Comparison of Approaches to Thermoelectric Modules Mathematical Optimization

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Abstract

For mathematical simulation and optimization of thermoelectric (TE) modules different methods are applied. The paper numerically compares two most rigorous ones and shows that these approaches provide close results.

TE pellets behaviour is described by the thermal conductance equation with temperature-dependent parameters. The usage of algebraic rate equations with effective parameters requires solving the thermal conductance equation as well. Usually a simulation of a pellet in operation is not sufficient as it is necessary to cope with the problem of optimization, commonly taking maximum coefficient of performance as a criterion. The Optimal Control Theory, based on the Pontriaguin maximum principle, provides an all-purpose approach to the problem. This paper proves that the method of effective parameters applied to TE module optimization yields a fairly good and reliable mathematical alternative.

Introduction

For a long time all calculations for TE modules have been carried out applying an elementary model supposing TE parameters to be independent of temperature (see, for example, [1]). Within this approach all the initial equations are written for a TE pellet (TE element) and simple algebraic expressions for its optimal modes of operation are found. This model has advantages of unsophistication and ostensive consistency.

Some complications of this approach involve effective TE parameters [2,3] (we shall refer to this approach as the *method of effective parameters*) that allow precise description of thermal balances on the ends of a pellet, preserving unsophisticated consistency as the main advantage.

On the other hand TE parameters temperature dependences were most stringently taken into account by the *Pontriaguin maximum method* [4,5]. This method gives mathematically formalized recipes for optimal solutions because the relations between TE parameters and results are not straightforward. This method is initially expressed in terms of a TE couple, not a pellet, which is an advantage. For this paper the derivation of the method equations has been redone and the result obtained and applied differs from the one offered earlier, for example in paper [4].

Let us compare the two approaches.

Basic Equations

In one dimension a TE pellet operation is described by the thermal conductance equation with temperature-dependent parameters:

$$\frac{d}{dx}\left(\kappa\frac{dT}{dx}\right)+\frac{j^2}{\sigma}\pm jT\frac{d\alpha}{dx}=0\,, \qquad (1)$$

Here $T(x)$ is temperature along a pellet, σ is electrical conductivity, κ is thermal conductivity, α is the Seebeck coefficient, and j is electric current density. The double sign before the first term is defined by the system of axes.

For a numerical solution of Eq. (1) it is convenient to transform this second-order equation into a system of two one-order equations (2) relating the independent variables $T(x)$ and the value proportional to $\pm\kappa(T)\frac{dT(x)}{dx}+\alpha(T)jT(x)$. This choice of variables is reasoned as the second variable is proportional to the pellet cooling capacity Q_0 on the one end and the heating capacity Q on the other [4].

$$\begin{aligned}\frac{dT}{dx}&=\frac{j}{\kappa}q-\frac{j\alpha T}{\kappa},\\ \frac{dq}{dx}&=-\frac{j}{\sigma}+\frac{\alpha j}{\kappa}q-\frac{j\alpha^2}{\kappa}T,\end{aligned}\,, \qquad (2)$$

where $q=\dfrac{\kappa\frac{dT}{dx}+\alpha jT(x)}{j}$. Here the TE pellet section and length are supposed to equal unity and the origin of coordinates corresponds to the pellet hot end. Then its cold end coordinate is unity. We consider electric current density $j>0$, irrespective of the current direction and the Seebeck coefficient related to the junction material $\alpha\geq 0$, irrespective of the true sign. Eqs. (2) are to be solved at the boundary conditions $q(0)=Q/sj$, $q(1)=Q_0/sj$, where s is the pellet section.

For the Cauchy problem it is necessary to set T and q on one end of the pellet. In all programming languages there is standard software for solving such-type problems (for example, see [6]). In TE problems the temperatures T_h and T_c are usually given. To reduce this task to the Cauchy one, the method of "shooting" can be applied [6]. Interpolating software for taking into account experimental TE parameters temperature dependences are also available. Thus, the thermal conductance equation solution is not too much of a challenge for computer-aided engineering.

The main problem is in optimizing the solutions obtained. As a rule it is necessary to find the optimal electric current

j_{opt} such that the heating coefficient μ be minimal possible:

$$\mu = \frac{Q}{Q_0} = \frac{q(0)}{q(1)}, \qquad (3)$$

Here due to the paper size restriction, we consider the problem within one cascade.

