{fin})}{mH_{fin}} \quad (66)$$

$$m = \sqrt{\frac{2h_{\text{ex}}}{\lambda_{\text{fin}} \delta_{\text{fin}}}} \quad (67)$$

where, A_b is the area of the base of the heat exchanger. η_{fin} , A_{fin} , H_{fin} , λ_{fin} , and δ_{fin} are the efficiency, area, height, thermal conductivity, and thickness of fins, respectively.

When the heat is transferred from the inner wall to the outer wall of the heat exchanger and heat sink, the conductive thermal resistances of the heat exchanger (R_{h_cond}) and heat sink (R_{c_cond}) can be defined by:

$$R_{h_cond/c_cond} = \frac{\delta_{b/sink}}{\lambda_{b/sink} A_{b/sink}} \quad (68)$$

where, δ and A are the thickness and cross-sectional area respectively. Subscripts sink and b denote heat sink and base of heat exchanger respectively.

When the heat moves from the heat exchanger (a bigger area) to the hot side of the TEG module (a smaller area), there is a constricted thermal resistance [88], which is defined by:

$$R_{\text{cons}} = \frac{\zeta \tau + 0.5 \sqrt{\pi} (1 - \zeta)^{\frac{3}{2}} \cdot \Theta}{\lambda_b \pi a} \quad (69)$$

with

$$\Theta = \frac{\tanh(\beta \tau) + \beta / \text{Bi}}{1 + (\beta / \text{Bi}) \tanh(\beta \tau)} \quad (70)$$

$$\zeta = \frac{a}{b} = \frac{\sqrt{A_{ce} / \pi}}{\sqrt{A_b / \pi}} \quad (71)$$

$$\tau = \frac{\delta_b}{b} \quad (72)$$

$$\beta = \pi + \frac{1}{\zeta \sqrt{\pi}} \quad (73)$$

$$\text{Bi} = \frac{1}{\pi \lambda_b b R_{h_conv}} \quad (74)$$

When the heat moves from the cold side of the TEG module (a smaller area) to the heat sink (a bigger area), there is a spreading thermal resistance [88], which can be expressed as:

$$R_{\text{sp}} = \frac{A_{\text{sink}}^{0.5} - A_{\text{ce}}^{0.5}}{\lambda_{\text{sink}} (\pi A_{\text{sink}} A_{\text{ce}})^{0.5}} \cdot \frac{\gamma \lambda_{\text{sink}} A_{\text{sink}} R_{\text{wa}} + \tanh(\gamma \delta_{\text{sink}})}{1 + \gamma \lambda_{\text{sink}} A_{\text{sink}} R_{\text{wa}} \cdot \tanh(\gamma \delta_{\text{sink}})} \quad (75)$$

with

$$\gamma = \frac{\pi^{\frac{3}{2}}}{A_{\text{sink}}^{0.5}} + \frac{1}{A_{\text{ce}}^{0.5}} \quad (76)$$

In addition, the conductive thermal resistances of the hot side ($R_{\text{h_ce}}$) and cold side ($R_{\text{c_ce}}$) ceramic plates can be estimated by Eq. (77). Generally, the area of the hot side ceramic plate is equal to that of the cold side ceramic plate, which is $A_{\text{h_ce}}=A_{\text{c_ce}}$.

$$R_{\text{h_ce/c_ce}} = \frac{\delta_{\text{ce}}}{\lambda_{\text{ce}} A_{\text{h_ce/c_ce}}} \quad (77)$$

Similarly, the conductive thermal resistances of the hot side ($R_{\text{h_co}}$) and cold side ($R_{\text{c_co}}$) of copper electrodes can be estimated by Eq. (78), and $A_{\text{h_co}}$ is generally equal to $A_{\text{c_co}}$.

$$R_{\text{h_co/c_co}} = \frac{\delta_{\text{co}}}{\lambda_{\text{co}} A_{\text{h_co/c_co}}} \quad (78)$$

As described above, all thermal resistances from exhaust gases to the hot side of thermoelectric legs and from the cold side of thermoelectric legs to cooling water are modeled completely. And thus, the total hot side and cold side thermal resistances of R_{h} and R_{c} can be defined by:

$$R_{\text{h}} = R_{\text{h_conv}} + R_{\text{h_cond}} + R_{\text{cons}} + R_{\text{h_ce}} + R_{\text{h_co}} \quad (79)$$

$$R_{\text{c}} = R_{\text{c_conv}} + R_{\text{c_cond}} + R_{\text{sp}} + R_{\text{c_ce}} + R_{\text{c_co}} \quad (80)$$

Finally, the overall hot side heat flux and cold side flux can be expressed as:

$$Q_{\text{h}} = \frac{T_{\text{ex}} - T_{\text{h_leg}}}{R_{\text{h}}} = \alpha_{\text{pn}} I T_{\text{h_leg}} + \frac{T_{\text{h_leg}} - T_{\text{c_leg}}}{R_{\text{leg}}} - \frac{1}{2} I^2 R_{\text{in}} \quad (81)$$

$$Q_{\text{c}} = \frac{T_{\text{c_leg}} - T_{\text{wa}}}{R_{\text{c}}} = \alpha_{\text{pn}} I T_{\text{c_leg}} + \frac{T_{\text{h_leg}} - T_{\text{c_leg}}}{R_{\text{leg}}} + \frac{1}{2} I^2 R_{\text{in}} \quad (82)$$

Therefore, the output power of the TEG module can be estimated by:

$$P = Q_{\text{h}} - Q_{\text{c}} \quad (83)$$

The electric current can be expressed as:

$$I = \frac{\alpha_{\text{pn}} (T_{\text{h_leg}} - T_{\text{c_leg}})}{R_{\text{in}} + R_{\text{L}}} \quad (84)$$

According to Eqs (81)-(84), there are six formulas with six unknowns of Q_{h} , Q_{c} , $T_{\text{h_leg}}$, $T_{\text{c_leg}}$, P , and I . Ultimately, the output power of the automotive TEG system can be computed, and the conversion efficiency is equal to the output power divided by the hot side heat flux, that is:

$$\eta = \frac{P}{Q_{\text{h}}} \quad (85)$$

1 In addition, by using the iterative method described in Fig. 4, the temperature-dependent
 2 thermoelectric material properties can be taken into consideration, which can further improve the
 3 reasonability of this model.

4 However, when T_{exo} and T_{wao} are not given, Eqs (81)-(84) can not solve eight unknowns of Q_{h} , Q_{c} ,
 5 T_{exo} , T_{wao} , $T_{\text{h_leg}}$, $T_{\text{c_leg}}$, P , and I , and two additional equations are needed. For this reason, the overall
 6 heat flux of the hot side and cold side can also be characterized by the change of internal energy of
 7 exhaust gases and cooling water, which are:

$$8 \quad Q_{\text{h}} = c_{\text{ex}} \dot{m}_{\text{ex}} (T_{\text{exi}} - T_{\text{exo}}) \quad (86)$$

$$9 \quad Q_{\text{c}} = c_{\text{wa}} \dot{m}_{\text{wa}} (T_{\text{wao}} - T_{\text{wai}}) \quad (87)$$

10 Based on the above analysis, the performance of the automotive TEG system can be evaluated with
 11 given temperature data, fluid parameters, geometric characteristics, and material properties. In Ref.
 12 [89], under the condition of neglecting the thermal resistances (R_{h} and R_{c}) and taking the exhaust gas
 13 temperature (T_{ex}) and cooling water temperature (T_{wa}) as the working temperature of the hot side and
 14 cold side of the TEG module directly, the thermal resistance-based analytical model of automotive
 15 TEG system was divided into different submodels according to different leg rows along the direction
 16 of exhaust gas downward flow. The submodels were computed by using engineering equation solver
 17 (EES) software. According to model results, a TEG module composed of $\text{Mg}_2\text{Si}/\text{Zn}_4\text{Sb}_3$ for high-
 18 temperature regions followed by Bi_2Te_3 for low-temperature regions was optimized by the authors.

19 With the consideration of convective and conductive thermal resistances, Wang et al. [90], Vale et
 20 al. [91], Mostafavi and Mahmoudi [92], and Marvão et al. [93] used the thermal resistance-based
 21 analytical model to evaluate the performance of automotive TEG system and to study the effects of
 22 exhaust mass flow rate, exhaust temperature, geometry size of fins and heat exchanger on the
 23 performance. Some useful findings were obtained in their research. Furthermore, the thermal
 24 resistance-based analytical model of the automotive TEG system was improved in Refs [87, 88] by
 25 considering the constricted thermal resistance (R_{cons}) and spreading thermal resistance (R_{sp}). However,
 26 the temperature dependence of thermoelectric material properties was omitted in Refs [88, 90, 92], or
 27 the average temperature of the hot side ($T_{\text{h_leg}}$) and cold side ($T_{\text{c_leg}}$) of TEG legs was adopted to
 28 evaluate the thermoelectric properties in Refs [87, 91, 93]. Therefore, the accuracy of the developed
 29 models can be further improved by using reasonable methods to deal with the temperature-dependent
 30 thermoelectric properties.

