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GENERALIZED THEORY OF THERMOELECTRIC ENERGY CONVERSION FOR PERMEABLE THERMOELEMENTS

A generalized theory of calculation of permeable thermoelements is presented, taking into account the dependences of the parameters of legs material on the temperature and current carrier concentration and changes in the conditions of heat transfer along the height of the leg. Methods for simulating the distributions of temperatures and heat flows in 1-D and 3-D dimensional models of a permeable thermoelement are described. The theory of calculating permeable thermoelements has been improved for the case of solving a multifactor optimization problem in order to achieve the maximum energy efficiency of thermoelectric energy conversion. Bibl. 12, Fig. 2.

Key words: generalized theory of permeable thermoelements, methods of designing a permeable thermoelement.

Introduction

Permeable thermoelements are thermocouples in which heat exchange with a heat source (sink) occurs not only on the surfaces of the junctions but also inside the thermoelement legs (Fig. 1).

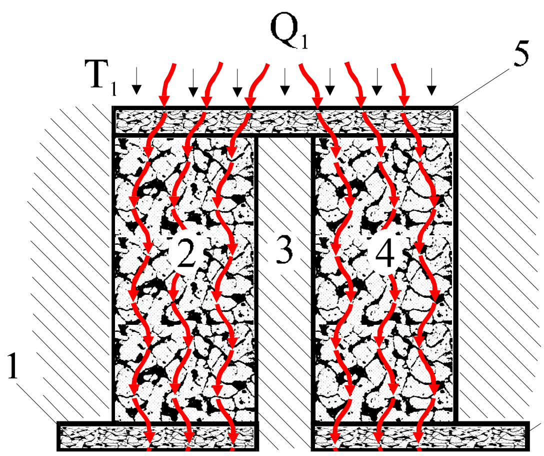

Fig. 1. A model of a permeable thermoelement in which heat carrier is passed from the hot to cold junctions ($T_1 > T_2$). 1,5,6 – connecting plates, 3 – adiabatic insulation, 2,4 – legs that have channels (pores), ↓ – heat flows;

– heat carrier flows.

In this case, the legs material is made permeable (has channels or pores) for pumping a heat carrier (liquid or gas) therethrough.

Since, thanks to the use of materials of high permeability, the inner surface of heat exchange can be sufficiently developed, the intensity of heat exchange increases, and the temperature difference between the media that exchange heat decreases. This leads to an increase in the useful temperature difference across the thermoelement, which makes it possible to increase the efficiency of energy conversion [1 – 3].

By changing the heat transfer conditions along the leg height, it is possible to influence the volumetric distribution of heat sources (sinks) in the legs of a permeable thermoelement. Thus, it becomes possible to influence the energy characteristics of the thermoelement – the efficiency or power of the generator or the coefficient of performance of coolers or air conditioners.

The parameters of porous structures were also studied in [4-6]. The estimation of the output power of a porous annular thermoelectric generator for waste heat harvesting was carried out in [4]. This article points out the fact that the porous TEGs have better performance than the bulk TEGs. However, in these works, the multiparameter optimization of permeable thermoelements was not carried out taking into account the change in heat transfer conditions along the height of the leg, the effect of contact resistances and connecting heat spreaders.

To do this, it is necessary to generalize the theory of calculation of permeable thermoelements taking into account the change of heat exchange conditions for 1D and 3D model of a permeable thermoelement, which is the purpose of this work.

Physical model and its mathematical description

The presence of heat exchange between the thermoelectric material and the heat carrier (Fig. 2) makes it necessary to solve the problem of finding the distributions of temperatures, electric potential and heat flows in the material conjugate with the equations of motion and heat transfer for the heat carrier.

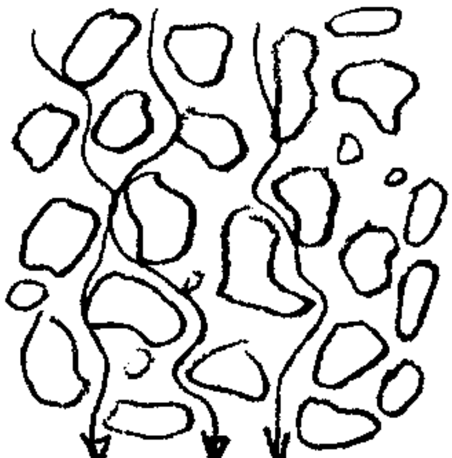

Fig.2. Pattern of heat carrier flow in a permeable material.

The system of the Navier-Stokes equation and the continuity equation is used to describe the motion of the heat carrier in the channel, and the heat conduction equation is used to describe the temperature distribution in the heat carrier.

