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Research on Integration of an Automotive Exhaust-Based Thermoelectric Generator and a Three-Way Catalytic Converter

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A key research topic related to thermoelectric generators (TEGs) for automotive applications is to improve their compatibility with the original vehicle exhaust system, which determines the quality of the exhaust gas treatment and the realization of energy conservation and emission reduction. A new TEG integrated with a three-way catalytic converter (CTEG) by reshaping the converter as the heat exchanger is proposed. A heat-flux coupling simulation model of the integrated TEG is established at the light-off stage of the original three-way catalytic converter (TWC). Temperature distribution maps of the integrated heat exchanger, thermoelectric modules, and cooling-water tank are obtained to present the process of energy flow among the parts of the CTEG. Based on the simulation results, the output power of the CTEG is calculated by a mathematical model. A minimum output power of 31.93 W can be obtained by conversion when the TWC starts working at steady conditions. Theoretically, this case study demonstrates the great potential for use of CTEGs in vehicles.

Key words: TEG, three-way catalytic converter, CTEG, temperature distribution map, output power

List of Symbols

Variables

A	Cross-sectional area (m^2)
l	Thermocouple length (m)
P	Output power (W)
r	Electrical resistance (Ω)
T	Temperature (°C)
U	Voltage (V)
X	Number of thermocouples

Greek Symbols

α	Seebeck coefficient (V/K)
ρ	Electrical resistivity (Ω m)

Subscripts

c	Cold side
h	Hot side
L	Load
m	Mean/average
max	Maximum
MD	Thermoelectric module
n	n-Type thermocouple
p	p-Type thermocouple

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INTRODUCTION

Currently, approximately 40% of the fuel energy is lost in the exhaust gas.[1] Automobile exhaust heat recovery not only is beneficial for reuse of waste heat energy but can also improve the engine fuel economy. Thermoelectric technology offers the possibility of recovering exhausted heat. Based on the Seebeck effect of thermoelectric materials, an automobile exhaust waste heat thermoelectric power generator can convert thermal energy into electric energy.[2]

An automobile exhaust waste heat thermoelectric power generation system consists of a heat exchanger, a cooling-water tank, and a clamping device.[3] Thermoelectric modules made of semiconductor material are placed between the heat exchanger and the cooling-water tank, enabling

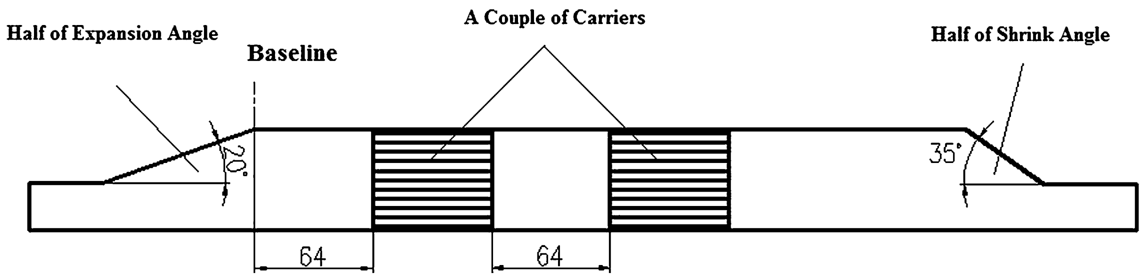

Fig. 1. Schematic diagram of integrated heat exchanger.

conversion of the temperature difference between the hot and cold sides into power.[4] Liu et al. constructed various heat exchangers, including maze-shaped, fishbone-shaped,[5] and chaos-shaped devices,[6] to analyze their thermal performance. As the cold side, Deng et al. proposed a TEG water-cooling unit inserted into the engine cooling system (called an "integrated cooling system" herein).[7]

However, attaching such a thermoelectric generator (TEG) directly into the automotive exhaust system may conflict with the target of lightweight automobiles and affect the layout of the overall system.[8] The TWC, a device for automotive exhaust purification, carries out redox reactions on its carrier. As a result, the temperature on its surface is extremely high. To take advantage of this considerable heat energy, a new TEG integrated with the converter (CTEG) is proposed in this work. A heat-flux coupling simulation model of the CTEG is established at the light-off stage of the catalytic converter. Temperature distribution maps of the integrated heat exchanger, thermoelectric modules, and cooling-water tank are obtained to present the process of energy flow among the parts of the CTEG. Based on the average temperatures of the hot side and cold side of the thermoelectric modules obtained from the temperature distribution simulation, a mathematical model for the CTEG output power is also established in Simulink. Extra power can be obtained by such conversion without affecting the light-off characteristics of the TWC.