31 The thermal resistance-based analytical model can also be used to evaluate the performance of some
 32 novel TEG system structures. Zhao et al. [94, 95] proposed an intermediate fluid TEG system in which

the exhaust waste heat is transferred by boiling and condensation of the intermediate fluid. Combined with the heat transfer analysis of the intermediate fluid, the output performance of the TEG system for automotive exhaust waste heat recovery was studied by using the thermal resistance-based analytical model. The results indicated that the peak output power of the proposed structure is significantly higher than that of the traditional structure. In addition, the model can be used to predict the performance of the TEG system with phase change materials [96].

In other fields of waste heat recovery, Meng et al. [7] utilized the thermal resistance-based analytical model to evaluate the performance of the TEG system for waste heat recovery from industrial gas, while ignoring the constricted and spreading thermal resistances and using constant thermoelectric material properties. Kristiansen et al. [97] constructed a TEG system to recover waste heat from a marine waste incinerator and used the thermal resistance-based analytical model to optimize the parameters of the heat exchanger and TEG module. The convective, conductive, and spreading thermal resistances (R_{h_conv} , R_{c_conv} , R_{h_cond} , R_{c_cond} , R_{h_ce} , R_{c_ce} , and R_{sp}) were considered in their theoretical analysis. The basic equations in Refs [7, 97] are consistent with those of the thermal resistance-based analytical model of the automotive TEG system.

On the other hand, the temperature and mass flow rate of automotive exhaust gas will change with the change in vehicle operating conditions. The steady-state performance analysis of the automotive TEG system can not reveal its dynamic response characteristics. Based on the temperature and mass flow rate data of exhaust gas at different time points, Gou et al. [98] and Lan et al. [99] used the thermal resistance-based analytical model to evaluate the dynamic performance of the TEG system applied to waste heat recovery. However, according to the transient numerical simulation of the TEG module [58], it can be observed that the transient response of output power and conversion efficiency has an obvious time delay phenomenon, which can not be considered by the thermal resistance model. Besides, when considering the transient fluid flow and heat transfer in fluid regions, the time delay may be more obvious, which leads to the larger error of the transient performance predicted by the thermal resistance-based analytical model of the TEG system for fluid waste heat recovery.

Table 2. Lists of recent thermal resistance-based analytical models of TEG system applied in fluid waste heat recovery.

| Steady/transient state | Thermal resistances consideration | in Temperature-dependent properties | thermoelectric material | Sources |
|------------------------|---|-------------------------------------|-------------------------|--------------|
| Steady state | No | Using constant properties | thermoelectric material | [89] |
| Steady state | R_{h_conv} , R_{c_conv} , R_{h_cond} , R_{c_cond} | Using constant properties | thermoelectric material | [92, 94, 95] |
| Steady state | R_{h_conv} , R_{c_conv} , R_{h_cond} , R_{c_cond} , R_{h_ce} , R_{c_ce} , | Using constant properties | thermoelectric material | [7] |
| Steady state | R_{h_conv} , R_{c_conv} , R_{h_cond} , R_{c_cond} , | Using constant properties | thermoelectric material | [97] |

| | | | |
|---|--|--|----------|
| Steady state | $R_{sp}, R_{h_{ce}}, R_{c_{ce}}, R_{h_{conv}}, R_{c_{conv}}, R_{h_{cond}}, R_{c_{cond}}, R_{h_{ce}}, R_{c_{ce}}, R_{h_{co}}, R_{c_{co}}$ | properties Using constant thermoelectric material properties | [90, 96] |
| Steady state | $R_{h_{conv}}, R_{c_{conv}}, R_{h_{cond}}, R_{c_{cond}}, R_{h_{ce}}, R_{c_{ce}}, R_{h_{co}}, R_{c_{co}}$ | Evaluated by using the average temperature of the hot side and cold side of TEG legs | [91, 93] |
| Steady state | $R_{h_{conv}}, R_{c_{conv}}, R_{h_{cond}}, R_{c_{cond}}, R_{cons}, R_{sp}, R_{h_{ce}}, R_{c_{ce}}$ | Using constant thermoelectric material properties | [88] |
| Steady state | $R_{h_{conv}}, R_{c_{conv}}, R_{h_{cond}}, R_{c_{cond}}, R_{cons}, R_{sp}, R_{h_{ce}}, R_{c_{ce}}, R_{h_{co}}, R_{c_{co}}$ | Evaluated by using the average temperature of the hot side and cold side of TEG legs | [87] |
| Steady state | $R_{h_{conv}}, R_{c_{conv}}, R_{h_{cond}}, R_{c_{cond}}, R_{cons}, R_{h_{ce}}, R_{c_{ce}}, R_{h_{co}}, R_{c_{co}}$ | Evaluated by using an iterative method | [25] |
| Transient state using the data at different time points | $R_{h_{conv}}, R_{c_{conv}}, R_{h_{cond}}, R_{c_{cond}}, R_{h_{ce}}, R_{c_{ce}}, R_{h_{co}}, R_{c_{co}}$ | Using constant thermoelectric material properties | [98] |
| Transient state using the data at different time points | $R_{h_{conv}}, R_{c_{conv}}, R_{h_{cond}}, R_{c_{cond}}, R_{h_{ce}}, R_{c_{ce}}, R_{h_{co}}, R_{c_{co}}$ | Evaluated by using the average temperature of the hot side and cold side of TEG legs | [99] |

1 Recent developed thermal resistance-based analytical models of the TEG system applied in fluid
2 waste heat recovery are tabulated in Table 2. In order to ensure high enough model accuracy, the
3 thermal resistances of $R_{h_{conv}}, R_{c_{conv}}, R_{h_{cond}}, R_{c_{cond}}, R_{h_{ce}}, R_{c_{ce}}$ are required to be comprehensively
4 considered, because the temperature changes greatly when the heat is transferred through these thermal
5 resistances. Due to the high thermal conductivity and small thickness of copper electrodes, ignoring
6 the conductive thermal resistances of $R_{h_{co}}$ and $R_{c_{co}}$ has little effect on the output performance, and
7 thus, the conductive thermal resistance of copper electrodes is ignored in a considerable number of
8 studies. The value of constricted and spreading thermal resistances is depended on the area difference
9 between the TEG module and contact surfaces of the heat exchanger and heat sink. When the area of
10 the hot side surface of the heat exchanger and cold side surface of the heat sink is larger than the cross-
11 sectional area of the ceramic plate, the corresponding thermal resistances of R_{cons} and R_{sp} should not
12 be neglected, and vice versa. In addition, the thermoelectric material properties are highly temperature-
13 dependent and nonlinear, therefore, appropriate methods should be adopted to ensure reasonability.

14 However, the thermal resistance-based analytical model is based on the assumption that there is no
15 heat loss between the TEG system and the surrounding environment, and there is no Thomson heat
16 along the TEG legs, which may lead to overestimation of output performance. The authors in Ref. [25]
17 conducted a comparison between the thermal resistance-based analytical model and the fluid-thermal-
18 electric multiphysics field coupled numerical model. Their results indicated that the numerical model
19 is more reasonable than the thermal resistance model, and the accuracy of the thermal resistance model
20 is highly affected by the exhaust temperature and mass flow rate. Details of the numerical model are
21 introduced in the following sections.

1 3.2.2 CFD models

2 In general, the TEG system for fluid waste heat recovery is composed of a heat exchanger, TEG
3 modules, heat sinks, and clamping devices. The heat exchanger is used to absorb heat from exhaust
4 gases and transfer the heat to the hot side of TEG modules, and the heat transfer performance of the
5 heat exchanger largely determines the output performance of the TEG system. The computational fluid
6 dynamics (CFD) model is a common method to study and optimize the performance of heat
7 exchangers, which is usually computed by using numerical analysis software such as ANSYS/Fluent
8 and COMSOL. According to CFD results, temperature distributions of the whole TEG system and
9 pressure distributions of fluids can be obtained. High hot side temperature, uniform hot side
10 temperature distribution, and low pressure drop are key parameters to evaluate the performance of the
11 heat exchanger. Besides, the obtained average surface temperature on both sides of TEG modules can
12 be used to calculate the output performance of the TEG system through a simple calculation of Seebeck
13 voltage. Furthermore, the average surface temperature can be used as the boundary conditions of the
14 thermal resistance model and thermal-electric numerical model of the TEG module, and then more
15 reasonable output performance can be predicted. These three methods based on the CFD model are
16 introduced as follows:

17 i. CFD model only

18 The governing equations of the CFD model for the TEG system used to recover fluid waste heat
19 include two parts: fluid regions and solid regions. In the fluid region of the exhaust channel and cooling
20 water channel, the steady-state fluid flow follows the basic conservations of mass, momentum, and
21 energy, which are:

$$22 \quad \nabla \cdot \vec{v} = 0 \quad (88)$$

$$23 \quad \nabla \cdot (\vec{v}\vec{v}) = -\frac{1}{\rho} \nabla p + \nabla \cdot (\mu \nabla \vec{v}) \quad (89)$$

$$24 \quad \nabla \cdot (\lambda \nabla T) = \rho c \vec{v} \cdot \nabla T \quad (90)$$

25 where \vec{v} is the fluid velocity vector. Eq. (88), Eq. (89), and Eq. (90) represent the mass, momentum,
26 and energy conservations, respectively.

