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TECHNIQUE FOR COMPACT MODELING OF THERMOELECTRIC SYSTEMS

E.V. Zavorotneva, D.A. Indeitsev, A.V. Lukin, I.A. Popov, P.P. Udalov Peter the Great St. Petersburg Polytechnic University, St. Petersburg, Russian Federation

This article describes a technique for modeling a thermoelectric module (TEM) based on a systematic approach using compact models. A finite-element model of a Peltier battery was built in the COMSOL software environment. A numerical analysis of the characteristics of TEM in the case of the dependence of material parameters on temperature is carried out. A compact dynamic TEM model has been constructed and verified on the basis of direct numerical modeling of a number of stationary and non-stationary problems for TEM. The presented approach facilitates the modeling of a thermoelectric module and its interrelationships with control units and other thermal elements under various boundary and initial conditions. The simulation results are in good agreement with the results obtained using other models described in the literature, as well as with numerical solutions. Based on numerical experiments, it is noted that the dependence of the physical parameters of the Peltier battery on temperature can distort the output parameters of the TEM and, if possible, should be taken into account in a compact model.

Keywords: thermoelectric module, system reduction, compact model, Matlab, COMSOL, sssMOR.

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МЕТОДИКА КОМПАКТНОГО МОДЕЛИРОВАНИЯ ТЕРМОЭЛЕКТРИЧЕСКИХ СИСТЕМ

Е.В. Заворотнева, Д.А. Индейцев, А.В. Лукин, И.А. Попов, П.П. Удалов

Санкт-Петербургский политехнический университет Петра Великого, Санкт-Петербург, Российская Федерация

Описана методика моделирования термоэлектрического модуля (ТЭМ) на базе системного подхода с применением компактных моделей. Построена конечно-элементная модель батареи Пельтье в программной среде COMSOL. Проведен численный анализ характеристик ТЭМ в случае зависимости материальных параметров от температуры. Выполнено построение компактной динамической модели ТЭМ и её верификация на основе прямого численного моделирования ряда стационарных и нестационарных задач для ТЭМ. Представленный подход облегчает моделирование термоэлектрического модуля и его взаимосвязей с блоками управления и другими тепловыми элементами при различных граничных и начальных условиях. Результаты моделирования хорошо согласуются с результатами, полученными с использованием других моделей, описанных в литературе, а также с численными решениями. Отмечено, что зависимость физических параметров батареи Пельтье от температуры может искажать выходные параметры ТЭМ и по возможности должна быть учтена в компактной модели.

Ключевые слова: термоэлектрический модуль, редуцирование систем, компактная модель, Matlab, COMSOL, sssMOR.

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Introduction

There are several techniques for thermoelectric process modeling. The first method consists in standard finite element modeling using well-known packages such as COMSOL, ANSYS [1–3]. The second method is based on the numerical integration of differential equations using platforms such as MATLAB Simulink [4, 5]. The third method is based on the construction of equivalent electrical circuits in the SPICE, PSPICE software packages [6–9].

Thermoelectric modules are used in cases where it is impossible to use classical methods or principles of thermostating, which are based on the use of refrigerants, and when active cooling or power generation is required. The field of application of thermoelectric devices is extremely large. Thermoelectric modules are used in solid-state and diode lasers, telecommunications equipment, electronics, various equipment in transport, spacecraft, and also in everyday life. One of the promising directions for the development and application of thermoelectric systems is the development of thermoelectric devices based on microelectromechanical systems (MEMS), which can be used to stabilize the temperature of various high-precision sensors [10, 11]. With the growth of requirements for the performance of microsystem technology, there is a fundamental need for the development of cooling systems for electronic devices. The purpose of this work is to develop a methodology for compact computationally efficient modeling of controlled thermoelectric processes in distributed systems.

Modern numerical tools make it easy to obtain solutions to various physical problems, but a single calculation is not always able to meet the design needs. A way out of this situation is to synthesize approximation models based on direct numerical modeling, which are much simpler in further analysis. It is convenient to combine compact models of individual parts of the system into a single system model of the object under study in Simulink or ANSYS TwinBuilder analysis systems, given that the general view of nonlinearities and the type of converters are not so convenient and clear in direct software implementation at the script level. The construction diagram of the proposed compact model of the thermostating system is shown in the Fig. 1.

