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COMPUTER SIMULATION OF A PERMEABLE GENERATOR THERMOELEMENT

The paper presents the results of computer studies of a 3D model of a permeable generator thermoelement. A physical model and design of a permeable thermoelement are given, and its mathematical description is presented. A method for calculating a thermoelement based on the Comsol Multiphysics software package has been developed. The dependences of the energy characteristics of a thermoelement made of Bi-Te-Se-Sb based materials on the height of the thermoelement leg are calculated. Bibl.11, Fig. 4.

Key words: permeable thermoelement, computer simulation, electric energy generation, energy characteristics.

Introduction

The widest application of thermoelectric energy converters is based on the use of a thermocouple element [1, 2]. Its energy conversion efficiency is determined by the figure of merit Z of materials used. Therefore, the search for materials with the maximum value of the figure of merit becomes the main task of thermoelectric materials science. However, despite intensive research, no significant increase in the figure of merit has been observed in this direction over the past 20–30 years [3, 4]. The maximum values of the dimensionless figure of merit of thermoelectric materials for industrial use remain at the level of 1 ÷ 1.2. Therefore, to improve efficiency, it is necessary to use new, unconventional approaches, which consist in the use of other non-traditional variants of physical models of thermoelements, which are the main component of a thermoelectric power converter.

One of them is the use of thermoelements with a developed internal heat exchange surface, i.e. permeable thermoelements. In such thermoelements, heat exchange with the heat source and heat sink occurs not only at the junctions, but also in the legs. Already the first theoretical [5] and experimental

[6] studies for cooling gas flows showed their promise. They point to the possibility of improving the energy conversion efficiency by a factor of 1.3 ÷ 1.4.

However, such studies were carried out for a model that is difficult to implement in practice. Therefore, it is necessary to create and study a more realistic 3D model of a permeable thermoelement, which is the purpose of this work.

Physical model and its mathematical description

The physical model of a permeable thermoelement, in which heat exchange with the heat carrier occurs not only through the interconnect plates, but also with the side surfaces of the leg, is shown in Fig. 1.

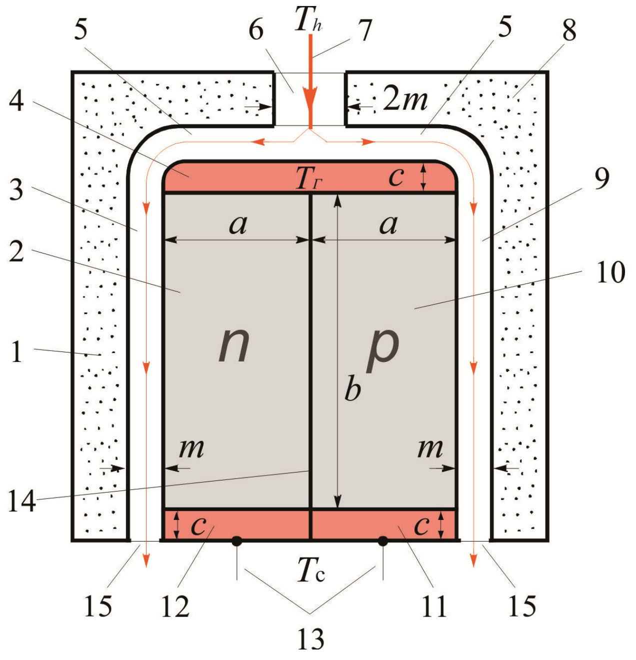


Fig. 1. Physical model of a permeable thermoelement:
1 – adiabatic isolation, 2 – n-type legs, 3 – channels,
4 – interconnect plate, 5 – channel, 6 – channel,
7 – heat carrier, 8 – adiabatic isolation, 9 – channel,
10 – p-type leg, 11, 12 – interconnect plates, 13 – electric contacts,
14 – layer between n- and p-type legs, 15 – channel outlets.