27 For the automotive TEG system, the flow pattern is usually turbulent and depended upon the
28 Reynolds number. Two-equation turbulence models are the most commonly used methods to simulate
29 the turbulent flow, including standard $k - \varepsilon$ model, renormalization group (RNG) $k - \varepsilon$ model, realizable
30 $k - \varepsilon$ model, and so on. Considering the high accuracy and high adaptivity of the RNG $k - \varepsilon$ model, it

1 has been widely adopted in previous studies [100, 101], which transport equations are:

$$2 \quad \frac{\partial}{\partial t}(\rho k) + \frac{\partial}{\partial x_i}(\rho k u_i) = \frac{\partial}{\partial x_j} \left(\alpha_k \mu_{eff} \frac{\partial k}{\partial x_j} \right) + G_k + G_b - \rho \varepsilon - Y_M \quad (91)$$

$$3 \quad \frac{\partial}{\partial t}(\rho \varepsilon) + \frac{\partial}{\partial x_i}(\rho \varepsilon u_i) = \frac{\partial}{\partial x_j} \left(\alpha_\varepsilon \mu_{eff} \frac{\partial \varepsilon}{\partial x_j} \right) + C_{1\varepsilon} \frac{\varepsilon}{k} (G_k + C_{3\varepsilon} G_b) - C_{2\varepsilon} \rho \frac{\varepsilon^2}{k} - R_\varepsilon \quad (92)$$

4 Detailed descriptions of the symbols in Eqs (91)-(92) can be found in the Fluent user's guide. The
 5 fluid flow and heat transfer in fluid regions can be completely worked out by Eqs (88)-(92). The heat
 6 is transferred between fluid regions and solid regions in the form of conjugate heat transfer, and the
 7 heat transfer in solid regions can be characterized by simple energy conservation, which is:

$$8 \quad \nabla \cdot (\lambda \nabla T) = 0 \quad (93)$$

9 Eqs (88)-(93) constitute the basic governing equations of the CFD model. By setting appropriate
 10 boundary conditions, the CFD model can be solved by numerical analysis software. For the automotive
 11 TEG system, the boundary conditions include inlet and outlet boundary conditions of exhaust gas and
 12 cooling water. In most research, the velocity inlet or mass flow rate inlet with constant inlet
 13 temperature is applied on the inlet surfaces of the fluid channel, while the pressure outlet is applied on
 14 the outlet surfaces. On the surfaces of the TEG system exposed to ambient air, the natural convective
 15 heat transfer boundary is defined. Ultimately, detailed fluid field and thermal field distribution
 16 characteristics of the TEG system are obtained. According to the average surface temperature on both
 17 sides of the TEG module, the output power can be expressed as:

$$18 \quad P = \frac{\alpha_{pn} (T_{h_{ce}} - T_{c_{ce}})}{R_{in} + R_L} \quad (94)$$

19 In a great number of works, to reduce the numerical simulation time, the TEG module is usually
 20 simplified to a whole cube for CFD simulation, to obtain the temperature of the hot side and cold side
 21 of the ceramic plate. Furthermore, considering the heat transfer of all components of the TEG module,
 22 including ceramic plates, copper electrodes, and thermoelectric legs, the average surface temperature
 23 on both sides of the legs ($T_{h_{leg}}$ and $T_{c_{leg}}$) can be obtained, and then more reasonable output power can
 24 be calculated by replacing $T_{h_{ce}}$ and $T_{c_{ce}}$ with $T_{h_{leg}}$ and $T_{c_{leg}}$ respectively.

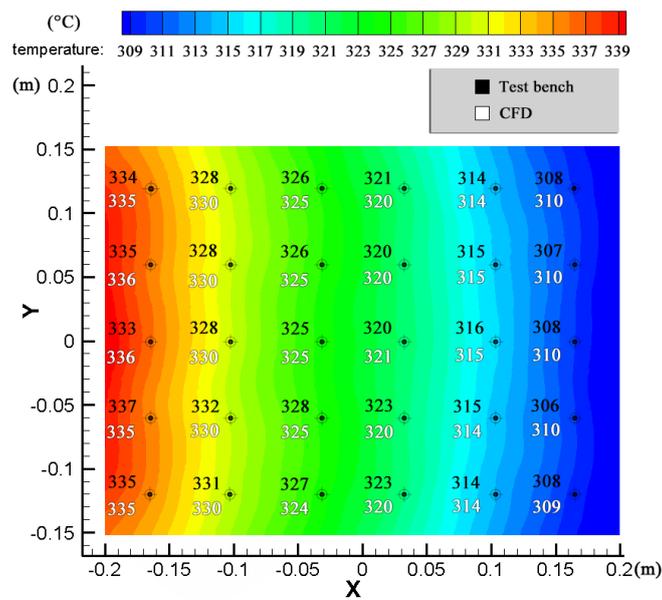
25 The optimization of the automotive TEG system mainly focuses on the improvement of the heat
 26 exchanger. The configuration of the fin structure in the heat exchanger increases the convective heat
 27 transfer area and the residual time of exhaust gas, thus increasing the temperature at the hot side of the
 28 heat exchanger, but the pressure drop will deteriorate. To balance the heat transfer performance and

1 pressure drop, it is necessary to determine the appropriate fin parameters. Liu et al. [101] and
2 Fernández-Yañez et al. [102] proposed several TEG system structures for automotive exhaust heat
3 recovery, in which the heat exchanger adopts different fin designs. The authors used the CFD model
4 to simulate the temperature and pressure distribution of the heat exchanger and studied the influence
5 of different fin parameters on the performance of the heat exchanger, including fin angle, fin size, fin
6 distribution, etc. Accordingly, some optimization design methods were put forward, which provide
7 meaningful guidance for researchers to determine the appropriate fin structure.

8 In addition to fin structure, the parameters of the heat exchanger itself are also crucial to the
9 performance of the TEG system. For a fixed exhaust pipe diameter, the heat exchanger can be designed
10 with different aspect ratios. The oversized heat exchanger length will lead to a large temperature drop
11 and pressure drop from inlet to outlet, and the oversized heat exchanger width will lead to low heat
12 transfer performance for areas away from the center of the exhaust flow. For this reason, Kempf and
13 Zhang [103] used the CFD model to analyze the thermal performance of the TEG system, and then
14 studied the influence of heat exchanger material and various TEG configurations with six different
15 TEG aspect ratios on the thermal performance. They reported that the optimal TEG aspect ratio
16 increases with the thermal conductivity of heat exchanger material under a fixed number of TEG
17 modules. Considering the space limitation of the vehicle exhaust system, Wan et al. [104] integrated a
18 catalytic converter and muffler into the heat exchanger of the TEG system and studied its thermal
19 performance through CFD simulation. Pacheco et al. [105] proposed a novel temperature-controlled
20 TEG system concept in a light-duty vehicle, in which the novel heat exchanger consists of corrugated
21 pipes embedded in the cast aluminum matrix and variable conductance heat pipes acting as spreaders
22 of excess heat along the longitudinal direction. The performance of the novel heat exchanger is
23 examined by the CFD model.

24 In Refs [101-105], the CFD model was only used to analyze the temperature and pressure
25 characteristics of the TEG system, but not to calculate its output performance. According to the average
26 surface temperature of the hot side and cold side of the TEG module predicted by the CFD model, the
27 output power of the TEG system can be calculated by Eq. (94). Weng and Huang [106], Bai et al.
28 [107], and Wang et al. [108, 109] proposed various TEG system configurations for vehicle exhaust
29 waste heat recovery, and used this method to predict their output performance. Fig. 16 shows the
30 temperature distribution on the hot side surface of the heat exchanger. The hot side working
31 temperature of the TEG module can be obtained by evaluating its hot side average surface temperature.
32 Similarly, the cold side working temperature can be obtained, so as to work out the output power of

1 the TEG system. However, in the above literature, the TEG module was simplified as a whole cube to
 2 facilitate CFD simulations, which may lead to the overestimation of output power due to ignoring the
 3 thermal resistances of ceramic plates and copper electrodes. In addition, it is difficult to accurately
 4 express the equivalent material properties of the simplified TEG module. The model error caused by
 5 this factor can be avoided by considering the complete three-dimensional geometry of the TEG module
 6 in CFD simulation and using the average temperature of T_{h_leg} and T_{c_leg} to calculate the output power,
 7 although it requires more calculating power and time. Furthermore, the temperature dependence of
 8 thermoelectric material properties should be considered in CFD simulation to ensure that the results
 9 are more reasonable. On the other hand, the temperature distribution on the hot side of the TEG module
 10 is not uniform, and the working temperature difference among different thermoelectric legs is not
 11 consistent. The overall output current of the TEG module will be limited by the smallest one among
 12 legs because all legs are connected in series. Consequently, the use of average surface temperature will
 13 affect the model accuracy.