CTEG STRUCTURE

To purify automobile exhaust, the TWC is an indispensable component of the automotive exhaust system. To balance the purification performance of the TWC and the power generation efficiency of the new TEG, two factors must be considered when designing the CTEG. One should avoid causing too many adverse effects on flow characteristics such as the uniformity and flow resistance to the carrier. Besides, most widely used thermoelectric modules are block-shaped and cannot be bent, and a smooth surface with a uniform temperature distribution is essential for the heat exchanger to provide better working conditions for the thermoelectric modules.

Yang[9] optimized the structure of a TWC based on flow characteristics including the expansion angle of

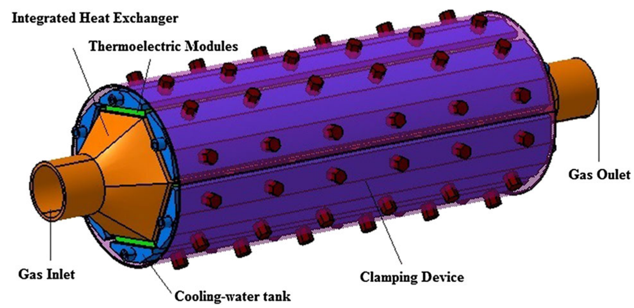

Fig. 2. Three-dimensional model of CTEG.

the inlet tube, the convergence angle of the outlet tube, the installation location of the carrier, and the spacing of the coupling carriers. As shown in Fig. 1, the TWC adopted in this paper has an expansion angle of 40° and a convergence angle of 70°. To achieve better performance, a couple of carriers are used in the model as well, the first part of which deviates from the baseline by 64 mm; the distance between the two carriers is designed as 64 mm. Taking the thermoelectric modules into consideration, modification of the TWC to a hexahedral CTEG is proposed, as shown in Fig. 2. In addition, a separate clamping force is applied on each module to ensure reliable contact between the hot side and cold side.

SIMULATION OF THE HEAT FLUX BETWEEN PARTS OF THE CTEG

Typical software for analyzing turbulent mechanics, i.e., computational fluid dynamics X, was adopted to simulate the heat flux among the parts of the CTEG. Temperature distribution maps of the integrated heat exchanger, the hot side and cold side of the thermoelectric modules, and the cooling-water tank were obtained.

Boundary Condition Setting

One-sixth of the hexagonal-prism-shaped heat exchanger was taken as the object of study due to its symmetry; the whole exchanger can be obtained based on the axial symmetry of the inlet and outlet.

Considering the light-off working condition of the TWC, the average flow rate of exhaust is 15 L/s and the temperature is 250°C. The inlet boundary