It includes n - and p - type legs (2, 10), covered by adiabatic isolation 1 and 8, which together form channels 5, 6, 9. Heat carrier 7 with temperature T_h flowing through channels 3, 5 and 5, 9 is supplied through channel 6. The legs are made of a homogeneous material based on *Bi-Te* with a maximum value of figure of merit Z in the temperature range 20 ÷ 320 °C. The temperature dependence of the material parameters should be taken into account. Interconnect plates c are made of copper, interconnect resistance is 10^{-6} Ohm·cm^2. The temperature T_0 of the lower interconnect plates is thermostatically controlled. The n - and p - type legs are interconnected by a thin layer 14, the thermal conductivity, electrical conductivity and thickness of which are neglected. The material of the legs is homogeneous and isotropic with known temperature dependences: electrical conductivity $\sigma(T)$, thermoelectric coefficient $\alpha(T)$, thermal conductivity $\kappa(T)$. In the thermoelectric medium, the volumetric effects of Thomson, Joule-Lenz and the near-contact Peltier effect are taken into account. The temperature of the heat carrier at the inlet to the thermoelement was assumed to be equal to the temperature of the hot junctions. The size of the thermoelement in the direction perpendicular to the plane of the figure is d, the value of $d = a$. The planes $d = 0$ and $d = a$ are the adiabatic isolations forming channels 5, 6, 9. There is no friction between the heat carrier and the adiabatic isolations 1, 8.

On the side surface of the legs 2 of the interconnect 4, which are in thermal contact with the heat carrier 7, heat transfer is described by the Newton-Richmann law:

$$q_0 = \alpha_T (t - T), \tag{1}$$

where α_T is the heat transfer coefficient, T is the temperature of the thermoelement leg, t is the heat carrier temperature.

The system of equations describing the distribution of temperature and potential in the thermoelectric medium is described by the fundamental laws of conservation of energy and current carriers [7]:

$$\vec{\nabla} \vec{W} = 0 \tag{2}$$

$$\vec{\nabla} \vec{i} = 0 \tag{3}$$

where $\vec{W} = \vec{q} + U\vec{i}$ is energy flow density.

Using the generalized Fourier and Ohm's laws for a thermoelectric medium:

$$\vec{q} = -\kappa \vec{\nabla} T + \alpha \vec{i}\, T \tag{4}$$

$$\vec{i} = -\sigma(\vec{\nabla} U + \alpha \vec{\nabla} T) \tag{5}$$

where U is the potential, κ is the thermal conductivity, α is the thermoelectric coefficient, σ is the electric conductivity, it is possible to obtain a system of differential equations for finding the distribution of temperatures and potentials:

$$\left.\begin{array}{l} \vec{\nabla}\kappa\vec{\nabla}T + \dfrac{i^2}{\sigma} - T\vec{i}\,\vec{\nabla}\alpha = 0; \\ \vec{\nabla}(-\sigma(\vec{\nabla}U + \alpha\vec{\nabla}T)) = 0. \end{array}\right\} \tag{6}$$

The Navier-Stokes equation and the continuity equation can be written as [8]:

$$\left.\begin{array}{l} \rho\dfrac{d\vec{\vartheta}}{dt} = \rho\vec{F} - \vec{\nabla}P + \mu\vec{\nabla}^2\vec{\vartheta} + \dfrac{1}{3}\mu\vec{\nabla}(div\vec{\vartheta}), \\ div\rho\vec{\vartheta} = 0. \end{array}\right\} \tag{7}$$

The left side of (7) represents the fluid inertia force. The first term on the right side of (7) 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 contiguous components of surface forces (internal friction forces).

Heat transfer in a liquid is described by thermal conductivity equation [9]:

$$\rho C_p\left(\frac{\partial T}{\partial t}+(\vec{\vartheta}\vec{\nabla})T\right)=-(\vec{\nabla}\vec{q})+\sum_{i,j}\tau_{\mathrm{ij}}S_{ij}-\frac{\mathrm{T}}{\rho}\frac{\partial\rho}{\partial T}\bigg|_{P}\left(\frac{\partial\rho}{\partial t}+(\vec{\vartheta}\vec{\nabla})P\right)+Q \tag{8}$$

where ρ is the density, C_p is the heat capacity, T is the temperature, $\vec{\vartheta}$ is the heat flux density, q is the heat flux density, P is the pressure, τ_{ij} is the viscous stress tensor, η is the viscosity, I is the unit tensor, $\vec{S}_{ij}$ is the strain rate tensor.