Construction order includes the following steps:

1. For the control object and all components of the thermostating system, except for the Peltier elements, a finite element model is built. The computational domain is obtained considering the construction of a denser mesh in places with large thermal gradients, in close proximity to areas of application of thermal loads and near objects of interest from the point of view of the simulation model.

2. The resulting finite element model using the finite element analysis system is uploaded in vector-matrix form to the Matlab software system.

3. On the basis of global matrices, a system in the state space is built and reduced, while the inputs of the model are heat fluxes on the pads of thermoelectric modules and all external loads, and the outputs are the temperatures of sites and those nodes in which the thermal field is of greatest interest. For relatively small models, it is possible to use the built-in functions of the Matlab system (Control System Toolbox). For large models, it is recommended to use the sssMOR methods, which are described in detail in [12].



Fig. 1. Scheme for constructing a compact model of a thermostating system

The order of the reduced model can be determined based on the accuracy requirements of the resulting model with respect to the estimates of the error rate for the Hankel singular eigenvalues of the controllability and observability Grammians.

4. The reduced model is placed in Simulink and connected to a model of effective thermoelectric module, compiled on the basis of the Matlab Simulink built-in tools or the revised scheme on the basis of elements Simscape software package (analog VHDL AMS), intended for modeling and calculation of the generalized Kirchhoff networks.

Compact Simulink TEM model

One of the main problems in the construction of compact models of thermoelectric systems is the mathematical description of a thermoelectric module (TEM) or a Peltier element. A typical TEM consists of an array of NP-pairs of some semiconductor materials. Each NP-pair is connected electrically in series with copper plates and thermally in parallel. The entire structure is enclosed between ceramic plates that form the mounting platforms for the module itself. The simplest view of the Peltier element and the principle of operation of a pair of NP-semiconductors are shown in Fig. 2.

There are five energy conversion processes in the thermoelectric module [13]:

• Conductive heat transfer: the process of transferring energy from warmer parts of the body to less heated parts;

• Peltier effect: the effect of energy transfer during the passage of an electric current at the point of contact of two dissimilar conductors;

• Thomson effect: a phenomenon which consists in the fact that in a homogeneous unevenly heated conductor where an electric current flow, not only heat will be released due to the Joule-Lenz law, but also Thomson's heat will be released or absorbed depending on the direction of the current flow;

• Seebeck effect: the phenomenon of EMF at the ends of series-connected dissimilar conductors, the contacts of which are at different temperatures;

• Joule effect: the heating effect observed in a conductor when an electric current is passed through the conductor.

In the literature, there are many methods for modeling thermoelements (TE). One of these methods is three-dimensional modeling in a coupled thermoelectric formulation, which is based on the finite element



Fig. 2. Scheme and principle of operation of TEM



Fig. 3. The proposed effective scheme for modeling a thermoelement

method (ANSYS, COMSOL, Fluent). Another method for modeling TE is based on the electrothermal analogy and the construction of equivalent RC circuits, calculated, for example, in SPICE. In work [6], an effective scheme for modeling TEM was proposed, shown in Fig. 3. This model of a thermoelectric module is divided into two main parts. The first simulates only thermoelements in a form of a thermoelectric physics simulation. This one-dimensional model divides the thermocouple into discrete lengths. This discretization simulates distributed heat flux and mass. The material properties of the fuser are calculated for each finite element.

The second part of the model describes the other components of that module, except for the thermoelectric elements themselves. Additionally, thermal boundary conditions on the TEM surface are set here. The advantage of such schemes is the ability to simulate essentially non-stationary processes [16–18]. It is known that when a current pulse is applied, an instantaneous lower temperature is achieved on the cold side of the TEM. The cold side temperature decreases to a minimum and then rises above the steady state value to a maximum. Then it decreases exponentially to a steady-state value. Increased Peltier cooling is a transient effect that only occurs at the cold junction of each pair.