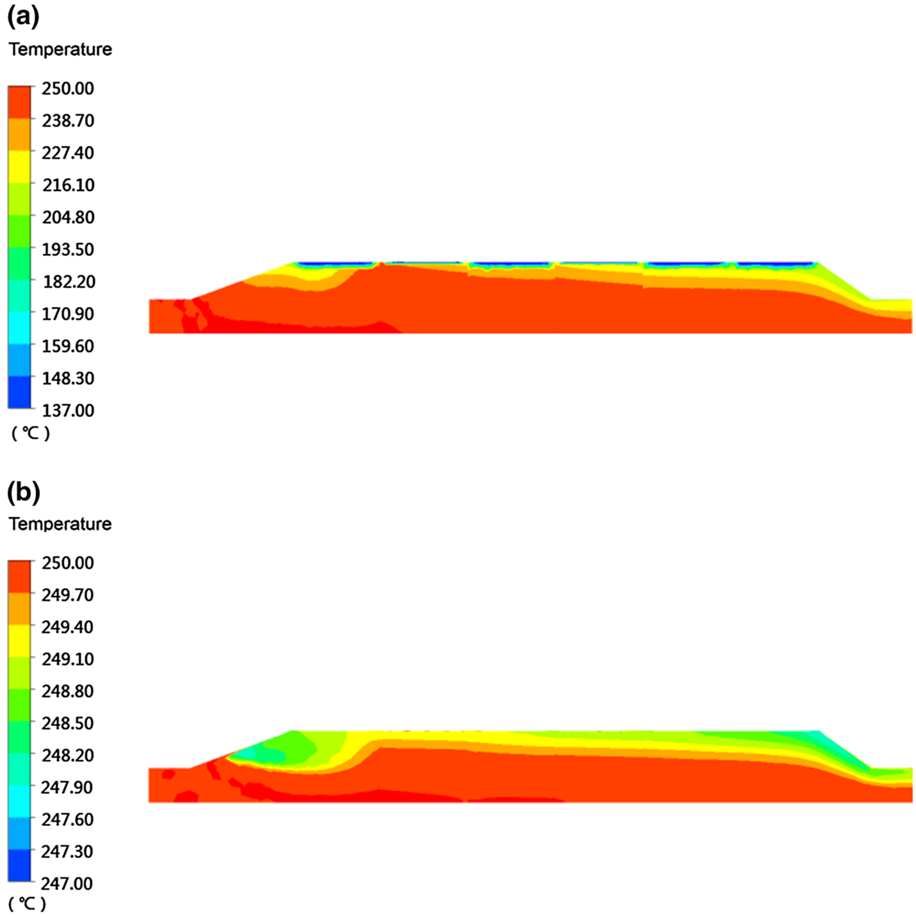

Fig. 3. Temperature distribution maps of the internal exhaust gas of (a) the CTEG heat exchanger and (b) the original TWC.

conditions of the CTEG are set as the former. The exit of the CTEG is connected to the entrance of the rear muffler, whose exit is connected to atmosphere, so the pressure at the exit of the exchanger is approximately standard atmospheric pressure, and so the back pressure at the exit can be set to 0 Pa. With the water-cooling unit of the CTEG inserted into the engine cooling system, the inlet temperature of the cooling-water tank is set to 67°C. The average inlet flow rate is set to 8 L/min, close to that of the traditional TEG device. The pressure at the outlet can also be set to 0 Pa. The materials of the heat exchanger, cooling-water tank, and carriers were defined as steel with thickness of 3 mm, aluminum with thickness of 2 mm, and common ceramic materials, respectively. The thermoelectric modules used in this study were made of Bi_2Te_3, so a new material was defined in the library. Additionally, the coefficient of convective heat transfer between the outer surface of the exchanger and the air was set to 15 W/(m^2 K).

To simplify the model, various assumptions were also made. Gas in this system is considered to be incompressible, and the flow to be fully turbulent. The molecular viscosity can be neglected in the simulation model, as well as heat radiation and the thermal contact resistance because of the reliable contact between the different parts of the CTEG. Regardless of the complicated working situation of the TWC at the light-off stage, all of the chemical reactions were not taken into account.

Simulation Results and Discussion

The temperature distribution maps of the internal exhaust gas of the CTEG heat exchanger and the original TWC are shown in Fig. 3a, b. The mean temperature of the exhaust gas in the CTEG is 239°C, lower than that of the original TWC by 10°C due to the heat absorption by the thermoelectric modules placed on its surface. When the temperature decreases, the catalytic converter may not ignite successfully. Based on the mean temperature of the internal exhaust gas and the carriers, different inlet temperature conditions were also considered, as shown in Fig. 4. When the temperature of the inlet reaches 260°C, the device works normally as a TWC and a TEG at the same time.

Figure 5 shows the interface temperature distribution map of the integrated CTEG heat exchanger when the inlet temperature was adjusted to 260°C. Along the exhaust flow direction (left to right), a temperature gradient is present on the surface of the integrated heat exchanger. With the exhaust flowing from the expansion tube into the hexagonal channel, the cross-sectional area of the channel gradually expands and the temperature drops to the outlet, where it is 225°C. Because of the heat absorption by the thermoelectric modules, the temperatures of the contact areas between the modules and the CTEG are significantly low.