Since this problem is considered for a steady-state case, the left side of the first equation of system (7) is equal to zero. The influence of mass forces is also neglected, so the first term in the left part of the same equation is also equal to zero. Equation (8) must also be written for the steady-state case, and heating of the liquid due to internal friction, compression of the liquid, and heating of the liquid due to internal heat sources are neglected. Then the system of Navier-Stokes, continuity and heat conduction equations for this problem will be written in the form:

$$\left.\begin{aligned}&-\vec{\nabla}P+\mu\vec{\nabla}^2\vec{\vartheta}+\frac{1}{3}\mu\vec{\nabla}(div\vec{\vartheta})=0,\\&div\rho\vec{\vartheta}=0,\\&\rho C_p(\vec{\vartheta}\vec{\nabla})T+\vec{\nabla}\vec{q}=0.\end{aligned}\right\} \tag{9}$$

Boundary conditions describing the conjugate problem used in this task have the following form:

– for thermoelectric medium:

$$\text{temperature - }\begin{aligned}&T|_0=300K\\&T|_{z_h}=\alpha_T(T_h-T)\end{aligned}, \tag{10}$$

$$\text{potential - }\begin{aligned}&U|_0=0\\&U|_{x_3}=U_0\end{aligned}, \tag{11}$$

– for heat carrier:

$$\text{velocity - }\begin{aligned}&\vartheta|_0=\vartheta_0\\&\vartheta|_{z_h}=P_0=0,\\&\vartheta|_{S_б}=0\end{aligned} \tag{12}$$

$$\text{inlet temperature - }t|_{z_h}=T_h \tag{13}$$

where ϑ_0 is the initial velocity of heat carrier, U_0 is a fixed potential value, S_0 is the side surface of thermoelement.

Implementation of given problem in the Comsol Multiphysics software package

To calculate the problem, the Comsol Multiphysics software package was chosen, namely, the equation in partial derivatives (PDE modes), where one of the ways to represent the equation is the coefficient form:

$$e_a \frac{\partial^2 \vec{u}}{\partial t^2} + d_a \frac{\partial \vec{u}}{\partial t} + \vec{\nabla}(-c\vec{\nabla}\vec{u} - \alpha\vec{u} + \gamma) + \beta\vec{\nabla}u + a\vec{u} = f \tag{14}$$

This equation is used for a thermoelectric medium and reduced to the form of $\vec{\nabla}(-c\vec{\nabla}\vec{u}) = 0$. For this, e_a, d_a, α, γ, β, a are set to zero, and the value c is written in the form of a matrix:

$$c = \begin{pmatrix} \kappa + \alpha^2\sigma T + \sigma U\alpha & \alpha T\sigma + \sigma U \\ \alpha\sigma & \sigma \end{pmatrix}. \tag{15}$$

Moreover, the vector $\vec{u}$ also has the form of a matrix:

$$\vec{u} = \begin{pmatrix} T \\ U \end{pmatrix}. \tag{16}$$

The Comsol Multiphysics – Non-Isothermal Flow module [11] is used to describe the motion and heat transfer of a fluid. The module includes a system of Navier-Stokes equations, a continuity equation and a heat transfer equation for a fluid, in a time-varying or steady-state mode. The calculation of the given model, in the steady-state mode, was carried out according to the relations:

$$\left.\begin{aligned} &\rho(\vec{\vartheta}\vec{\nabla})\vec{u}_2 = \vec{\nabla}\left[-PI + \mu(\vec{\nabla}\vec{\vartheta} + (\vec{\nabla}\vec{\vartheta})^T) - \frac{2}{3}\mu(\vec{\nabla}\vec{\vartheta})I\right], \\ &\vec{\nabla}(\rho\vec{\vartheta}) = 0, \\ &\rho C_p\vec{\vartheta}\vec{\nabla}T + \vec{\nabla}(\kappa\vec{\nabla}T) = 0. \end{aligned}\right\} \tag{17}$$