Pontriaguin Maximum Method

First we consider optimization (3) by the Pontriaguin maximum method [7]. The variables ψ_1 and ψ_2 conjugated to T and q are introduced and Hamiltonian H is written:

$$H = \psi_1 \frac{dT}{dx} + \psi_2 \frac{dq}{dx} \qquad (4)$$

From the Hamilton function (4) Equations for ψ_1 and ψ_2 are found:

$$\frac{d\psi_1}{dx} = -\frac{\partial H}{\partial T}, \; \frac{d\psi_2}{dx} = -\frac{\partial H}{\partial q}. \qquad (5)$$

The solution minimizing (3) is sought. The variables ψ_1 and ψ_2 boundary conditions are found from transversality requirements. If necessary, additional restrictions on pellet operation are taken into account. In this case the number of equations is doubled, which, however, does not create any specific difficulties. Equating the Hamilton function to zero in any point (.) x, it is possible to find the optimal control. In TE cooling problems, the optimal control is commonly expressed by one parameter j_{opt}, which can be written as:

$$j_{opt} = \frac{\psi_2 \alpha T\big|_0^1}{\int_0^1 \left[\left(\frac{\psi_2}{\sigma}(1-ZT) - \frac{q\psi_1}{\kappa}\right) + \frac{\psi_2 T}{\kappa}\frac{d\alpha}{dT}(q-\alpha T)\right]dx} \qquad (6)$$

where $Z = \frac{\alpha^2 \sigma}{\kappa}$ is Figure-of-Merit. It is important that Eq. (5) obtained and used for calculations in this work differs from the one given earlier in paper [4].

As this method is applied for a TE couple, the variables T and q are introduced for each type of conductivity; therefore in Eq. (4) there appears a sum over n- and p-types and the number of ψ_1 and ψ_2 doubles. Eqs. (5) are written separately for each conductivity type and in Eq. (6) summarizing is carried out both in the numerator and in the denominator.

Method of Effective Parameters

Let us consider the method of effective parameters. For temperature-independent TE parameters there are well known approaches for finding j_{opt} [1]. For temperature-dependent TE parameters the following heat rate equations for the pellet ends can be written [2,3]:

$$\begin{aligned} &\alpha_c T_c j - \frac{1}{2} j^2 \rho_c - k_{eff}\Delta T = q(1), \\ &\alpha_h T_h j + \frac{1}{2} j^2 \rho_h - k_{eff}\Delta T = q(0), \end{aligned} \qquad (7)$$

Here $\Delta T = T_h - T_c$. The values $\alpha_h, \alpha_c, \rho_h, \rho_c$ for a unity length and section of a pellet are obtained as:

$$k_{eff} = \bar{\kappa} = \frac{1}{\int_0^1 \frac{dx}{\kappa(T_x)}} \qquad (8)$$

$$\alpha_c = \alpha(T_c) + \frac{\bar{\kappa}}{T_c}\int_0^1 T_y \frac{d\alpha(T_y)}{dT}\frac{dT}{dy}dy \int_y^1 \frac{dx}{\kappa(T_x)} \qquad (9)$$

$$\alpha_h = \alpha(T_h) - \frac{\bar{\kappa}}{T_h}\int_0^1 T_y \frac{d\alpha(T_y)}{dT}\frac{dT}{dy}dy \int_0^y \frac{dx}{\kappa(T_x)} \qquad (10)$$

$$\rho_c = 2\bar{\kappa}\int_0^1 \rho(T_y)dy \int_y^1 \frac{dx}{\kappa(T_x)} \qquad (11)$$

$$\rho_h = 2\bar{\kappa}\int_0^1 \rho(T_y)dy \int_0^y \frac{dx}{\kappa(T_x)} \qquad (12)$$

These equations differ from those offered in [8] as they are precise and not restricted by the assumption of the heat flux along the pellet being constant. Among five parameters (8)-(12) three are independent, as α_c and α_h are related as:

$$\alpha_h T_h - \alpha_c T_c = \bar{\alpha}\Delta T = \int_{T_c}^{T_h} \alpha(T)dT, \qquad (13)$$

whereas ρ_c and ρ_h are:

$$\rho_h + \rho_c = 2\bar{\rho} = 2\int_0^1 \rho(T_x)dx, \qquad (14)$$

For calculating these parameters it is necessary to solve system (1) and then pass over to integrals (8) – (12). It is worth remembering that Eqs. (7) give the precise description of the pellet behaviour. The Thomson effect results in the inequality of the values α_c and α_h, and the fact that the Joule heat fluxes are divided not equally between the pellet ends results in the difference of the values ρ_c and ρ_h.