Based on the Seebeck effect, the output power of the CTEG was determined from the temperature difference between the hot side and cold side of the thermoelectric modules directly. The temperature distribution maps of the hot side and cold side of the thermoelectric modules are shown in Fig. 6a, b, in which the modules are labeled as no. 1 to no. 6 from top to bottom. Affected by the coupling carriers, the mean temperatures of modules no. 2 and no. 4 are higher than the others, being 132°C and 127°C, respectively. The temperature of the last module is the lowest because of the impact of the cooling water. For the cold side of the modules, which is in contact with the cooling-water tank surface, the temperature is lower and more uniform overall, as shown in Fig. 6b. The temperature rises by 4°C from module no. 1 to no. 6. Figure 6c shows the temperature distribution map of the cooling-water tank, which is in good agreement with the cold side of the thermoelectric modules.

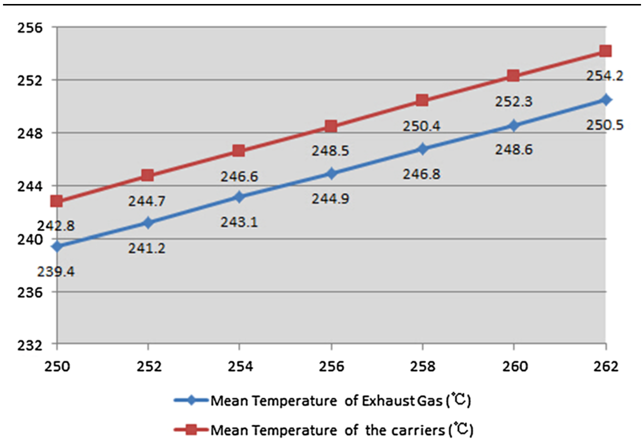

Fig. 4. Mean temperature of internal exhaust gas and carriers for different inlet conditions.

ANALYSIS OF THE OUTPUT PERFORMANCE OF THE CTEG

In this work, low-temperature modules made of Bi_2Te_3, which are capable of withstanding temperatures below 300°C, were adopted. The output power of the thermoelectric module was determined from the performance parameters of the semiconductor material, such as the Seebeck coefficient, electrical resistivity, and thermal conductivity.

Performance Parameters of the Thermoelectric Module

On the basis of extensive testing of thermoelectric materials, Hi-Z Company found that the performance parameters of p-type and n-type thermoelectric materials, including the Seebeck coefficient, electrical resistivity, and thermal conductivity, are dependent on temperature. They obtained the fitting functions between these parameters and the mean temperature of the thermoelectric modules.[10] Then the open-circuit voltage of a single p–n thermocouple (U_{in}) can be calculated based on the Seebeck effect as shown in Eq. 1.

$$U_{\mathrm{in}} = \alpha_{pn}(T_{\mathrm{h,m}} - T_{\mathrm{c,m}}), \tag{1}$$

where α_{pn} is the relative thermoelectric Seebeck coefficient, i.e., the difference between α_p and α_n.

The internal resistance of a single thermocouple, i.e., r_{in}, is given by Eq. 2. The output voltage U_{L} with a load resistance connected in the circuit is calculated by Eq. 3.

$$r_{\mathrm{in}} = \frac{\rho_n l_n}{A_n} + \frac{\rho_p l_p}{A_p}, \tag{2}$$

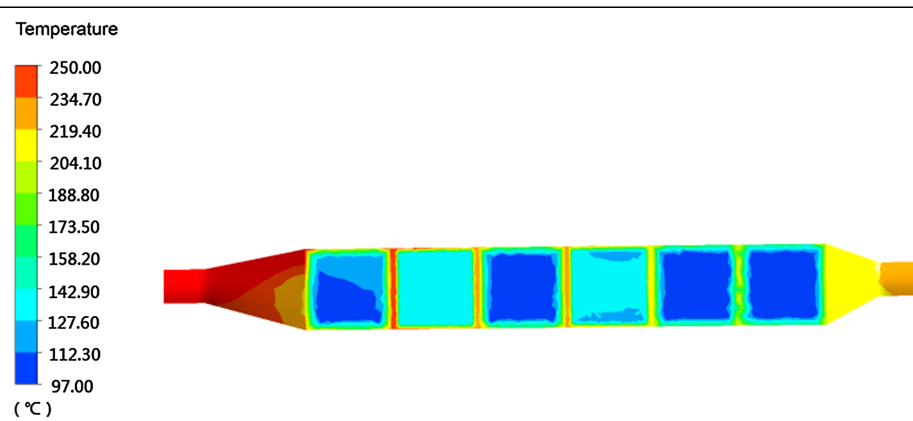

Fig. 5. Interface temperature distribution map of integrated heat exchanger of CTEG.