The value of the electric current was calculated through the integral over the cross-sectional area S_V::

$$I = \iint\limits_{S_V} I_n dS_V\ , \tag{19}$$

where $I_n = n_x I_x + n_y I_y + n_z I_z$ is electric current density vector. The values of I_x I_y I_z were determined by the relations:

$$I_x = -\sigma \frac{\partial U}{\partial x} - \sigma\alpha \frac{\partial T}{\partial x}, \tag{20}$$

$$I_y = -\sigma \frac{\partial U}{\partial y} - \sigma\alpha \frac{\partial T}{\partial y}, \tag{21}$$

$$I_z = -\sigma \frac{\partial U}{\partial z} - \sigma\alpha \frac{\partial T}{\partial z}. \tag{22}$$

The heat carrier flow rate was determined by integrating the velocity *υ* over the cross-sectional area of the channel S_{V1}:

$$G = \iint\limits_{S_{V1}} \vartheta dS_{V1} \tag{23}$$

Electrical power of the thermoelement $W = I \cdot U$, heat flux entering the thermoelement $Q_h = GC_p\Delta t$

The main parameter characterizing the efficiency of the thermoelement in the electric power generation mode is the efficiency factor, determined by the relation:

$$\eta = \frac{W}{Q_h}. \tag{24}$$

Results of computer research on the characteristics of a permeable thermoelement based on *Bi-Te-Se –Sb* materials

Calculation was made for materials based on *Bi-Te-Se-Sb* with functional dependences of material parameters, i.e. the Seebeck coefficient α, thermal conductivity κ and electric conductivity σ on temperature [3].

The simulation of the permeable thermoelement was carried out in the Comsol Multiphysics program for the following basic design (Fig. 1): height *b* = 10 *mm*, length 10 *mm*, width *a* = 10 mm. Dimensions of the lower interconnect: height *c* = 1 *mm*, length 10 *mm*, width *a* =10 mm; of the upper interconnect: height *d* = 1 mm, length *c* = 10 *mm*, width *a* = 10 *mm*. The interconnect material is copper. The slots in interconnects, together with the legs, form a system of channels for pumping the heat carrier. The design takes into account the presence of a transient layer of solder with a thickness of 0.3 mm. Fig. 2 shows the partition of such a design into finite elements.

At the inlet gas temperature of 600K, the temperature distributions in the heat carrier in Fig. 3 and the thermoelement material in Fig. 4 were obtained.