The Navier-Stokes equation and the continuity equation can be written as [7]

$$\left.\begin{aligned}&\rho\frac{d\vec{\vartheta}}{dt}=\rho\vec{F}-\vec{\nabla}P+\mu\vec{\nabla}^2\vec{\vartheta}+\frac{1}{3}\mu\vec{\nabla}(div\vec{\vartheta}),\\&div\ \rho\vec{\vartheta}=0.\end{aligned}\right\}\qquad(1)$$

The left-hand side of the first equation (1) is the inertial force. The first term on the right-hand side of this equation is the mass force, the second is the action of surface pressure forces (normal stresses), and the last two terms are the action of the tangential components of surface forces (internal friction forces).

Heat exchange in liquid is described by thermal conductivity equation

$$\rho C_p\left(\frac{\partial T}{\partial t}+(\vec{\vartheta}\vec{\nabla})T\right)=-(\vec{\nabla}\vec{q})+\sum_{i,j}\tau_{ij}S_{ij}-\frac{T}{\rho}\frac{\partial\rho}{\partial T}\bigg|_P\left(\frac{\partial\rho}{\partial t}+(\vec{\vartheta}\vec{\nabla})P\right)+Q\qquad(2)$$

where ρ is density, C_p is heat capacity, T is temperature, $\vec{\vartheta}$ is liquid velocity vector, q is heat flow density, P is pressure, τ_{ij} is viscous stress tensor, $\vec{S}_{ij}$ is strain rate tensor, Q are internal heat sources.

The generalized mathematical model for a thermoelectric medium is based on the equations of heat balance in solid phases, mass transfer of gas components, continuity equations, filtration hydrodynamics and equations of state. In addition, it is necessary to formulate the appropriate boundary conditions. It is advisable to solve this problem by computer tools using specially developed applications, such as COMSOL Multiphysics.

The results of such studies, carried out for a permeable thermoelement in a 3D model, were first obtained in [8] for cooling liquid and air flows. The influence of the rate of heat carrier pumping and the supply voltage of the thermoelement on the temperature difference and the characteristics of energy conversion is investigated. The optimal values of the water (air) supply rate at the inlet to the channels and the potential difference across the thermoelement, whereby the maximum cooling capacity is realized during cooling, are determined in this paper. Optimization for other parameters in a 3D model was a significant challenge.

Therefore, to carry out multiparameter optimization of a permeable thermoelement, a 1D-dimensional model and the mathematical theory of optimal control are used [9, 10]. In this case, the steady-state one-dimensional heat conductivity equation for the thermoelectric leg material is given by

$$\frac{d}{dx}\left(\kappa\left(T,\xi(x)\right)\frac{dT}{dx}\right)+i^2\rho\left(T,\xi(x)\right)-Ti\frac{d\alpha\left(T,\xi(x)\right)}{dx}-\frac{\alpha_T P_K^1 N_K}{\left(S-S_K\right)}\left(T-t\right)=0\,,\qquad(3)$$

where P_K^1 is channel perimeter; N_K is the number of channels; S_K is cross-sectional area of all channels; S is cross-section of a leg together with channels; t is heat carrier temperature at point x; T is leg temperature at point x; α_T is heat exchange coefficient; i is current density ($i=\dfrac{I}{S-S_K}$); $\alpha(T,\ \xi(x)),\ \kappa(T,\ \xi(x)),\ \rho(T,\xi(x))$ - the Seebeck coefficient, thermal conductivity and resistivity of leg material are functions of temperature T and parameter of material inhomogeneity $\xi(x)$. In the capacity of $\xi(x)$, we can use the concentration of current carriers in semiconductor, doping impurities, or other value that characterizes thermoelectric structure inhomogeneity along the height of thermoelement legs. It should be noted that the thermoelectric medium parameters α,κ,ρ are interdependent. The system of these relations assigns a certain set $G\xi$ for possible values of the inhomogeneity parameter ξ. Specifying the physical model, one should assign such relations, for instance, in the form of theoretical or experimental dependences α, κ, ρ on ξ and T, and thus determine the set $G\xi$.

In the one-dimensional steady-state case on the leg section dx the change in heat carrier temperature dt is determined by the law of conservation of energy given by the expression

$$Gc_P dt = \alpha_T P_K^1 N_K \left(t - T\right) dx \ , \tag{4}$$

where G is mass flow rate of heat carrier through the leg of thermoelement; c_P is heat capacity of heat carrier.