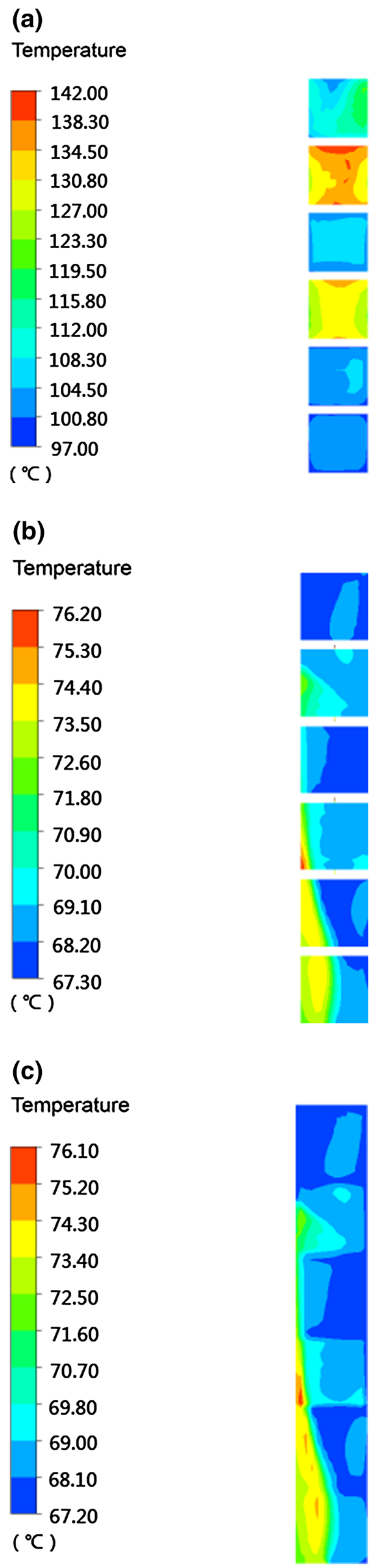

Fig. 6. Temperature distribution maps of (a) hot side and (b) cold side of thermoelectric modules and (c) cooling-water tank.

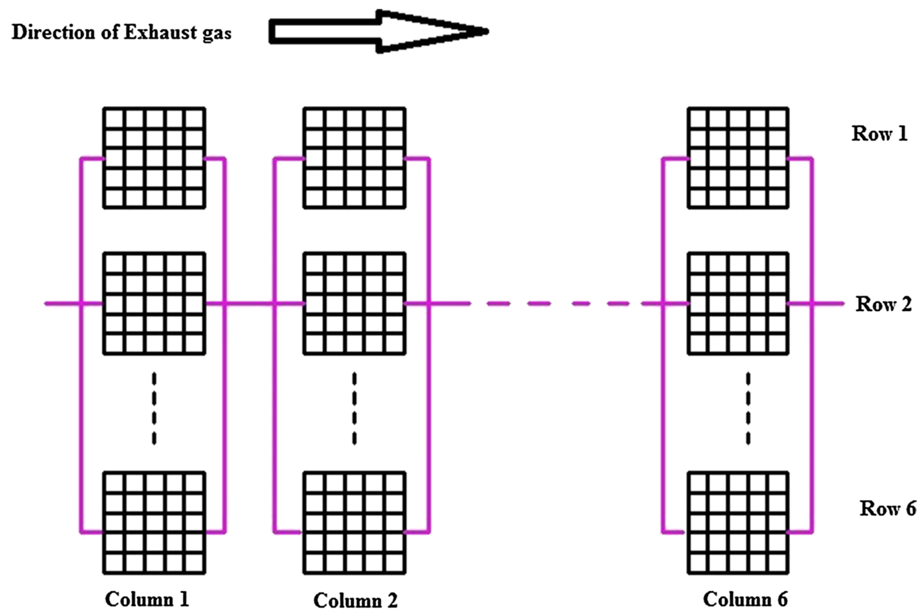

Fig. 7. Topological graph of the thermoelectric generator modules.