14
 15 Fig. 16. The average hot-side temperature of the TEG module obtained by CFD [109].

16 ii. CFD model combined with thermal resistance model

17 After obtaining the average surface temperature of the hot side and cold side of the TEG module by
 18 the CFD model, taking the given temperature data as the boundary condition of the thermal resistance
 19 model of the TEG module, the output power and conversion efficiency of the TEG system can be
 20 calculated, which is a more reasonable method than using CFD model alone to predict the output
 21 performance of TEG system. Li et al. [110] combined the CFD model with the thermal resistance
 22 model of the TEG module to evaluate the performance of a fluid-based TEG system. The hot side and

1 cold side temperature data were extracted from the CFD simulation, and the output performance of the
2 TEG module was calculated by the thermal resistance model. In their study, both the complete three-
3 dimensional geometry of the TEG module and the temperature dependence of thermoelectric materials
4 were taken into account, which provides useful guidance for researchers to analyze the performance
5 of the TEG system theoretically.

6 iii. CFD model combined with thermal-electric numerical model

7 Considering that the accuracy of the numerical model is higher than that of the thermal resistance
8 model, the CFD model can also be combined with the thermal-electric numerical model of the TEG
9 module to predict the output performance of the TEG system. Massaguer et al. [24] proposed a novel
10 method to evaluate the fuel economy of the automotive TEG system, accounting for its output power,
11 backpressure, weight, and coolant pumping power. The benefit of the TEG system applied to a vehicle
12 was analyzed. In their work, firstly, the CFD simulation of the whole TEG system was completed by
13 using ANSYS/Fluent, and the average temperature of the hot side and cold side of the TEG module
14 was obtained, which was used as temperature boundary conditions of TEG module, and then the
15 thermal-electric numerical simulation of the TEG module was completed by using ANSYS/Thermal-
16 Electric, and the open-circuit output voltage of the module was obtained, which was used to predict
17 the output power of TEG system. Their research provides a new idea for analyzing the potential of the
18 TEG system in automotive waste heat recovery.

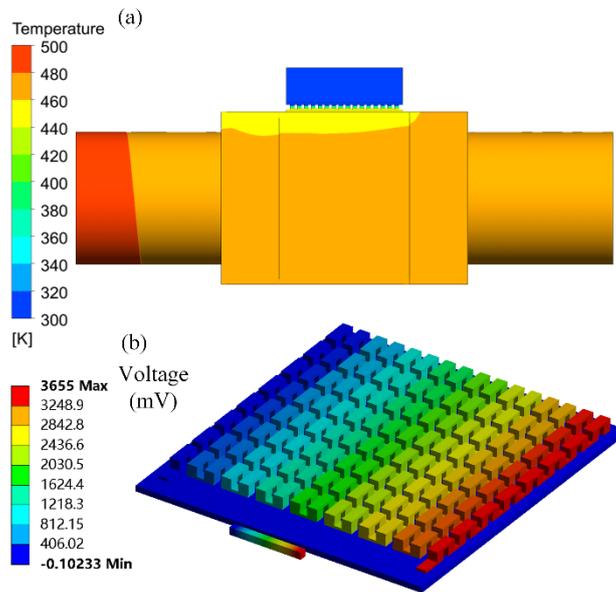
19 3.2.3 Fluid-thermal-electric multiphysics field coupled numerical models

20 In practice, the fluid field, thermal field, and electric field of the TEG system interact simultaneously.
21 These three physical fields should be considered in the comprehensive numerical simulation of the
22 TEG system. However, the CFD model can not consider the electric field, and the thermal-electric
23 numerical model can not consider the fluid field. To accurately predict the performance of the TEG
24 system for fluid waste heat recovery, it is necessary to establish a complete fluid-thermal-electric
25 multiphysics field coupled numerical model. Also, it can be extended into a transient model to study
26 the dynamic response characteristics of the TEG system under conditions of transient change in
27 exhaust temperature and mass flow rate.

28 i. Steady state

29 For the steady-state fluid-thermal-electric multiphysics field coupled numerical model, its governing
30 equations include Eqs (88)-(93) of the CFD model and Eqs (34)-(40) of the thermal-electric numerical
31 model. Reddy et al. [111] integrated the source terms of the energy conservation equation of the TEG

1 module into the energy conservation equation of the CFD model by using the user-defined scalar
2 (UDS) function of Fluent. Combined with reasonable boundary conditions, a fluid-thermal-electric
3 multiphysics field coupled numerical model of a simplified TEG system was established by the
4 authors, and the output performance was predicted by the numerical simulation of Fluent. However,
5 the simplified TEG system only contains one p-type TEG leg and one n-type TEG leg, which is far
6 from the actual situation. The existing reports using Fluent/UDS to study the behavior of TEG devices
7 or TEG systems are all based on a single thermoelectric couple. The reason for this is that the surfaces
8 of each TEG leg need to be redefined by UDS, which means a huge workload for a TEG module, and
9 it is easy to make human or software errors in the process of redefinition.

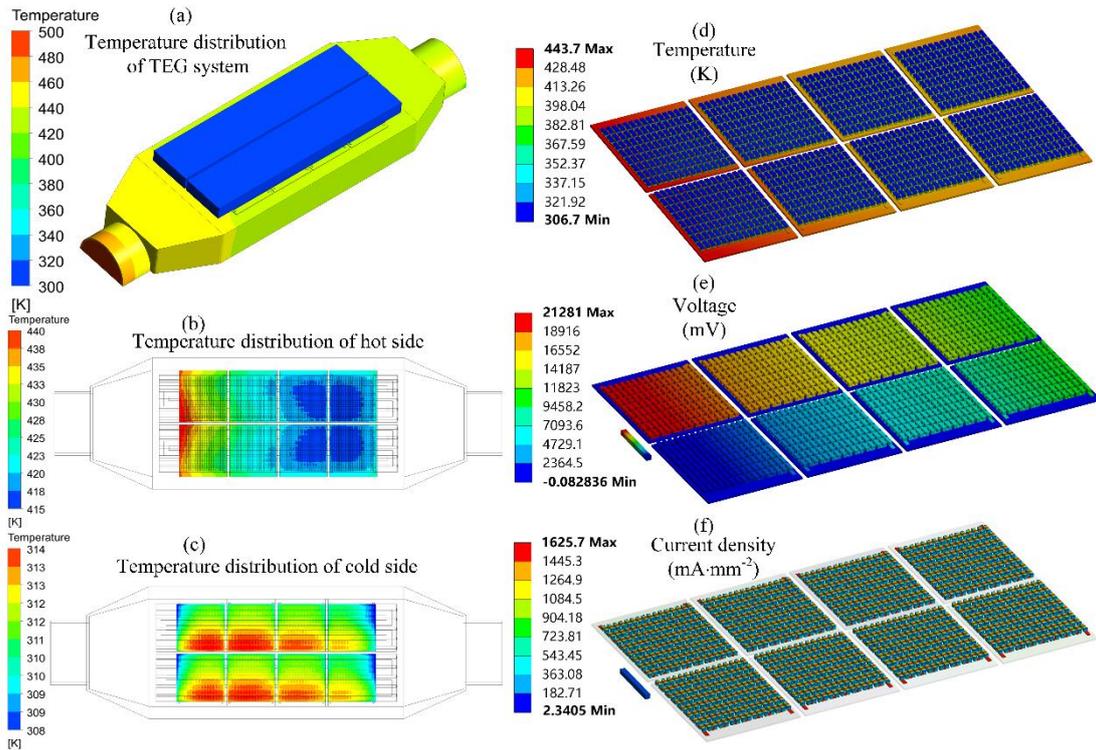


10
11 Fig. 17. Numerical results of a one-TEM-contained TEG system predicted by the fluid-thermal-electric multiphysics field
12 coupled numerical model in Ref. [26]. (a) Temperature distribution of the whole TEG system. (b) Voltage distribution of
13 the TEG module.

14 To extend the fluid-thermal-electric multiphysics field coupled numerical model from the simplified
15 TEG system containing one single thermoelectric couple to a TEG system containing one TEG
16 module, Luo et al. [23, 26] proposed a novel approach to solve the model via the coupling simulation
17 of ANSYS/Fluent and ANSYS/Thermal-Electric. In their study, the CFD model was used to solve the
18 primary temperature distribution of the TEG system, and the obtained temperature distribution of the
19 TEG module was used as the temperature boundary condition of the thermal-electric numerical model
20 to solve its electrical outputs. The obtained numerical results were shown in Fig. 17. Based on the
21 numerical results, they proposed an effective optimization method to overcome the overall output
22 current limitation of the TEG module due to uneven temperature distribution, in which, the length of

1 each TEG leg was determined by its specific temperature difference.