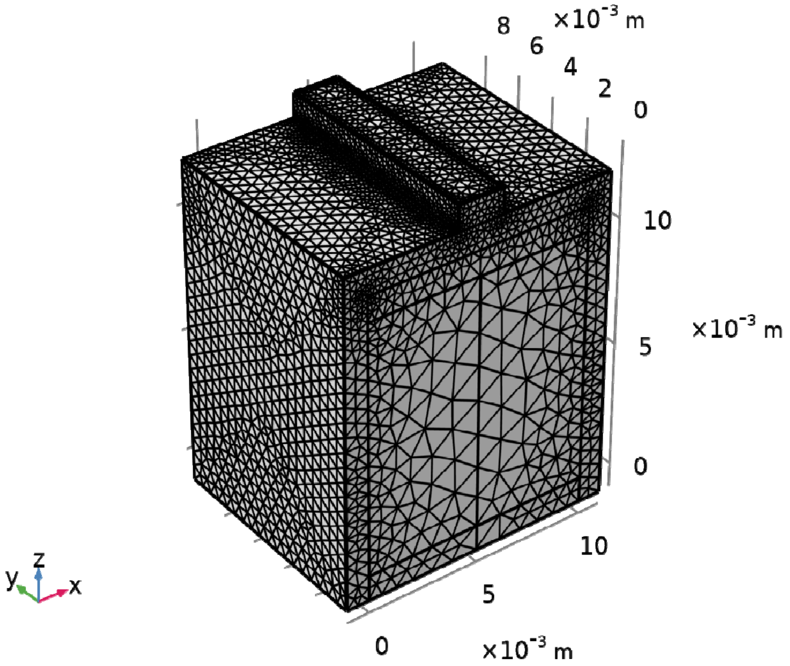
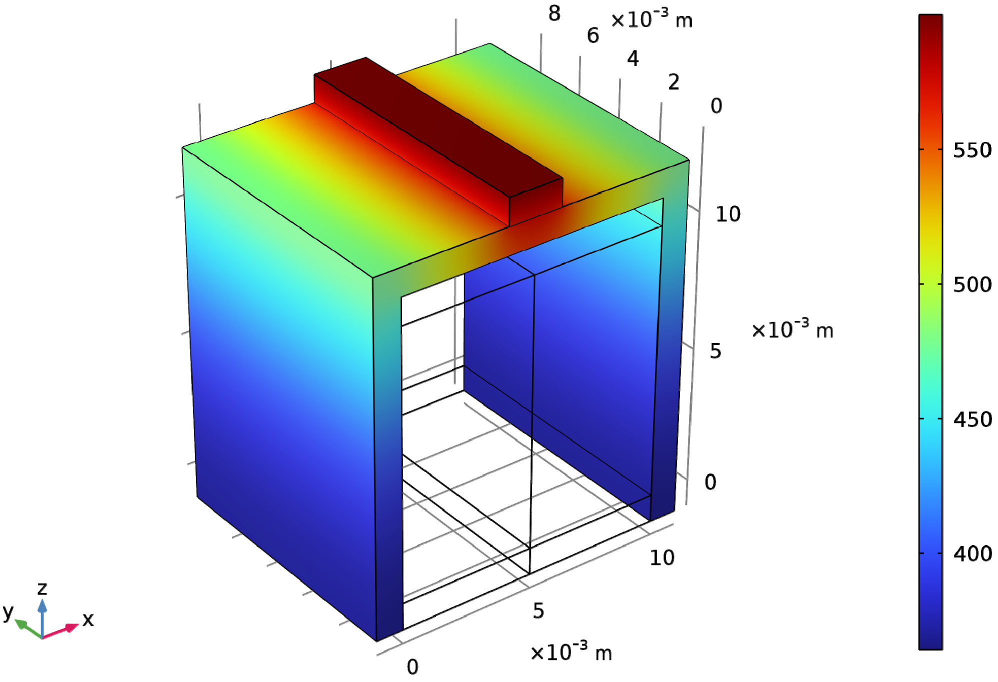
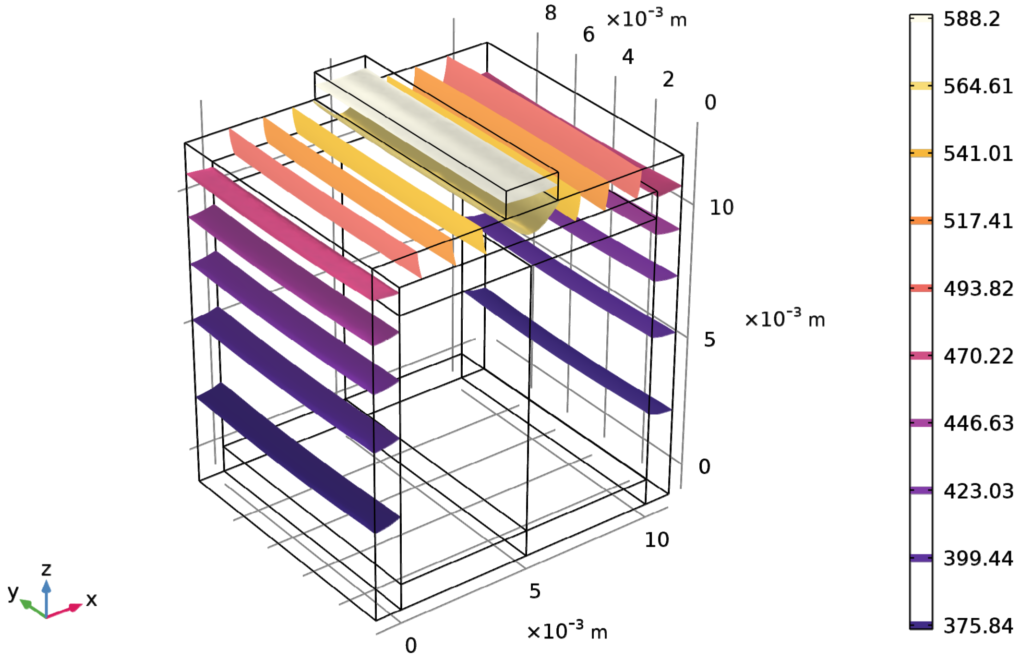