In this work, we neglect the heat release associated with the Thomson effect. This is due to the objective smallness of the arising heat sources. The idea of synthesizing an effective model of a Peltier element is to describe the heat fluxes developed by it as functions of the temperatures of the cold and hot sides, as well as the applied electric voltage or current. According to [14], the total heat flux through the cold and hot sides of the NP-junction has the form:

$$q_c = \frac{\Delta T}{\Theta_m} + \alpha_m T_c I - \frac{I^2 R_m}{2},\tag{1}$$

$$q_h = \frac{\Delta T}{\Theta_m} + \alpha_m T_h I + \frac{I^2 R_m}{2},\tag{2}$$

$$\alpha_m = \alpha N, \tag{3}$$

$$R_m = RN,\tag{4}$$

$$\Theta_m = \Theta/N, \tag{5}$$

where N – number of thermocouples; $R = \frac{L(\tilde{\rho}_n + \tilde{\rho}_p)}{A}$ – electrical resistance, Ohm; L – conductor length, m; A – cross-sectional area, m²; $\tilde{\rho}_n, \tilde{\rho}_p$ – resistivity of n and p semiconductors, Ohm·m; $\theta = \frac{L}{(k_n + k_p)A}$ – thermal resistance of the conductor, K/W; k_n, k_p – thermal conductivity coefficients

of *n* and *p* type materials, $W/m \cdot K$.

The electrical part of the system is described by the following expression:

$$V = \alpha_m T_e - \alpha_m T_a. \tag{6}$$

The approach of compact modeling of TEM is based on an exact analytical solution to the problem of the thermal state of a homogeneous conducting material, considering thermoelectric effects. A detailed solution to this problem is given in the article [14]. The obtained relation for the profile of temperature and heat fluxes makes it possible to analyze the regime of the maximum temperature difference and give an estimate for the parameters of this regime: the flowing current and voltage. In the TEM specifications, the manufacturer always indicates the parameters ΔT_{max} , I_{max} and V_{max} , since they are the main characteristics when completing the system and choosing the required module. The final ratios can be written as follows:

$$\Delta T_{\max} = T_h + \frac{1 - \sqrt{1 + 2T_h Z}}{Z},\tag{7}$$

$$I_{\max} = \frac{\sqrt{1 + 2T_h Z} - 1}{\alpha_m \Theta_m},\tag{8}$$

$$V_{\max} = \alpha_m T_h, \tag{9}$$

where the material parameter $Z = \frac{\alpha_m \Theta_m}{R_m}$; ΔT_{max} – maximum temperature difference between the cold and hot sides of the TEM; I_{max} – current providing maximum temperature difference ΔT_{max} ; V_{max} – voltage corresponding to optimal current I_{max} .

Solving the above system of equations with respect to the model parameters $(\alpha_m, R_m, \Theta_m)$, we obtain the following formulae for determining the parameters of the effective model:

$$R_m = \frac{V_{\max} \left(T_h - \Delta T_{\max} \right)}{I_{\max} T_h} [\Omega], \tag{10}$$

$$\Theta_m = \frac{2\Delta T_{\max} T_h}{I_{\max} V_{\max} \left(T_h - \Delta T_{\max}\right)} \left[\frac{\mathbf{K}}{\mathbf{W}}\right],\tag{11}$$

$$\alpha_m = \frac{V_{\text{max}}}{T_h} \left[\frac{\mathbf{V}}{\mathbf{K}} \right]. \tag{12}$$

Since the calculated material parameters are the characteristics of the entire module, and to build an effective TEM model, the parameters of each individual element are required, it is necessary to calculate these parameters using the manufacturer's database. Following the web-site of the manufacturer Kryotherm [15], a universal abbreviation of the type TB-N-C-h is used for the names of single-stage modules. TB stands for thermoelectric battery (module); N is the number of thermoelectric pairs in the module; C is the length of the edge of the base of the thermoelectric element (in millimeters); h is the height of the thermoelectric element (in millimeters). The manufacturer also provides information on the dimensions of the thermoelectric module, namely the total height of the module and the width of the ceramic plates. The material of ceramic plates in standard delivery conditions is Al₂O₂ ceramics. Material properties for copper conductors in TEM can be neglected due to their relatively small size. This means that using the obtained generalized material properties of TEM and knowing the properties of the material and the geometry of ceramic insulators, one can find the necessary parameters for constructing the RC TEM model. The total thermal resistance will now be the sum of two terms, the first is responsible for thermoelectric elements, the second is for ceramic plates. In this case, the effective Seebeck coefficient and electrical resistance do not need to be divided into components, since these effects occur only in a thermoelectric element and have no relation to ceramics:

$$\Theta_m = \Theta_{te} + \Theta_c \left[\frac{\mathrm{K}}{\mathrm{W}}\right]. \tag{13}$$

The thermal resistance of a ceramic plate can be calculated using the formula for the thermal resistance of a section of a constant section circuit:

$$\Theta_c = \frac{l}{\lambda S} \left[\frac{\mathbf{K}}{\mathbf{W}} \right],\tag{14}$$

where l – thermal circuit length, m; λ – material thermal conductivity coefficient, W/(m·K); S – cross-sectional area of a site, m².