2 In subsequent works [112, 113], Luo et al. further extended the fluid-thermal-electric multiphysics
3 field coupled numerical model from a one-TEM-contained TEG system to a multiple-TEMs-contained
4 TEG system. Similarly, in the numerical simulation, the temperature distribution of the hot side and
5 cold side of TEG modules was used as the temperature boundary condition, and all TEG modules were
6 set to be connected in series. A complete numerical simulation of the whole TEG system was reported
7 for the first time, as shown in Fig. 18, which took into account the temperature dependence of
8 thermoelectric materials and the topological relationship of load resistance. Different from the method
9 of combining the CFD model with the thermal-electric numerical model, the thermal boundary
10 condition loaded on both sides of TEG modules adopts temperature distribution in this model instead
11 of average surface temperature. The influence of two modeling approaches on the output power of the
12 TEG system was studied in Ref. [113], and the results showed that the output power predicted by
13 average surface temperature is about 1% higher than that predicted by temperature distribution, which
14 means the temperature distribution should not be ignored in predicting the output performance of TEG
15 systems for fluid waste heat recovery.



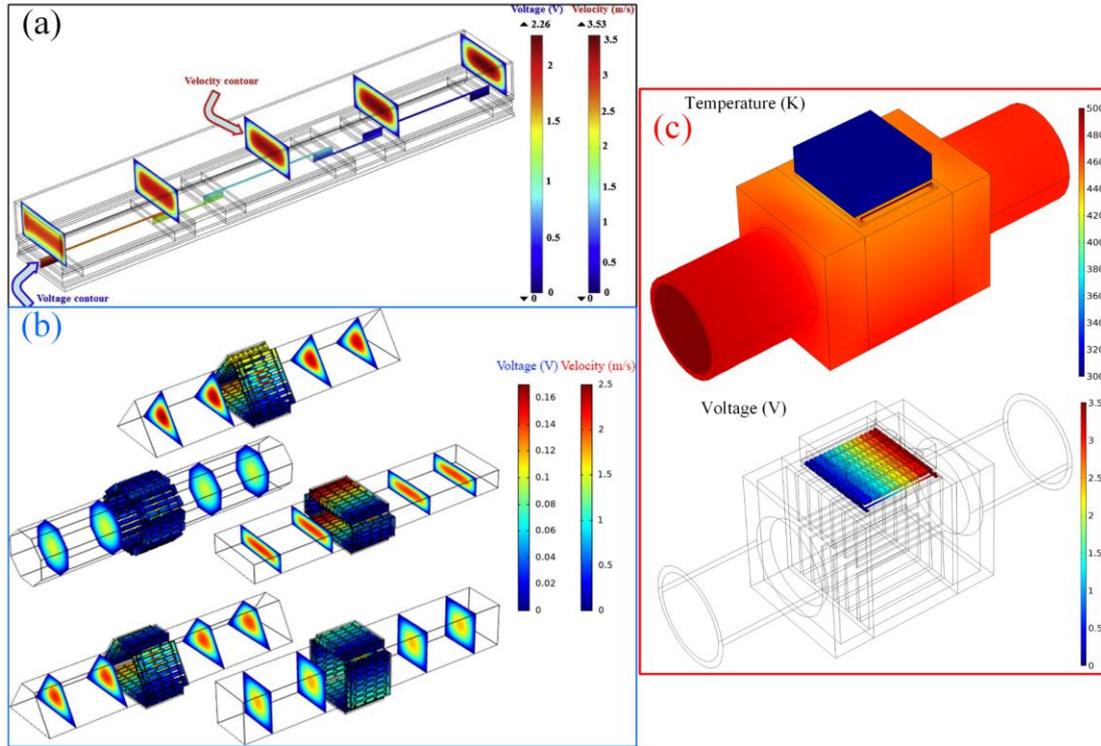
16
17 Fig. 18. Numerical results of multiple-TEMs-contained TEG system predicted by the fluid-thermal-electric multiphysics
18 field coupled numerical model in Ref. [113]. (a) Temperature distribution of the whole TEG system. (b) Hot side
19 temperature distribution of TEG modules. (c) Cold side temperature distribution of TEG modules. (d) Temperature
20 distribution of TEG modules. (e) Voltage distribution of TEG modules. (f) Current density distribution of TEG modules.

1 However, the solution of the fluid-thermal-electric multiphysics field coupled numerical model by
2 the coupling numerical simulation of ANSYS/Fluent and ANSYS/Thermal-Electric can not solve the
3 fluid field, thermal field, and electric field at the same time. In this method, the fluid-thermal
4 multiphysics coupled field is calculated first, and then the thermal-electric multiphysics coupled field
5 is calculated. The influence of parasitic heat (including Joule heat and Peltier heat) generated by the
6 thermoelectric effect on the thermal field and fluid field of the TEG system cannot be considered,
7 which may cause additional model errors. A more reasonable solution needs to be developed.

8 By simplifying the TEG module with multiple TEG legs to a module containing only one pair of
9 TEG legs, and assuming that the thermoelectric material properties were constant, Ma et al. [114]
10 established a fluid-thermal-electric multiphysics field coupled numerical model to study the
11 thermoelectric-hydraulic performance of a simplified TEG system. In their study, the fluid field,
12 thermal field, and electric field were computed at the same time, and numerical simulations were
13 performed on the COMSOL platform, as shown in Fig. 19(a). Compared with ANSYS, COMSOL has
14 the advantages of multiphysics field coupled simulation, which can realize the complete simulation of
15 a fluid-based TEG system. Considering the temperature dependence of thermoelectric materials, Yan
16 et al. [115] studied the effect of heat exchanger channels with different cross-sectional shapes on the
17 TEG system performance through the fluid-thermal-electric multiphysics field coupled numerical
18 simulation on the COMSOL platform, as shown in Fig. 19(b). The research results showed that the
19 TEG system with a rectangular-shaped channel can provide the highest output power and conversion
20 efficiency. However, the cooling device was ignored and the cold side surfaces of TEG modules were
21 directly set as a constant temperature in Ref. [115]. Besides, the load response characteristics were not
22 considered in Refs [114, 115], and only the open-circuit voltage distribution was predicted.

23 To make the multiphysics numerical model closer to reality and with higher availability, Luo et al.
24 [54] improved the model and used it to predict the performance of a TEG system containing one TEG
25 module, taking into account the complete geometry of the TEG system, the temperature dependence
26 of thermoelectric materials, and the topological connection of load resistance. Fig. 19(c) shows the
27 temperature distribution of the whole TEG system and the voltage distribution of the TEG module. By
28 comparing the numerical results of COMSOL coupled solver, COMSOL separate solver, and ANSYS,
29 the influence of ignoring parasitic heat on the output performance of the TEG system was also studied.
30 The prediction process of the COMSOL solver for TEG system performance was the same as that of
31 ANSYS, wherein the fluid-thermal field was computed first, and then the thermal-electric field. It was
32 reported that the neglect of parasitic heat will induce lower predictions of output performance and

1 parasitic internal resistance, and an unreasonable prediction of maximum power point. The
 2 multiphysics model predicted by COMSOL coupled solver was more reasonable because the fluid
 3 field, thermal field, and electric field were calculated simultaneously. The research provides an
 4 effective method to predict the performance of the TEG system in fluid waste heat recovery, which
 5 can take all the actual conditions into account.



6
 7 Fig. 19. Numerical results of the fluid-thermal-electric multiphysics field coupled numerical model obtained by COMSOL.
 8 (a) Velocity and voltage distributions of a simplified TEG system [114]. (b) Fluid velocity contour in channels and voltage
 9 distribution of TEG modules [115]. (c) Temperature distribution of the whole TEG system containing one TEG module
 10 and voltage distribution of the TEG module [54].

11 ii. Transient state

12 Furthermore, the COMSOL platform also provides a transient solver, which can be used to predict
 13 the dynamic response characteristics of the TEG system. However, ANSYS/Thermal-Electric can only
 14 conduct steady-state numerical simulations. Taking the previously developed TEG system as the
 15 research objective, Luo et al. [116] proposed a transient fluid-thermal-electric multiphysics field
 16 coupled numerical model and carried out the numerical simulation by COMSOL software. The
 17 transient governing equations of mass, momentum, and energy in the fluid region of the heat exchanger
 18 and heat sink channels can be expressed as:

19
$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = 0 \quad (95)$$

$$\frac{\partial}{\partial t}(\rho\vec{v}) + \nabla \cdot (\rho\vec{v}\vec{v}) = -\nabla p + \nabla \cdot [\mu(\nabla\vec{v} + \nabla\vec{v}^T)] \quad (96)$$

$$\rho c \frac{\partial T}{\partial t} + \rho c \vec{v} \cdot \nabla T - \nabla \cdot (\lambda \nabla T) = 0 \quad (97)$$

where, t represents the time. Compared with the steady-state CFD model, the transient transport terms were included in the governing equations. Similarly, the $k - \varepsilon$ model can be used to compute the turbulence flow of the fluid region, as represented in Eqs (91)-(92).