The optimal electric current for the pellet with given values T_h and T_c is written as:

$$j_{opt} = \frac{\bar{\alpha}\Delta T}{\bar{\rho}(M_{eff} - 1)}, \qquad (15)$$

where M_{eff} is equal to:

$$M_{eff} = \sqrt{1 + ZT_{eff}}, \; Z = \frac{\bar{\alpha}^2}{\bar{\rho}\bar{\kappa}}, \qquad (16)$$

The effective temperature value is given by:

$$T_{eff} = \frac{T_c \frac{\alpha_c}{\alpha} \frac{\rho_h}{\rho} + T_h \frac{\alpha_h}{\alpha} \frac{\rho_c}{\rho}}{2} = \\ = T_c \frac{\alpha_c}{\alpha} + \frac{\Delta T}{2} \frac{\rho_c}{\rho} = T_h \frac{\alpha_h}{\alpha} - \frac{\Delta T}{2} \frac{\rho_h}{\rho} \quad (17)$$

There is no need to obtain $\mu_{min}, q(0), q(1)$ by approximate formulae for the reason that knowing j_{opt} and solving the thermal conductance equation one can find these values to the necessary extent of accuracy. As the optimal current is found separately for n- and p-type pellets, its resulting value is taken average.

For numerical calculations experimental temperature dependences of TE parameters for solid solutions based on bismuth-antimony chalcogenides are approximated by third order polynomial functions of temperature. To interpolate curves for any concentration of charge carriers, factors of these polynomials are similarly approximated by the functions of the Seebeck coefficients $|\alpha^{300}|$ at room temperature. Thus, for any value of α within (200 – 290) μV/K TE parameter temperature dependences are calculated in the temperature range (150 – 330) K. All the further calculations are carried out with these curves.

Both the Pontriaguin maximum method and the method of effective parameters involve a multi-iteration calculation. For a zero-approach electric current $j_{opt}^{(0)}$ the set of Eqs. (2) is solved and a new value of the optimal electric current is calculated for the first method by Eq. (6) and for the second one by Eq. (15). Then this new value is used in system (2) and the procedure is repeated until the results of two successive iterations differ less than by 0.2%. This is about the error with which TE parameters are defined and a higher accuracy of the calculation is unreasonable. It is convenient to take $j_{opt}^{(0)}$ calculated by Eq. (15) where the value of any TE parameter $\bar{p}$ is calculated as:

$$\bar{p} = \frac{p(T_h) + p(T_c)}{2} \quad (18)$$

$$T_{eff} = \frac{T_h + T_c}{2} \quad (19)$$

Results and Discussion

The results of calculations of the optimal mode by the two methods and different temperatures of the TE module cold and hot sides are given in Table 1.

Table 1: *Comparison of the results of the optimal electric current calculations by the Pontriguin method and by the method of effective parameters*

#	T_c, K	T_h, K	$\lvert\alpha_n^{300}\rvert$, μV/K	α_p^{300}, μV/K	Pontriaguin Maximum method		Method of effective parameters		Methods difference	
					j_{opt}, A/cm^2	μ	j_{opt}, A/cm^2	μ	δj_{opt}, %	$\delta\mu$, %
1	250	300	210	210	31.126	4.185	31.503	4.165	1.2	-0.5
2	220	250	230	230	21.88	3.012	22.43	3.013	2.5	0.0
3	250	300	210	230	26.026	3.878	28.77	4.162	9.5	6.8
4	220	250	230	250	19.776	3.276	20.011	3.067	1.2	-6.8

From Table 1 we can conclude that both the Pontriaguin Maximum method and the method of effective parameters yield very close results in case TE parameters of p- and n-type match well (this case is applied as a rule). The calculation of the optimal current for a couple as averaged for the pellets is a rather acceptable approach even if the pellets' TE properties are quite different (see Table 1, cases #3, 4).

