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COMPUTER SIMULATION OF SINGLE-STAGE THERMOELECTRIC GENERATOR MODULE

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• *Program for computer design of single-stage thermoelectric generator modules was elaborated with regard to temperature dependences of material parameters, thermal losses in ceramic and connecting plates, as well as electrical losses on the contacts and connections of thermoelements. The program allows a detailed optimization of module parameters to be made during its design phase, owing to which generator modules with improved parameters can be elaborated and produced.*

Introduction

Design and analysis of possibilities for improvement of thermoelectric generator modules have become classical problems of theory of thermoelectricity [1-4].

The well-established methods of thermoelectric modules design are based on the use of the simplest thermocouple model. These models utilize averaged values in the operating temperature range of thermoelement [2, 3]. Besides, account of thermal and electrical losses is approximate. Such models offer the advantage of simplicity and evidence. Design parameters and power characteristics are described by simple, accessible for analysis, algebraic expressions. Though the calculated results do not suppose high precision, the analytical methods have proven well and are successfully used in the design of thermoelectric products today [5].

Strict account of temperature dependences of module material parameters, a well as contact phenomena, is possible only with the use of numerical methods. However, exactly contact losses impose restrictions on the reduction of thermoelement leg height, hence, on the reduction of such parameters as power per unit area and cost.

Classical numerical methods for solving similar problems are methods of optimal control theory in thermoelectricity [6, 7]. They are successfully used in the design of single- and multi-stage thermoelectric modules. The essence of calculation lies in solving second-order one-dimensional differential equations with temperature-dependent coefficients and with account of contact phenomena [8, 9].

There is a series of papers dedicated to precise three-dimensional simulation of thermoelement under conditions of the electric current generation [10, 11] with the use of commercial software packages of finite-element simulation Ansys [12] and Comsol Multiphysics [13]. Taking into account their high cost and the awkwardness of calculation, it can be concluded that for industrial production such studies are unnecessary.

For practical purposes the one-dimensional models characterize module work with a fair degree of precision. Therefore, one of the main factors in the design of thermoelectric generator modules is the use of up-to-date fast algorithms assuring absolute convergence.

The purpose of this paper is development of method and program for design of single-stage thermoelectric generator module, convenient for work and analysis, as well as easily adaptable according to customer-manufacturer's requirements.

1. Physical model of thermoelectric generator module

Single-stage generator module consists of a series of equal pairs of thermoelectric legs connected electrically in series and thermally in parallel. The legs are arranged uniformly in the module. Taking these facts into account, for the analysis and design of the thermoelectric generator module the paper deals with one unit cell of module – the thermocouple.

Physical model of thermocouple analyzed in this paper is given in Fig. 1. It comprises *n*-and *p*-type thermoelectric legs 1, electric connection of legs 2, as well as a pair of ceramic plates 3 that make the entire construction stiff.

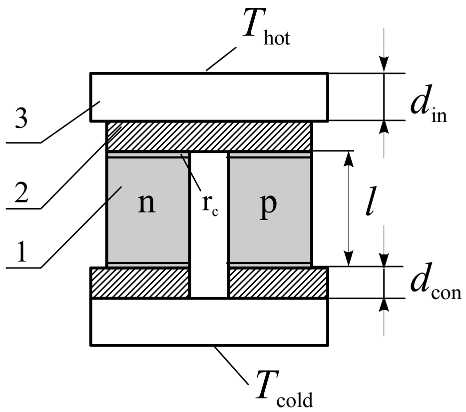

Fig. 1. Physical model of a thermocouple
1 – n- and p-type legs, 2 – electric connection, 3 – ceramic plates.

The surfaces of plates are at constant temperatures T_{hot} and T_{cold}, respectively.

In the general case all material parameters, including parameters of electric connections and ceramic plates, are functions of temperature:

$\alpha_n(T),\ \alpha_p(T)$ – the Seebeck coefficients of n- and p–type leg materials;

$\sigma_n(T),\ \sigma_p(T)$ – electric conductivity of leg materials;

$\kappa_n(T),\ \kappa_p(T)$ – thermal conductivity of leg materials;

$\sigma_{con}(T)$, $\kappa_{con}(T)$ – electric conductivity and thermal conductivity of connecting material;

$\kappa_{ins}(T)$ – thermal conductivity of ceramic plate.

The contacts between thermoelectric legs and connecting plates are characterized by contact electric resistivity $r_c(T)$ which is also a function of temperature. The space between the legs is filled with the air of thermal conductivity κ_{air}, and in this airspace there is heat exchange between the hot and cold ceramic plates.