As for the solid region, including the heat exchanger, heat sink, and the whole TEG module, the transient energy conservation can be defined by:

$$(\rho c)_m \frac{\partial T}{\partial t} = \nabla \cdot (\lambda_m \nabla T) + \dot{S}_m \quad (98)$$

where, subscript m represents different solid region materials. The first term denotes the transient term of internal energy change, the second term denotes the transient Fourier heat conduction, and the last term \dot{S}_m represents the energy source term. For different solid regions, the source term can be expressed as:

$$\dot{S}_m = \begin{cases} \sigma_p^{-1}(T) \vec{J}^2 - T \vec{J} \cdot \nabla \alpha_p(T) - \frac{\partial \alpha_p(T)}{\partial T} T \vec{J} \cdot \nabla T_p; & \text{p-type thermoelectric unit} \\ \sigma_n^{-1}(T) \vec{J}^2 - T \vec{J} \cdot \nabla \alpha_n(T) - \frac{\partial \alpha_n(T)}{\partial T} T \vec{J} \cdot \nabla T; & \text{n-type thermoelectric unit} \\ \sigma_{co}^{-1} \vec{J}^2; & \text{copper} \\ \sigma_L^{-1} \vec{J}^2; & \text{load resistance} \\ 0; & \text{heat exchanger, heat sink, and ceramic} \end{cases} \quad (99)$$

where, the energy source terms of p-type and n-type thermoelectric legs include Joule heat, Thomson heat, and Peltier heat. Since there is no Seebeck coefficient, only Joule heat is included in the source terms of copper electrodes and load resistance. For the heat exchanger, heat sink, and ceramic plates, there is no energy source because only Fourier heat conduction is involved.

The electric field conservation equations of the transient multiphysics numerical model are the same as those of the steady-state one, which are:

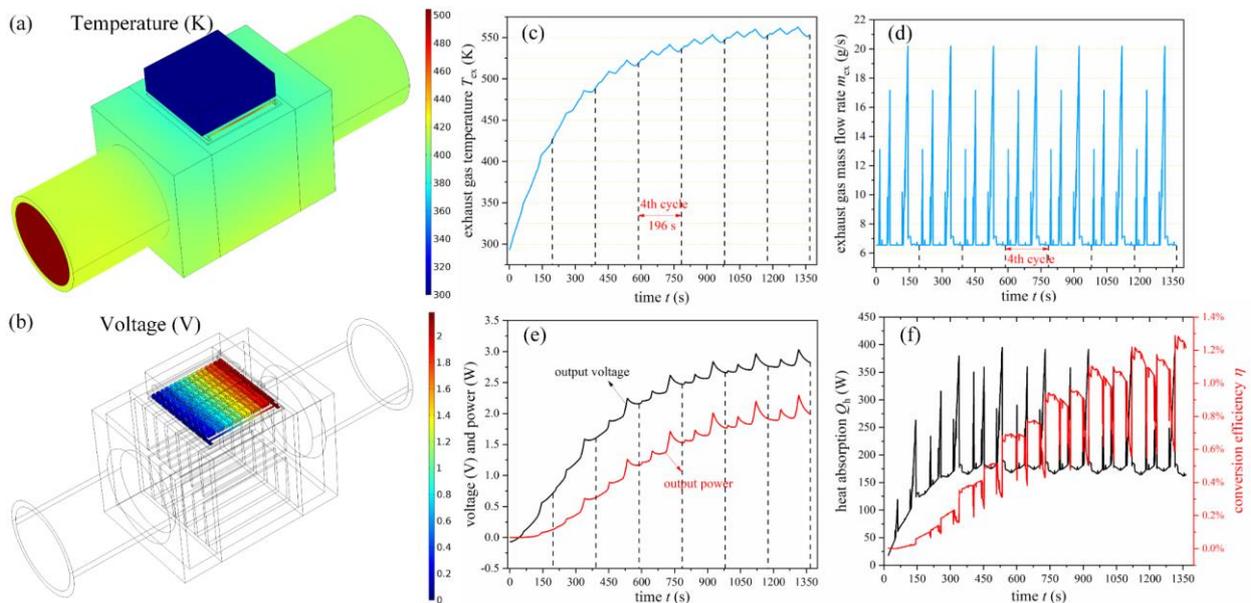
$$\vec{E} = -\nabla \phi + \alpha_{p,n}(T) \nabla T \quad (100)$$

$$\vec{J} = \sigma_m \vec{E} \quad (101)$$

$$\nabla \cdot \vec{J} = 0 \quad (102)$$

Combined with transient thermal boundary conditions, such as transient exhaust temperature and

1 transient mass flow rate, the dynamic response characteristics of a fluid-based TEG system can be
 2 predicted by numerical simulations on the COMSOL platform. To study the dynamic characteristics
 3 of the TEG system applied to vehicles, Luo et al. [116] first simulated the transient exhaust temperature
 4 and mass flow rate of a light-duty vehicle under seven Economic Commission of Europe (ECE) driving
 5 cycles through the vehicle simulation software of ADVISOR, as shown in Fig. 20 (c) and (d), and then
 6 used them as the transient boundary inputs of transient fluid-thermal-electric multiphysics field
 7 coupled numerical model of TEG system. Finally, the dynamic response characteristics of the TEG
 8 system were obtained by numerical simulation of COMSOL. Fig. 20 (e) shows the dynamic output
 9 voltage and output power, and Fig. 20 (f) shows the dynamic heat absorption and conversion
 10 efficiency. The authors performed the complete transient fluid-thermal-electric multiphysics field
 11 coupled numerical simulation for the first time, which provides an effective method to predict the
 12 dynamic performance of the TEG system.



13
 14 Fig. 20. Steady-state numerical results using the average exhaust parameters and transient characteristics of the TEG system
 15 [116]. (a) Temperature distribution and (b) voltage distribution of the whole TEG system predicted by the steady-state
 16 multiphysics numerical model. (c) Transient exhaust temperature and (d) transient exhaust mass flow rate under seven ECE
 17 driving cycles. (e) Dynamic output voltage and output power. (f) Dynamic heat absorption and conversion efficiency.

18 In previous studies, the output performance of an automotive TEG system under a complete driving
 19 cycle was usually predicted by steady-state performance analysis using average exhaust parameters.
 20 To analyze the performance difference between steady-state fluid-thermal-electric multiphysics field
 21 coupled numerical model and transient one. Luo et al. [116] also predicted the steady-state
 22 performance under the conditions of average exhaust temperature and average exhaust mass flow rate

1 of seven ECE cycles. Fig. 20 (a) and (b) show the temperature distribution and voltage distribution of
2 the whole TEG system respectively. The steady-state numerical results were compared with transient
3 numerical results. It was discovered that the total output power predicted by transient numerical
4 simulation is 12.6% lower than that predicted by steady-state numerical simulation. Therefore, in
5 practical situations, the transient fluid-thermal-electric multiphysics field coupled numerical model
6 should be used to predict the dynamic performance of the TEG system, but not replaced by steady-
7 state performance analysis. In addition, some meaningful findings were reported in their study, which
8 brings a new perspective to the dynamic response characteristics of the TEG system.

9 3.2.4 Summary of numerical models for thermoelectric generator system

10 Section 3.2.2 and section 3.2.3 introduce the recent advances in the numerical model for TEG system
11 applied to fluid waste heat recovery, from CFD models to complete fluid-thermal-electric multiphysics
12 field coupled numerical models and from steady-state to transient state, as listed in Table 3. CFD model
13 can accurately simulate the fluid flow in channels of the heat exchanger and heat sink. The heat
14 exchanger is responsible for collecting heat from the hot fluid, and its performance determines the
15 output performance of the entire TEG system. Therefore, the CFD model is widely used in thermal
16 performance and pressure performance analysis of heat exchangers. According to the characteristics
17 of temperature and pressure distribution predicted by the CFD model, the geometric parameters of the
18 heat exchanger can be optimized.

19 Furthermore, the average surface temperature of the hot side and cold side of the TEG module
20 predicted by the CFD model can be used as the temperature boundary conditions of the thermal
21 resistance model and thermal-electric numerical model of the TEG module, and then the output
22 performance of the TEG system can be estimated. In many studies, to reduce the execution time, the
23 TEG module is simplified to a cube for CFD simulation. Generally, the CFD model combined with
24 the numerical model can predict more reasonable results than the CFD model combined with the
25 thermal resistance model. However, the temperature distribution on both sides of the TEG module is
26 not uniform, and the output power predicted by the average surface temperature will be overestimated.