In Fig. 1 we offer the dependence $\mu(j)$ obtained by the method of effective parameters for cases #1, 2 of Table 1.

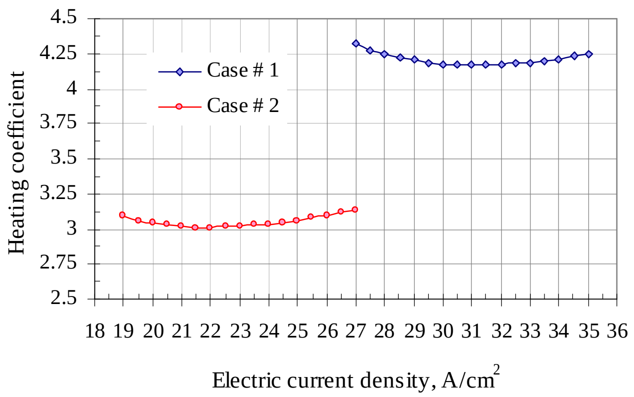

Figure 1: *Heating coefficient as a function of electric current density for cases # 1 and 2 of Table 1*

As the dependence $\mu(j)$ is quite flat (see Fig. 1) in the optimum vicinity this difference in n- and p-type optimal currents does not influence μ significantly, thus a (1-4 %) estimation accuracy of μ is sufficient. From Table 1 we can see that the two methods disagreement is less than this value (0.5 %).

Tables 2, 3 yield the difference between the effective TE parameters $p_{c,h}$ calculated by Eq. (9)-(12) and the actual values $p(T_{c,h})$ at the corresponding values of the optimal current of Table 1.

Table 2: *Effective Seebeck coefficient at the optimal electric current*

Type	T_h, K	T_c, K	Seebeck Coefficient, μV/K				
			$\alpha(T_h)$	$\alpha(T_c)$	$\bar{\alpha}$	α_h	α_c
p	300	250	210	185.9	199.1	201.6	202.1
n	300	250	209.8	192.7	202.1	204	204.4
p	250	220	206.7	186.8	197.1	198.9	197.1
n	250	220	213	197	205	206.7	206.9

Table 3: *Effective electric resisitivity at the optimal electric current*

Type	T_h, K	T_c, K	Electrical Resistivity·10^6, Ohm·cm				
			$\rho(T_h)$	$\rho(T_c)$	$\bar{\rho}$	ρ_h	ρ_c
p	300	250	1076	790	955	985	925
n	300	250	1055	828	962	982	942
p	250	220	1053	831	955	977	933
n	250	220	1059	885	982	995	968

From Tables 2,3 we see that α_h and α_c differ very slightly. That follows from Eq. (13) and is explained by the Thomson heat fluxes. On the other hand the difference between ρ_h and ρ_c is rather appreciable; we also see that $\rho_h > \bar{\rho} > \rho_c$, which is the evidence that the Joule heat flux to the pellet cold end is smaller than that to the hot one.

Conclusions

The accuracy of calculation of heating coefficients is of vital concern in TE modules mathematical simulation and optimization. However it is not worth overestimating this accuracy as TE properties of the pellets in a couple are not identical and each pellet is characterized by its own optimal current. The disagreement of the two methods: the *Pontriaguin maximum method* and *the method of effective parameters* for well fitting materials (a case of practical interest) does not exceed a usual (1-4)% mismatch of a TE couple n- and p-type materials – see Table 1.

The method of effective parameters provides a clear and evident relation between the initial data and the calculated result and not lesser degree of accuracy than the Pontriaguin maximum method. Moreover with the help of this method the investigation not only of the optimum but its vicinity is quite easier and natural.

Optimization of a multistage TE module is usually more troublesome. The Pontriaguin maximum method allows calculating the optimal temperature distribution on the cascades – see [4,5].

The method of effective parameters is also applicable for finding the optimal temperature distribution. For TE parameters being constant within a cascade this method was developed in [9]. The approach [9] can be generalized for precise expressions (6)-(19). It can be shown that the calculations by the two methods give close results for multistage TE modules as well. Therefore for the engineering mathematical simulation the method of effective parameters is a less sophisticated but albeit a consistent alternative to the methods of the Optimal Control theory.

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