Taking into account the relation (4), the equation for temperature distribution of heat carrier t can be represented as

$$\frac{dt}{dx} = \frac{\alpha_T P_K^1 N_K}{Gc_P}\left(t - T\right) \cdot \tag{5}$$

The solution of the system of differential equations (3) and (5) is temperature distribution in the materials of legs and the heat carrier.

We convert this system of equations to the form convenient for solving the problem. To do this, we introduce new symbols

$$j = il \ , \ \ q = \frac{1}{j}\left(\alpha jT - \kappa\frac{dT}{dx}\right), \quad \mathrm{x} = \frac{x}{l}, \ \alpha_e = \alpha_T P_K^1 N_K l \ , \tag{6}$$

where α_e is effective heat transfer coefficient, l is the height of thermoelement legs, q is specific heat flow.

Let us direct the x-axis from the cold to hot junctions. The change in the type of conductivity is carried out simultaneously with the change in the direction of the current, so that the condition $\alpha j<0$ is met in the n- and p- type thermoelement legs. Then it is possible to make the change $\alpha j = -|\alpha j|$ and then use the absolute values of the parameters α and j for the legs of both types of conductivity.

With regard to (6), the system of differential equations will take on the form:

$$\left.\begin{aligned} &\frac{dT}{d\mathrm{x}} = -\frac{\alpha\ j}{\kappa}\ T - \frac{j}{\kappa}q, \\ &\frac{dq}{d\mathrm{x}} = \frac{\alpha^2 j}{\kappa}T + \frac{\alpha\ j}{\kappa}q + j\rho + \frac{\alpha_e l}{\left(S - S_K\right) j}\left(t - T\right), \\ &\frac{dt}{d\mathrm{x}} = \frac{\alpha_e}{Gc_P}\left(t - T\right). \end{aligned}\right\}_{n,p} \tag{7}$$

The system of differential equations (7) written for n- and p- type legs (denoted by indices n and p, respectively) makes it possible to find the distributions of temperatures in the material of legs and the heat carrier, to determine heat flows. Based on this system of differential equations, one can find the optimal parameters and operating modes of permeable thermoelements, study their energy characteristics.

The values of specific heat flows on the cold and hot thermoelement junctions $q(1)$ and $q(0)$ will be determined with regard to the Joule heat release on the contact r_c and connecting resistances in the following way [10]:

$$\left.\begin{aligned} q(1) &= \sum_{n,p}\left[q^{n,p}(1)+\frac{j^{n,p}}{l}r_c^{n,p}\right]+\frac{2r_{com}I}{h_{com}}\left(K_{com}-\frac{2}{3}\right) \\ q(0) &= \sum_{n,p}\left[q^{n,p}(0)-\frac{j^{n,p}}{l}r_c^{n,p}\right]-\frac{2r_{com}I}{h_{com}}\left(K_{com}-\frac{2}{3}\right)\end{aligned}\right\}. \tag{8}$$

Consider the problem of maximum energy efficiency of thermoelectric cooling at fixed temperatures of heat sources T_h and T_c.

The problem reduces to finding maximum coefficient of performance ε and efficiency η

$$\varepsilon=\frac{Q_c}{Q_h-Q_c} \tag{9}$$

The efficiency is determined by the relation of the thermoelement power to the change in the enthalpy of the heat carrier as follows:

$$\eta=\frac{W}{\sum\limits_{n,p}Gc_p\left(T_m-T_C\right)} \quad . \tag{9*}$$

in the case of differential constraints (7) and the boundary conditions

$$T_{n,p}(0)=T_{\mathrm{h}},\quad T_{n,p}(1)=T_c,\quad t_{n,p}(0)=T_s, \tag{10}$$

where T_h is the temperature of the hot surface of junctions, T_c is the temperature of the cold surface of junctions, T_s is the initial temperature of heat carrier, Q_h, Q_c are heat flows that

the thermoelement exchanges with external heat sources

$$Q_h=Q_n(0)+Q_p(0),$$

$$Q_c=Q_n(1)+Q_p(1)+Q_L;$$

here Q_L is heat which is supplied due to internal heat transfer from the cooled heat carrier $Q_L=\sum\limits_{n,p}Vc_PS_R\left(t(0)-t(1)\right)$.

Hereinafter, instead of maximum ε it is convenient to consider functional minimum $\Im$:

$$\Im=\ln q(0)-\ln q(1), \tag{11}$$

where

$$q(0)=\frac{Q_h}{I}=q_n(0)+q_p(0),$$

$$q(1)=\frac{Q_c}{I}=q_n(1)+q_p(1)+\frac{Q_L}{j\left(S-S_K\right)}l,$$

here $q_n(1)$, $q_p(1)$, $q_n(0)$, $q_p(0)$ are the values of specific heat flows on the cold and hot thermoelement junctions for *n*- and *p*-type legs that are determined from solving the system of differential equations (7) with regard to (8).