27 Consequently, based on the coupling simulation of ANSYS/Fluent and ANSYS/Thermal-Electric, a
28 fluid-thermal-electric multiphysics field coupled numerical model is proposed, in which the
29 temperature distribution of the TEG module is directly loaded on both sides of the TEG module to
30 predict the output performance of TEG system. The established model can predict the output
31 characteristics of the whole TEG system considering all actual conditions and has high accuracy.
32 Nevertheless, this method first computes the fluid-thermal field and then the thermal-electric field,

1 thus, the effect of parasitic heat (including Joule heat and Peltier heat) on the fluid-thermal field can
 2 not be considered.

3 There are two methods to solve the fluid field, thermal field, and electric field of the TEG system at
 4 the same time: one is to use the Fluent-UDS function to integrate the source term of the energy
 5 conservation equation into the CFD model; the other is to use professional multiphysics software of
 6 COMSOL to solve the fluid-thermal-electric multiphysics field coupled numerical model. On this
 7 basis, the numerical model for the fluid-based TEG system is further improved. However, it is difficult
 8 for Fluent-UDS to deal with the whole TEG module with multiple legs, and the research objective of
 9 existing reports mainly focuses on one pair of the thermoelectric leg. Unlike Fluent-UDS, COMSOL
 10 can perform the complete numerical simulation of the TEG system, which does not require any
 11 simplification and assumption.

12 On the other hand, the fluid-thermal-electric multiphysics field coupled numerical model can be
 13 extended from a steady state to a transient state on the COMSOL platform. In the field of automotive
 14 exhaust waste heat recovery, the research on the transient numerical analysis of TEG systems under
 15 transient driving cycles has been witnessed [116]. As well, the transient fluid-thermal-electric
 16 multiphysics field coupled numerical model can be used for the dynamic performance prediction of
 17 the TEG system in other application scenarios.

18 However, there is no report of transient numerical simulation using other numerical models. For the
 19 coupling simulation of ANSYS/Fluent and ANSYS/Thermal-Electric, it can not solve the transient
 20 fluid-thermal-electric multiphysics field coupled numerical model, because ANSYS/Thermal-Electric
 21 only provides a steady-state solver. For the CFD model, it can be used to conduct the transient CFD
 22 simulation, and the transient characteristics of the average surface temperature on both sides of the
 23 TEG module can be estimated. Furthermore, the transient output performance of the TEG system can
 24 be predicted by the thermal resistance model with temperature data under different time points, and
 25 predicted by the transient thermal-electric numerical model with higher accuracy. It is necessary to
 26 analyze the transient performance of the TEG system because the heat source is not static in an actual
 27 situation. Shortly, there may be a great number of studies on the dynamic performance of the TEG
 28 system using the above modeling approaches. Besides, some efforts need to be made to compare
 29 different transient numerical modeling methods to provide further guidance.

30 Table 3 Recent advances in numerical models for the TEG system applied to fluid waste heat recovery.

| Model name | Steady state or transient state | Solver | Geometry and material simplifications | Features | Sources |
|----------------|---------------------------------|--------------|---------------------------------------|----------------------------|---------|
| CFD model only | Steady state | ANSYS/Fluent | • TEG module is | • performance analysis and | [101- |

| | | | | | |
|---|--------------|---|--|--|--------------------|
| | | | simplified into a cube | optimization for heat exchanger | [105] |
| CFD model only | Steady state | ANSYS/Fluent | <ul style="list-style-type: none"> constant thermoelectric properties TEG module is simplified into a cube constant thermoelectric properties | <ul style="list-style-type: none"> no theoretical output performance prediction performance analysis and optimization for heat exchanger output performance predicted by the average surface temperature difference | [106-109] |
| CFD model combined with thermal resistance model | Steady state | ANSYS/Fluent | <ul style="list-style-type: none"> no geometry simplification temperature-dependent thermoelectric properties | <ul style="list-style-type: none"> using the average temperature of hot side and cold side TEG module predicted by CFD model as boundary conditions output performance predicted by the thermal resistance model | [110] |
| CFD model combined with thermal-electric numerical model | Steady state | ANSYS/Fluent and ANSYS/Thermal-Electric | <ul style="list-style-type: none"> TEG module is simplified into a cube in CFD simulation temperature-dependent thermoelectric properties | <ul style="list-style-type: none"> using the average temperature of hot side and cold side TEG module predicted by CFD model as boundary conditions output performance predicted by the thermal-electric numerical model can not take into account the temperature distribution | [24] |
| Fluid-thermal-electric multiphysics filed coupled numerical model | Steady state | ANSYS/Fluent combined with Fluent-UDS | <ul style="list-style-type: none"> only one p-type leg and one n-type leg are included in the TEG module temperature-dependent thermoelectric properties | <ul style="list-style-type: none"> using Fluent-UDS to define the source terms of the energy conservation equation difficult to handle the whole TEG module containing multiple legs | [111] |
| Fluid-thermal-electric multiphysics filed coupled numerical model | Steady state | ANSYS/Fluent and ANSYS/Thermal-Electric | <ul style="list-style-type: none"> no geometry simplification temperature-dependent thermoelectric properties | <ul style="list-style-type: none"> using the temperature distribution of the TEG module predicted by the CFD model as boundary conditions of the thermal-electric numerical model calculating the fluid-thermal field first and then the thermal-electric field can not take into account the effect of parasitic heat on the fluid-thermal field | [23, 26, 112, 113] |
| Fluid-thermal-electric multiphysics filed coupled numerical model | Steady state | COMSOL | <ul style="list-style-type: none"> only one p-type leg and one n-type leg are included in the TEG module constant thermoelectric properties | <ul style="list-style-type: none"> calculating the fluid field, thermal field, and electric field at the same time open circuit a complete multiphysics numerical model but with some assumptions | [114] |
| Fluid-thermal-electric multiphysics filed coupled numerical model | Steady state | COMSOL | <ul style="list-style-type: none"> ignoring the heat sink and cooling source temperature-dependent thermoelectric properties | <ul style="list-style-type: none"> calculating the fluid field, thermal field, and electric field at the same time open circuit a complete multiphysics numerical model but with some | [115] |

| | | | | |
|---|-----------------|--------|---|--|
| Fluid-thermal-electric multiphysics filed coupled numerical model | Steady state | COMSOL | <ul style="list-style-type: none"> • no geometry simplification • temperature-dependent thermoelectric properties | assumptions <ul style="list-style-type: none"> • considering the load response characteristics • a complete multiphysics numerical model [54] |
| Fluid-thermal-electric multiphysics filed coupled numerical model | Transient state | COMSOL | <ul style="list-style-type: none"> • no geometry simplification • temperature-dependent thermoelectric properties | <ul style="list-style-type: none"> • the firstly developed transient multiphysics numerical model • record high reasonability to predict the dynamic performance of the TEG system [116] |

1 **4. Recommendations for the theoretical analysis of thermoelectric generation**

2 *4.1 Suggestions for improving model accuracy*

3 The theoretical models for predicting the performance of TEGs include the thermal resistance model,
 4 numerical model, and analogy model. To improve the model accuracy, it is suggested to take into
 5 account the temperature-dependent thermoelectric material properties, including the Seebeck
 6 coefficient, thermal conductivity, and electrical resistivity. In detail, the thermal resistance model
 7 widely adopts the average temperature to evaluate the thermoelectric properties, however, this method
 8 may inevitably lead to errors because the thermoelectric properties are highly nonlinear. More
 9 reasonable methods, such as mentioned in Fig. 4, can make the thermal resistance model more accurate.
 10 Besides, the thermal resistances of ceramic plates and copper electrodes should not be ignored. The
 11 thermal-electric numerical model can accurately predict the output performance of TEGs. By
 12 introducing a load resistance into the circuit, the load response characteristics of TEGs can be studied,
 13 which is closer to the actual situation than the open circuit performance analysis. The analogy model
 14 is based on the basic equations of the thermal resistance model, and thus, the suggestions of the thermal
 15 resistance model are also applicable to the analogy model.

16 The theoretical models for predicting the performance of TEG systems can be grouped into two
 17 categories: TEG system directly contacted with the heat source and TEG system for fluid waste heat
 18 recovery. Similarly, the thermal resistance-based analytical model and thermal-electric numerical
 19 model are two commonly used methods to assess the performance of the TEG system directly
 20 contacted with the heat source. Both of them should consider the temperature-dependent
 21 thermoelectric material properties. For the thermal resistance-based analytical model, a complete
 22 thermal resistance network from the heat source to the hot side of the TEG module and from the cold
 23 side of the TEG module to the cooling source should be established. When heat is transferred from a

larger cross-sectional area to a smaller cross-sectional area or from a smaller cross-sectional area to a larger cross-sectional area, the corresponding constricted thermal resistance and spreading thermal resistance should be integrated into the thermal resistance network. In the case of the thermal-electric numerical model, the complete geometry of the heat transfer unit between the heat (cooling) source and the TEG module should be considered in numerical simulation.