$$U_{\mathrm{L}} = \frac{r_{\mathrm{L}}}{r_{\mathrm{L}} + r_{\mathrm{in}}} U_{\mathrm{in}}. \quad (3)$$

When the load resistance is equal to the internal resistance, the output power reaches its maximum value of

$$P_{\max} = \frac{U_{\mathrm{in}}^2 r_{\mathrm{L}}}{(r_{\mathrm{L}} + r_{\mathrm{in}})^2} = \frac{U_{\mathrm{in}}^2}{4r_{\mathrm{in}}}. \quad (4)$$

The thermoelectric module mentioned above is composed of several *p–n* thermocouples in series. On the basis of the performance parameters of the thermocouples, the open-circuit voltage, internal resistance, and maximum output power of the thermoelectric module are given by Eqs. 5, 6, and 7.

$$U_{\mathrm{MD}} = X\alpha_{pn}(T_{\mathrm{h,m}} - T_{\mathrm{c,m}}), \quad (5)$$

$$r_{\mathrm{MD}} = Xr_{\mathrm{in}}, \quad (6)$$

$$P_{\mathrm{MD,max}} = \frac{U_{\mathrm{MD}}^2}{4r_{\mathrm{MD}}} = XP_{\max}. \quad (7)$$

Topology of Modules

To improve the consistency and uniformity of the module outputs, the rule for electrical connection is that modules of the same output capacity, that is, with resistance and open-circuit voltage equal or very close to one another, are connected in parallel, and then connected with the modules of other levels in series.[11] To describe the topology of the modules, they are labeled using two-dimensional coordinates (row, column). Modules arranged along the flow direction of the exhaust gas are defined as row 1, 2, … m (m = 6), and modules arranged around the hexahedral heat exchanger are labeled as column 1, 2, … n (n = 6). Considering the structure of the CTEG used in this paper, the topology of the modules is shown in Fig. 7.

The open-circuit voltage and internal resistance of the CTEG are as follows:

$$U_{\mathrm{CTEG}} = U_{\mathrm{col\_1}} + U_{\mathrm{col\_2}} + \cdots + U_{\mathrm{col\_6}}, \quad (8)$$

$$r_{\mathrm{CTEG}} = r_{\mathrm{col\_1}} + r_{\mathrm{col\_2}} + \cdots + r_{\mathrm{col\_6}}, \quad (9)$$

where $U_{\mathrm{col\_1}}$ and $r_{\mathrm{col\_1}}$ are the open-circuit voltage and internal resistance of the column 1 thermoelectric modules in parallel groups, and so on. Similarly, when the internal resistance of the CTEG is equal to the load resistance, the output power of the CTEG reaches its maximum of

$$P_{\mathrm{CTEG,max}} = \frac{U_{\mathrm{CTEG}}^2}{4r_{\mathrm{CTEG}}^2}. \quad (10)$$

Modeling and Results

According to the above parameters, a mathematical model for the output power of the whole CTEG was built in Simulink as shown in Fig. 8.

The inputs of the model are the temperatures of the cold side and hot side of the thermoelectric