2. Mathematical description of the model

Let us construct a mathematical model oriented at achievement of maximum generator efficiency

$$\eta = \frac{Q_h - Q_c}{Q_h} = 1 - \varphi\,, \tag{1}$$

where Q_c, Q_h are external heat flows on the cold and hot surfaces of generator module, respectively.

Function $\varphi = \dfrac{Q_c}{Q_h}$ can be considered as a minimized functional of the problem set. Let us move to equivalent logarithmic functional $J = \ln\varphi$:

$$J = \ln q_c - \ln q_h \tag{2}$$

where

$$q_c = \frac{Q_c}{nI}, \qquad q_h = \frac{Q_h}{nI}, \tag{3}$$

are specific heat flows on the cold and hot thermocouple junctions, respectively.

To calculate the boundary heat flows q_c and q_h, it is necessary to use a system of four differential equations of nonequilibrium thermodynamics

$$\left.\begin{aligned} \frac{dT(x)}{dx} &= -\frac{\alpha(T)j}{\kappa(T)}T(x) - \frac{j}{\kappa(T)}q(x) \\ \frac{dq(x)}{dx} &= \frac{\alpha(T)^2 j}{\kappa(T)}T(x) + \frac{\alpha(T)j}{\kappa(T)}q(x) + \frac{j}{\sigma(T)} \end{aligned}\right\}_{n,p}, \tag{4}$$

where x is dimensionless coordinate, $0 \le x \le 1$, $j_{n,p} = \dfrac{Il}{s_{n,p}}$ is specific current density in thermoelement legs. The boundary conditions for system (7) are of the form:

$$T(0) = T_{cold} + \delta T_c, \quad T(1) = T_{hot} - \delta T_h \tag{5}$$

where the losses in temperature difference on the ceramic and connecting plates δT_c and δT_h are determined like in [8] but with regard to difference in parameters of ceramic and connecting materials on the cold and hot sides:

$$\left.\begin{aligned} \delta T_c &= -\frac{q_c}{l\left(\dfrac{1}{j^n} + \dfrac{1}{j^p}\right)}\left(\frac{d_{ins}}{\kappa_{ins}(T_{cold})K_{ins}} + \frac{d_{con}}{\kappa_{con}(T_{cold})K_{con}}\right), \\ \delta T_h &= -\frac{q_h}{l\left(\dfrac{1}{j^n} + \dfrac{1}{j^p}\right)}\left(\frac{d_{ins}}{\kappa_{ins}(T_{hot})K_{ins}} + \frac{d_{con}}{\kappa_{con}(T_{hot})K_{con}}\right). \end{aligned}\right\}, \tag{6}$$

where K_{ins}, K_{con} are fill factors of ceramic and connecting plates.

The expressions for heat flows q_h and q_c with regard to temperature dependence of contact electric resistance will take on the form

$$\left.\begin{aligned} q_h &= \sum_{n,p}\left[q^{n,p}(1) + \frac{j^{n,p}}{l}r_c\right] + q_{con} \\ q_c &= \sum_{n,p}\left[q^{n,p}(0) + \frac{j^{n,p}}{l}r_c\right] - q_{con} \end{aligned}\right\}, \tag{7}$$

where the specific Joule heat released in connecting plate $q_{con}^{h,c}$ is calculated with the use of expression [4] as follows:

$$q_{con}^h = \frac{2I^2 r_c(T_{hot})}{d_{con}}\left(K_{con} - \frac{2}{3}\right), \; q_{con}^c = \frac{2I^2 r_c(T_{cold})}{d_{con}}\left(K_{con} - \frac{2}{3}\right). \tag{8}$$

Heat flows q_c and q_h depend on specific current density $j_{n,p}$. One should find such their values which impart minimum to functional *J*.

Optimal control theory [7, 9] provides a solution of the problem set. Solution of this problem is realized by numerical method of successive approximations and allows calculating optimal density of generated current to provide maximum efficiency of thermoelectric generator.

Through selection of the geometric dimensions and the number of thermoelements one can achieve the assigned voltage and power of thermoelectric generator module.

3. Description of computer program

The above described algorithm was used to create the TEG Designer computer program for design of single-stage thermoelectric generator modules. The program allows calculating optimal design parameters and power characteristics of module.

Program interface comprises two windows: a window for entry of input data and output of design results; a window for entry of polynomial coefficients for the approximation of thermoelectric material parameters.