The optimization problem is to select from the set of admissible controls $\xi \in G_\xi$ such concentration functions $\xi^{n,p}(x)$ and simultaneously assign such a specific mass velocity of the heat carrier in the channels $V=V_0$, whereby in the case of constraints (7) - (11) and under the condition

$$q_n(1)+q_p(1)=0 \tag{12}$$

the functional $\Im$ will take on the lowest value, in which case the coefficient of performance ε will be maximum [10, 11].

Finding the efficiency maximum reduces to a search for the functional minimum

$$\Im = \ln[\sum_{n,p}\left\{Gc_P\left(T_m - T_C\right)\right\}] - \ln[\sum_{n,p}\left\{Gc_P\left(T_m - t(0)\right) + q(0)\frac{j\left(S-S_K\right)}{l} - I\left(\frac{r_0}{S_n}+\frac{r_0}{S_p}\right)\right\}]. \tag{13}$$

For further solutions, the mathematical theory of optimal control developed under the guidance of L.S. Pontryagin is generally used [12].

Method for solving the problem

Next, the problem is reduced to finding control $\xi(x)$, parameter vectors ω and their respective solution $X(x)$ of system (7), (10) such that the functional $\Im$ acquires a minimum value. The problem set in this way is called optimization. Its solution in the most general form was first formulated by Pontryagin in the form of the maximum principle, which yields the necessary optimality condition in the problems of optimal control.

The maximum principle is formulated by the following theorem.

Let $\xi^*(x)$ be optimal control, ω^* - optimal parameter vector, $X^*(x)$ - optimal trajectory. Then there is such a vector of pulses $\psi^*(x)$, that for each x the following conditions are met:

1. The Hamiltonian function which is written as equation

$$H(X_*(x),\xi_*(x),\psi_*(x),\omega_*,x) = (\psi, f\ ) \tag{14}$$

(in our case f_1, f_2, f_3 are the right-hand sides of equation system (7)), with respect to variable ξ reaches its maximum:

$$H(X^*(x),\xi^*(x),\psi^*(x),\omega^*,x) = \max_{\xi\in G_\xi} H\ \ (X^*(x),\xi,\psi^*(x),\omega^*,x). \tag{14*}$$

2. Parameter vector ω must satisfy a system of integral differential equations

$$-\frac{\partial\Im(x(x),\omega)}{\partial\omega_i} + \int\sum_{j=1}^{n}\psi_j\cdot\frac{\partial f_j^k(x,\xi,\omega)}{\partial\omega_i}dt = 0, \qquad i=1,..,r. \tag{15}$$

Pulse vector $\psi(x)$ satisfies a system of differential equations of the form

$$\frac{d\psi}{dx} = -\frac{\partial H}{\partial X}, \tag{16}$$

which is canonically conjugate with system (7), where $X(X_1, X_2, X_3)$ is vector function of phase variables (in our case with components $X_1 = T$, $X_2 = q$, $X_3 = t$), with the boundary conditions

$$\psi(x) = -\frac{\partial J}{\partial X}. \tag{17}$$

The solution of optimal problems which is based on the use of the maximum principle can be realized by numerical methods with the development of corresponding computer programs.

With its help it is possible to investigate various problems of optimal control, differing in the way of assigning the functional (Lagrange, Mayer, Boltz problems), constraints, etc.

We specify the previously stated formalism of the mathematical theory of optimal control in relation to our problem.

Introduce the Hamiltonian function

$$H = \psi_1 f_1 + \psi_2 f_2 + \psi_3 f_3 , \tag{18}$$

here f_1, f_2, f_3 are the right-hand sides of the system of equations (7):

$$f_1 = -\frac{\alpha\ j\ T}{\kappa} - \frac{q}{\kappa},\quad f_2 = \frac{\alpha^2 j}{dx}T + \frac{\alpha\ j}{\kappa}q + i^2\rho - \frac{\alpha_T P_K^1 N_K l^2}{(S - S_K)\,j}(T - t),$$
$$f_3 = \frac{\alpha_T P_K^1 N_K l}{V c_P S_R}(T - t).$$