There are two theoretical models to predict the performance of the TEG system applied in fluid waste heat recovery: the thermal resistance-based analytical model and the numerical model. With the consideration of the factors mentioned above, the thermal resistance-based analytical model can exhibit high accuracy and reasonability. As for the numerical model, it includes the CFD model, CFD model combined with thermal resistance model, CFD model combined with a thermal-electric numerical model, and fluid-thermal-electric multiphysics field coupled numerical model. There is a great temperature drop from exhaust inlet to exhaust outlet, which leads to the change of material properties of exhaust gas. Therefore, the temperature-dependent material properties of both thermoelectric material and exhaust gas should be featured in the numerical simulation. In addition, geometry simplification is not recommended, because the temperature distribution plays a significant role in the output performance.

4.2 Usage of theoretical models in different scenarios

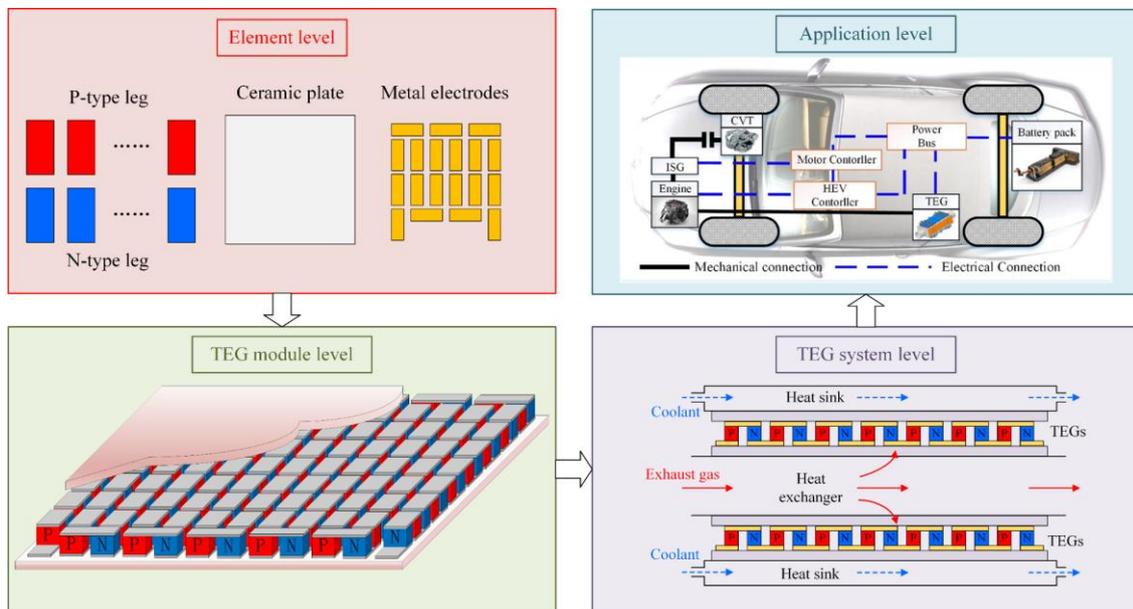


Fig. 21. The development process of the TEG system from element level to application level.

The application of thermoelectric generation technology in specific scenarios needs to go through four levels: element level, TEG module level, TEG system level, and application level, as shown in

1 Fig. 21. From the element level to the TEG module level, it is necessary to determine the optimal
2 parameters of the thermoelectric leg, ceramic plate, and metal electrode, including material and
3 geometrical parameters. To achieve this goal, the thermal resistance model and numerical model of
4 the TEG module are widely adopted. Due to the unavoidable simplification and assumptions of the
5 thermal resistance model, its model accuracy is worse than the numerical model. However, the thermal
6 resistance model can quickly obtain the output performance under different parameters, which is
7 suitable for the preliminary performance evaluation, structural design, and performance optimization
8 of TEG components before manufacturing. The numerical model needs more calculation time than the
9 thermal resistance model, but it can take all actual conditions into account. After the preliminary
10 structural design of the TEG module is obtained, the numerical model can be used for further
11 performance optimization to determine the final design scheme. The analogy model has the advantage
12 of transient simulation and coupling simulation with the energy recovery circuit. It is suitable for the
13 design and performance analysis of the energy recovery circuit, especially the maximum power point
14 tracking (MPPT) circuit.

15 Similarly, from the TEG module level to the TEG system level, the thermal resistance-based
16 analytical model is suitable for the preliminary performance analysis and structural design of the TEG
17 system. Furthermore, to determine the optimal parameters and the final design schema of the TEG
18 system, numerical models should be adopted to study the effect of different parameters on the output
19 performance of the TEG system. For the TEG system applied in fluid waste heat recovery, the CFD
20 model can be used to optimize both the thermal and pressure performance of the heat exchanger.
21 However, CFD models are not recommended to be used to predict the performance of the TEG system
22 under actual conditions, because the temperature distribution and other factors can not be considered
23 in the CFD simulation. More accurately, the fluid-thermal-electric multiphysics field coupled
24 numerical model should be used to predict the output characteristics, further optimize the performance,
25 and determine the final design of the whole TEG system.

26 From the TEG system level to the application level, the transient characteristics of the heat source
27 will affect the output performance of the TEG system. It is recommended to use the transient fluid-
28 thermal-electric multiphysics field coupled numerical model to study the dynamic response
29 characteristics of the TEG system under practical transient boundary conditions. And then, the
30 obtained dynamic output voltage and output power can guide the use and the management of electricity
31 produced by the TEG system.

1 5. Conclusions

2 In recent years, researchers have been developing theoretical models that can accurately predict the
3 performance of thermoelectric generators (TEGs) and TEG systems. Compared with the experimental
4 method, a reasonable theoretical model can reduce the cost of prototype development and save time.
5 Therefore, the purpose of this work is to perform a comprehensive review of theoretical models in
6 recent literature. TEG is the basic power generation unit of the TEG system, and the theoretical model
7 of the TEG system can be regarded as an extension of the model of TEG. For this reason, the theoretical
8 models of TEGs are reviewed first, and then the theoretical models of the TEG system.

9 With regards to the theoretical models of TEG, the thermal resistance model is the earliest used
10 model to predict TEG performance, which is based on the balance of energy. By considering the
11 temperature dependence of thermoelectric material and the thermal resistances of other components,
12 the accuracy of the thermal resistance model can be further improved. However, the numerical model
13 of TEG can take into account all actual conditions and predict more reasonable results than the thermal
14 resistance model. In particular, some commercial finite element software programs, such as ANSYS
15 and COMSOL, have integrated the governing equations of TEG into the software package, which
16 promotes the utilization of numerical models among researchers. Moreover, based on the analogy
17 between thermal circuit and electric circuit, the analogy model of TEG is developed on the platform
18 of SPICE software. The analogy model facilitates the coupling simulation with the energy recovery
19 circuit, which exhibits the potential use in the field of TEG recovery circuit development.

20 With regards to the theoretical models of TEG systems, they are classified into two groups:
21 theoretical models of TEG systems directly contacted with heat source and theoretical models of TEG
22 systems for fluid waste heat recovery. In the former case, the theoretical models of TEG can be applied
23 to predict its performance by adding the thermal resistances and energy conservation equations of heat
24 transfer units into the thermal resistance model and numerical model, respectively. In the case of the
25 TEG system for fluid waste heat recovery, the thermal resistance-based analytical model can also be
26 used to preliminarily evaluate the performance of the TEG system. To make the results more accurate,
27 it is suggested to adopt the fluid-thermal-electric multiphysics field coupled numerical model.

28 On the other hand, different theoretical models have different application scenarios. Although
29 numerical models can predict reasonable results, but suffer from the long execution time, especially
30 for the TEG system applied in fluid waste heat recovery. On the contrary, thermal resistance models
31 can quickly obtain the performance of TEG and TEG systems under different parameters. Therefore,
32 thermal resistance models are suitable for preliminary performance evaluation, structural design, and

1 performance optimization of TEGs and TEG systems before manufacturing. And numerical models of
2 TEGs and TEG systems are suitable for further performance optimization to determine the final design
3 scheme and the performance prediction under actual conditions. Moreover, the analogy model is
4 convenient for the design of the energy recovery circuit, while the CFD model is suitable for the
5 optimization of the heat exchanger. Combined with the advantages of each model, the development
6 time of the TEG and TEG system can be shortened, and ensure optimal performance at the same time.

7 Finally, the transient thermal-electric numerical model of the TEG module and the transient fluid-
8 thermal-electric multiphysics field coupled numerical model have been developed in recent research,
9 which can take the dynamic characteristics of the heat source into account. The transient performance
10 analysis of TEGs and TEG systems will remain a hot research field in the upcoming years.

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