The main window is shown in Fig.2.

The left panel of the main window is used for entry of input data for calculations. In the mode of input data entry the right side of the window is auxiliary and comprises a schematic of thermoelectric generator module with the required input parameters.

The input data are:

1. Hot side module temperature T_{hot}.
2. Cold side module temperature T_{cold}.
3. Module electric power W.
4. Module electric voltage V.
5. Contact electric resistivity $r_c(T)$.
6. Leg height l.
7. Ceramics thickness d_{ins}.
8. Ceramics thermal conductivity $\kappa_{ins}(T)$.
9. Connection thickness d_{con}.
10. Thermal conductivity of connecting material $\kappa_{con}(T)$.
11. Electric conductivity of connecting material $\sigma_{con}(T)$.
12. Distance between the legs a.
13. Materials of module legs.

Input parameters are entered into the respective marked fields with observance of the indicated dimensions.

Selection of materials for module legs is done on the input data entry panel. Drop-down lists enable selection from material library.

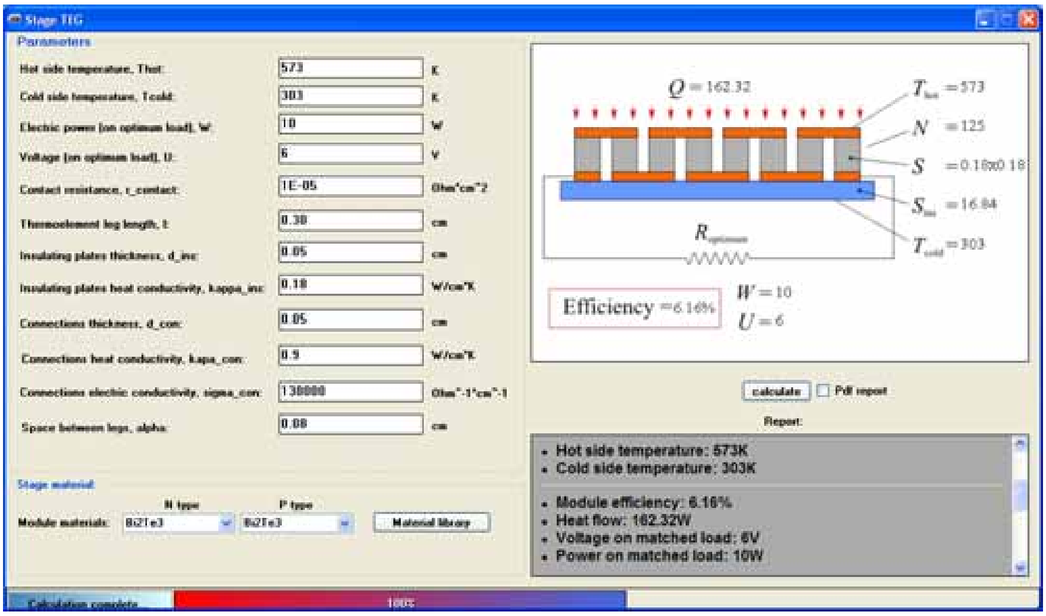

Fig. 2. Program main window.

Editing of material library is available in "Material library" dialogue window. It is shown in Fig. 3. The library comprises several positions of preset conventional materials. Choosing material from the list, one can browse the plots of temperature dependences of kinetic coefficients.