Fig. 2. Geometric grid.

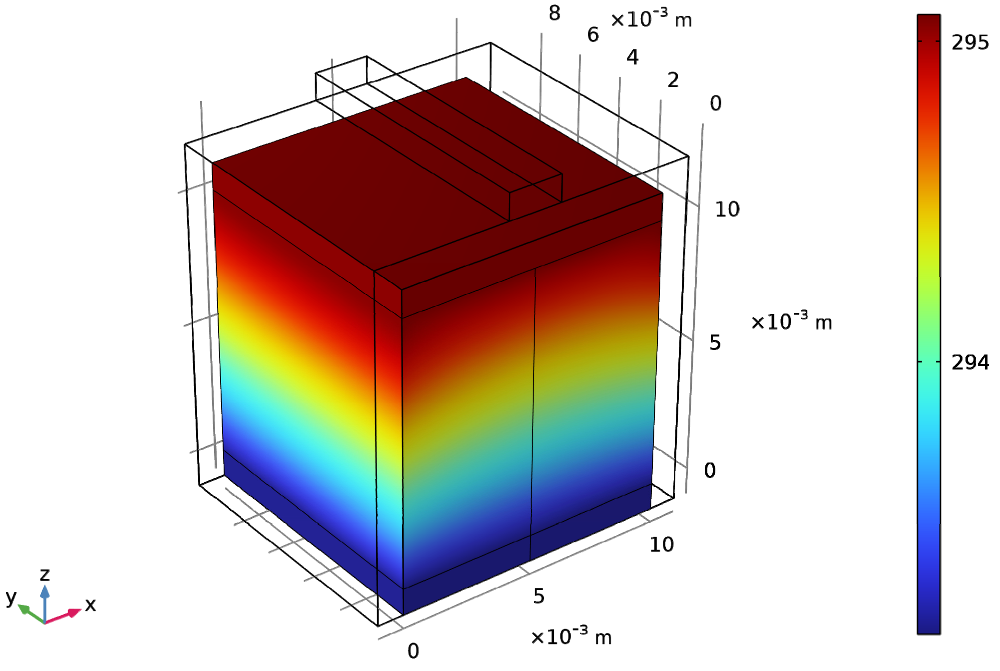


a)

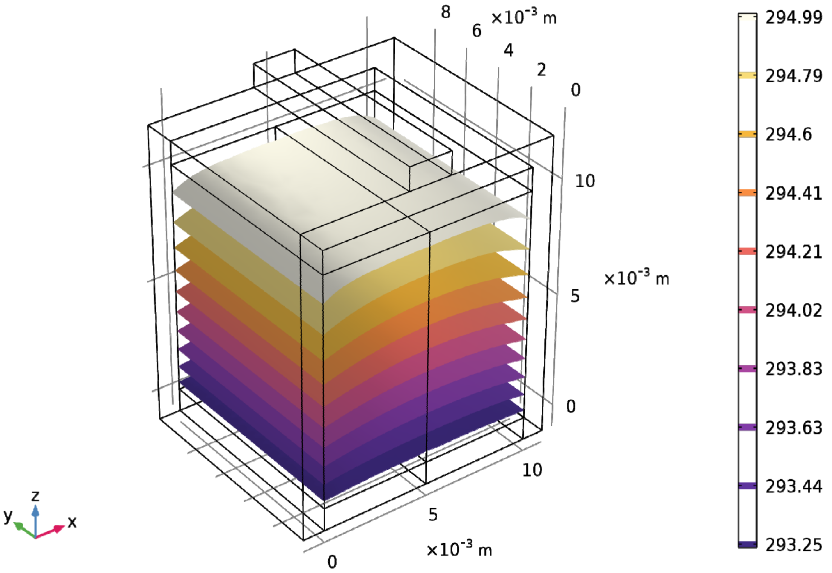


b)