Functions $\psi(x)$ (pulses) must satisfy a system of equations (with regard to (7) and (17)):

$$\begin{cases} \dfrac{d\psi_1}{dx} = \dfrac{\alpha\ j}{\kappa}R_1\psi_1 - \left(\dfrac{\alpha\ j}{\kappa}R_2 - \dfrac{\alpha_T P_K^1 N_K l^2}{(S - S_K)\,j}\right)\psi_2 - \dfrac{\alpha_T P_K^1 N_K l}{V c_P S_R}\psi_3, \\ \dfrac{d\psi_2}{dx} = \dfrac{j}{\kappa}\psi_1 - \dfrac{\alpha\ j}{\kappa}\psi_2, \\ \dfrac{dt}{dx} = -\dfrac{\alpha_T P_K^1 N_K l^2}{(S - S_K)\,j}\psi_2 + \dfrac{\alpha_T P_K^1 N_K l}{V c_P S_R}\psi_3, \end{cases}_{n,p} \tag{19}$$

where

$$\begin{cases} R_1 = 1 + \dfrac{d\ln\alpha}{dT}T - \dfrac{d\ln\kappa}{dT}\left(T + \dfrac{q}{\alpha}\right) \\ R_2 = R_1 + \dfrac{1}{Z_K}\dfrac{d\ln\sigma}{dT} + \dfrac{d\ln\kappa}{dT}\left(T + \dfrac{q}{\alpha}\right) \end{cases}_{n,p}$$

are canonically conjugate with system (7).

With the following boundary conditions (transversality conditions)

$$\psi(0)=\left.\frac{\partial \bar{J}}{\partial y}\right|_{x=0}, \quad \psi(1)=-\left.\frac{\partial \bar{J}}{\partial y}\right|_{x=1}, \tag{20}$$

where $\bar{J}=J+\sum(\nu, g)$ is extended functional; ν, g are vectors of undetermined constant Lagrange multipliers and the boundary conditions (10).

Then the boundary conditions for the conjugate system will acquire the form

$$\psi_2^{n,p}(0)=\frac{1}{q_n(0)+q_p(0)},$$
$$\psi_2^{n,p}(1)=-\frac{(S-S_K)\,j}{lVc_P S_R\left(2t(0)-t_n(1)-t_p(1)\right)},$$
$$\psi_3^{n,p}(1)=-\frac{1}{2t(0)-t_n(1)-t_p(1)}.$$

Using the systems of differential equations (7), (19) with regard to (10), (20) and numerical solution methods, it is possible to create a program of computer design of optimal inhomogeneity functions of thermoelectric material $\xi(x)$ (or optimally homogeneous material for thermoelement legs from (15)), the optimal velocity of heat carrier V_0, the parameter of electric current density j and others, in order to achieve maximum energy efficiency of permeable cooling thermoelements and electricity generation.

Conclusions

1. Theory of thermoelectric energy conversion is generalized for the case of heat sources and sinks in a permeable thermoelectric medium. Methods for simulation of such thermoelements in 3-D and 1-D space are described. The influence of connecting plates and contact resistances at points of connection of legs is taken into account.
2. Theory of calculation of permeable thermoelements for the case of solving a multifactor optimization problem (optimal inhomogeneity functions of thermoelectric material ξ(x), optimal heat carrier flow rate *G,* optimal heat carrier velocity V_0, parameter of electric current density j and others) is improved for the purpose of achieving maximum energy efficiency of thermoelectric energy conversion.

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ОБОБЩЕННАЯ ТЕОРИЯ ТЕРМОЭЛЕКТРИЧЕСКОГО ПРЕОБРАЗОВАНИЯ ЭНЕРГИИ ДЛЯ ПРОНИЦАЕМЫХ ТЕРМОЭЛЕМЕНТОВ

Представлена обобщенная теория расчета проницаемых термоэлементов с учетом зависимостей параметров материала ветвей от температуры и концентрации носителей тока и изменения условий теплообмена вдоль высоты ветви. Описаны методы моделирования

распределений температур и тепловых потоков в 1-D и 3-D мерной модели проницаемого термоэлемента. Усовершенствована теория расчета проницаемых термоэлементов в случае решения многофакторной оптимизационной задачи с целью достижения максимальной энергетической эффективности термоэлектрического преобразования энергии. Бібл. 12, рис. 2.
Ключевые слова: обобщенная теория проницаемых термоэлементов, методы проектирования пропницаемого термоэлемента.

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Представлена обобщенная теория расчета проницаемых термоэлементов с учетом зависимостей параметров материала ветвей от температуры и концентрации носителей тока и изменения условий теплообмена вдоль высоты ветви. Описаны методы моделирования распределений температур и тепловых потоков в 1-D и 3-D мерной модели проницаемого термоэлемента. Усовершенствована теория расчета проницаемых термоэлементов в случае решения многофакторной оптимизационной задачи с целью достижения максимальной энергетической эффективности термоэлектрического преобразования энергии. Библ. 12, рис. 2.
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