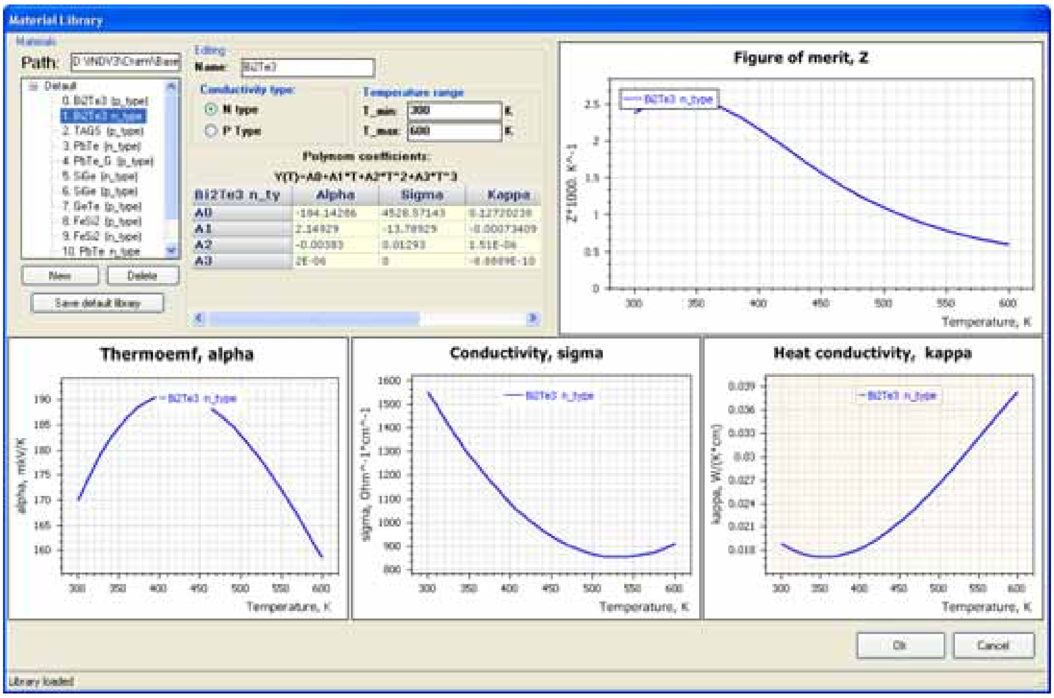

Fig. 3. Edit box of material library.

There is an opportunity of material library expansion by introducing polynomial coefficients for temperature dependences of the Seebeck coefficient $\alpha_{n,p}(T)$, electric conductivity $\sigma_{n,p}(T)$, thermal conductivity $\kappa_{n,p}(T)$, as well as indicating the operating temperature range. Polynomials are assigned as

$$F(T) = \sum_{i=0}^{n} A_i T^i \ , \tag{9}$$

where $A_0,\ldots,A_n$ are polynomial coefficients.

To calculate the generator module parameters, one should press "Calculate" button in the main window. After completing the calculations, the main characteristics will be shown in the figure. A detailed design report is output to "Report" panel with the opportunity of saving the results as PDF-file. The report file comprises full information on the results of design of single-stage thermoelectric generator module.

Report results include:

- temperatures of heat-absorbing and heat-releasing module surfaces;
- module efficiency;
- thermal flow through the module;
- voltage on matched load;
- power on matched load;
- number of thermoelement pairs;
- cross-sectional area of thermoelement legs;
- area of module heat-absorbing surface;
- areas of heat-absorbing and heat-releasing module surfaces.

4. Design results

To analyze the work of the program, a generator module of electric power 10 W and voltage 6 V operating in the temperature range 30÷300ºC was designed as an example. Parameters of thermoelectric materials are given in Fig. 3. Temperature dependences of Al_2O_3 ceramic and copper connecting materials are determined from [14]. Temperature dependence of contact electric resistance is given in [15]. Design results have shown that such module must comprise 125 thermocouples with leg dimensions 1.8x1.8x3 mm^3, located on ceramics of area 40x40 mm^2. The module efficiency will make 6.2%.

To analyze the effect of temperature dependences of module material parameters on design precision, a calculation was made by means of the referred program whereby certain values were assumed temperature independent. According to calculation results, simulation was made in Comsol Multiphysics medium by the procedure described in [16], and power and efficiency of designed generator module were determined.

The table gives the results of estimating the error in producing the necessary electric power and efficiency of generator module depending on the reductions made in physical model.

Table

Effect of physical model reductions on module design precision

Reductions		Error of module output parameters	
		Electric power	Efficiency
1	Kinetic coefficients are temperature independent	2.2%	5.4%
2	Contact resistance is temperature independent	4%	3%
3	Thermal and electric conductivity of connecting material are temperature independent	2%	0.6%
4	Thermal conductivity of ceramics is temperature independent	0.6	2%
5	There is no heat exchange in the air gap between the legs	1%	1%
	items 1–5 combined	~8.6%	~9.4%

Conclusions

The elaborated program of computer design of thermoelectric generator modules takes into account temperature dependences of material parameters, thermal losses in ceramic and connecting plates, as well as electric losses on the contacts and connections between thermoelements. The program allows making calculation and analysis of module parameters more precisely. Design error can be reduced by almost 10%.

The program enables a detailed optimization of module parameters to be made during its design phase, owing to which staged generator modules with improved parameters can be elaborated and produced.

The authors express their sincere gratitude to NASU academician L.Anatychuk for the all-round support of the work, consultations and constructive discussions.

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Submitted 25.03.2010.