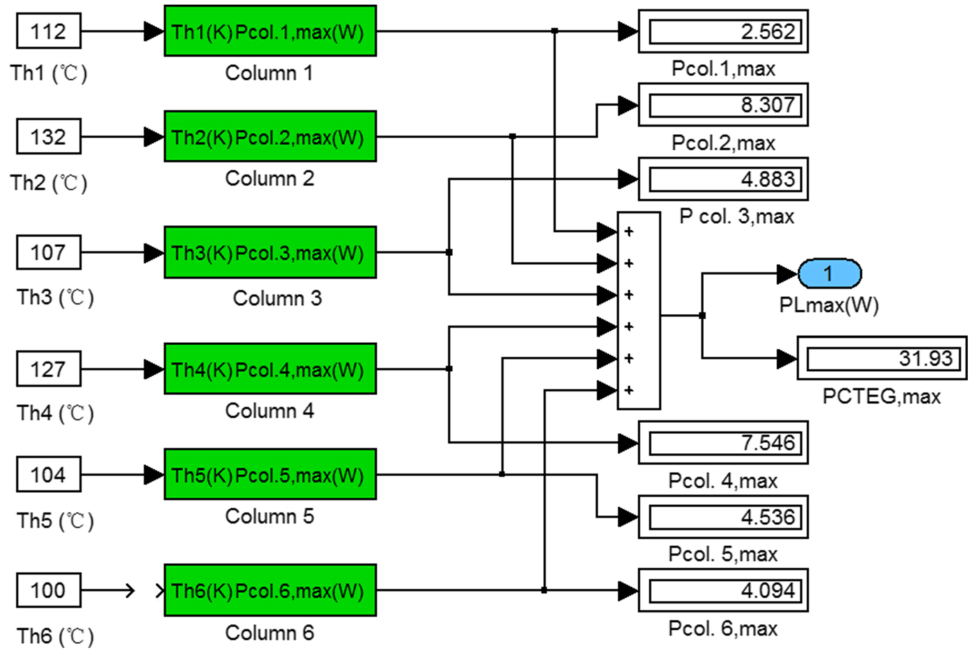

Fig. 8. Simulink mathematical model of output power for CTEG.

modules. Assuming that the modules in each column have the same parameters, it is reasonable to select the mean temperature of the modules for each side. Based on the simulation results, the hot-side temperatures of the modules are 112°C, 132°C, 107°C, 127°C, 104°C, and 100°C, in turn. For the cold side, whose temperature distribution is uniform on the whole, a mean temperature of 67°C was set. Based on the calculation using the mathematical model, the output power of the CTEG was obtained as 31.93 W.

CONCLUSIONS

To improve the compatibility with the original vehicle exhaust system, a new TEG integrated with the TWC, i.e., a CTEG, is proposed in this paper. According to the simulation results, the light-off temperature increases slightly by 10°C, due to the heat absorption by the thermoelectric modules placed on the surface of the CTEG. The process of energy flow among the various parts of the CTEG is presented using a heat-flux coupling simulation model. Based on the temperature difference between the two sides of the thermoelectric modules, a mathematical model for the output power is built. Without affecting the air purification function of the CTEG as a catalytic converter, extra power of 31.93 W is obtained through recovery of exhaust heat energy.

The current study focuses on the light-off stage of the TWC, and the minimum output power of the CTEG is obtained. In fact, the heat energy on the surface of the TWC is much greater after light-off, when the converter is exothermic. In that case, more heat will be used for generation and $CoSb_3$ thermoelectric modules, which can bear higher temperatures, will be applied. The Economic Commission for Europe (ECE) operating cycle, characterized by low vehicle speed, low load, and low exhaust temperature, will also be used to test the CTEG on vehicles in future study.

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REFERENCES

1. J. Yang and F.R. Stabler, *J. Electron. Mater.* 38, 1245 (2009).
2. D.T. Crane, C.R. Koripella, and V. Jovovic, *J. Electron. Mater.* 41, 1524 (2012).
3. J. Vazquez, *Proceedings of 7th European Workshop on Thermoelectrics*, Pamplona, Spain, 2002.
4. D.M. Rowe and G. Min, *J. Power Sources* 73, 193 (1998).
5. Y.D. Deng and X. Liu, *J. Electron. Mater.* 42, 1634 (2013).
6. X. Liu, C.G. Yu, and S. Chen, *J. Electron. Mater.* 43 (2014) (in press).
7. Y.D. Deng, X. Liu, and S. Chen, *J. Electron. Mater.* 43 (2014) (in press).
8. S.E. Votzs, C.R. Morgan, and D. Liederman, *Ind. Eng. Chem. Res.* 12, 194 (1973).
9. L. Yang and Y. Yao, *Auto Eng.* 11, 43 (2010).
10. D.T. Allen and D. Nathan, Space Technology and International Forum (Albuquerque, NM, Feb 2004).
11. R. Quan and S.H. Quan, *J. Shanghai Jiaotong Univ.* 1006 (2011).