Fig. 3. a) temperature distribution;
b) isothermal surfaces



a)



b)

Fig.4. a) temperature distribution;
b) isothermal surfaces

The height of the thermoelement legs was set equal to 1mm, 5 mm, 10 mm, 15 mm, 20 mm. The coefficient of heat exchange between water and thermoelement - α_T, in the Newton-Richmann law, was 1000 $W/(m^2{\cdot}K)$.

For these parameters, the mean integral characteristics of the thermoelement were determined: air temperature at the thermoelement outlet - t_{out}; thermoelement electromotive force - EMF; the value of electric current I, A; air consumption - G; electric power W; efficiency η. The dependences of these parameters on the leg height l, for the case when the air temperature at the inlet to the thermoelement was 600K, are presented in the table.

Table

l, mm	t_{out}, K	EMF, V	I, A	G, m^3/s	W, 10^{-8} W	η (%)
1	473.60	0.00003	0.0004782	0.00047	1.43	1.57
5	414.13	0.00017	0.0001539	0.00680	2.62	1.84
10	365.01	0.00038	0.0001355	0.00599	5.13	2.87
15	335.62	0.00062	0.0000822	0.00582	5.09	1.56
20	299.98	0.00243	0.0000215	0.00480	5.22	0.83

Thus, there are such rational heights of the thermoelement legs whereby the efficiency has maximum values. To reveal the extreme possibilities of a permeable thermoelement, it is necessary to carry out multi-parameter optimization of its structural and thermophysical parameters.

Conclusions

1. A 3*D* model of a permeable thermoelement for cooling liquid and gas flows has been developed in the Comsol Multiphysics software package.
2. Temperature distributions in the material of the thermoelement legs and heat carrier, potentials in the thermoelement, air velocities and energy characteristics of a permeable thermoelement made of *Bi-Te-Se-Sb* based materials are determined.
3. It is necessary to carry out multi-parametric optimization of the structural and thermophysical parameters of a permeable thermoelement, which will make it possible to determine the maximum characteristics

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КОМП'ЮТЕРНЕ МОДЕЛЮВАННЯ ПРОНИКНОГО ГЕНЕРАТОРНОГО ТЕРМОЕЛЕМЕНТА

В роботі представлені результати комп'ютерних досліджень 3D моделі проникного генераторного термоелемента. Приведено фізичну модель та конструкцію проникного термоелемента, представлено її математичний опис. Створено метод розрахунку термоелемента на основі пакета прикладних комп'ютерних програм Comsol Multiphysics. Розраховано залежності енергетичних характеристик термоелемента з матеріалів на основі Bi-Te-Se-Sb від висоти вітки термоелемента. Бібл. 11, рис.4, табл.1.

Ключові слова: проникний термоелемент, комп'ютерне моделювання, генерація електричної енергії, енергетичні характеристики.

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КОМПЬЮТЕРНОЕ МОДЕЛИРОВАНИЕ ПРОНИЦАЕМОГО ГЕНЕРАТОРНОГО ТЕРМОЭЛЕМЕНТА

В работе представлены результаты компьютерных исследований 3D модели *проницаемого генераторного термоэлемента. Описаны физическая модель и конструкция проницаемого термоэлемента, представлено ее математическое описание. Создан метод расчета термоэлемента на основе пакета прикладных компьютерных программ Comsol Multiphysics. Рассчитаны зависимости энергетических характеристик термоэлемента из материалов на основе Bi-Te-Se-Sb от высоты ветки термоэлемента. Библ. 11, рис.4, табл.1.*

Ключевые слова: проницаемый термоэлемент, компьютерное моделирование, генерация электроэнергии, энергетические характеристики.

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