Thermoelements in TEM have parallel resistance, which means that the thermal resistance of one thermoelement is calculated as:

$$\Theta_N = 2N \left(\Theta_m - 2\Theta_c\right) \left[\frac{\mathrm{K}}{\mathrm{W}}\right],\tag{15}$$

where N – number of thermocouples in TEM.

The value for electrical resistance and the Seebeck coefficient are calculated similarly:

$$R_N = \frac{R_m}{2N} [\Omega], \tag{16}$$

$$\alpha = \frac{\alpha_m}{2N} \left[\frac{V}{K} \right]. \tag{17}$$

Since the effective model proposed in the section divides the thermoelement into discrete elements along their length, which are connected in series both thermally and electrically, the material properties of each individual discrete element are calculated as

$$R = \frac{R_N}{n} [\Omega], \tag{18}$$

$$\Theta = \frac{\Theta_N}{n} \left[\frac{\mathrm{K}}{\mathrm{W}} \right],\tag{19}$$

where n – number of discrete elements along the length of one thermoelement.

Analysis of formulas (7)–(8) shows that the integral parameters of the thermoelectric module are calculated at a certain temperature. In order to determine the accuracy of the model built using the basic parameters, it is necessary to calculate these parameters for a certain range of temperature values and estimate how strongly the parameters depend on temperature. Consider the TB 31-1.0-2.5 module, one of the thermoelectric cooling modules available on the Kryotherm manufacturer's website [15]. For $T_h \in [260 \text{ K}, 400 \text{ K}]$, a calculation was performed to find the integral characteristics of the module ΔT_{max} , I_{max} and V_{max} , taking into account that the material properties of the thermoelectric element are constants and the material parameters are direct functions of temperature. The boundary conditions are shown in the Fig. 4.

Fig. 5-7 show the dependence of the module parameters on the change in the hot side temperature. Obviously, these dependencies cannot be neglected, just as it is assumed that the module parameters are constants.

From the analysis of the results obtained, it can be concluded that when modeling thermoelectric processes in TEM, it is necessary to consider the dependence of the operating characteristics of the module on the operating temperature. It is also necessary to consider the dependence of material properties on the temperature.



Fig. 4. Boundary conditions for calculating the maximum characteristics of TEM



Fig. 5. Maximum temperature difference ΔT_{max} depending on the temperature on the hot side (-) – functional parameters; (- -) – constant parameters



Fig. 6. Maximum voltage V_{max} depending on the temperature on the hot side (-) – functional parameters; (- -) – constant parameters



Fig. 7. Maximum current I_{max} depending on the temperature on the hot side (-) – functional parameters; (- -) – constant parameters

Based on the obtained dependencies, as well as the diagram shown in Fig. 3, a compact model for TB-31-1.0-2.5 was built in the Matlab Simulink software package, shown in Fig. 8. Using an electrical analogy, heat effects are represented by an equivalent electrical circuit in which temperature and heat flux are given as voltage and current, respectively. Resistors and capacitors consider the thermal resistance and thermal capacitance of the finite element, and the current source characterizes the heating. Inside each unit element (region C) there is one current source responsible for Joule heating, two series-connected resistors responsible for the thermal resistance of the element, and three capacitors responsible for the heat capacity. The electrical part (area B) consists of an electrical resistance (resistor) in series with the electrical current. An additional voltage source simulates the Seebeck voltage. The complete circuit contains two additional current sources responsible for the Peltier effect. They are located on both sides of the thermoelement submodel, since the Peltier effect occurs precisely at the material boundary. The studied TEM consists of several thermoelements, which means that it is necessary to put a current amplifier (heat flow) at the junction of materials in the circuit. Further, on both sides of the circuit, only ceramic plates are modeled using two series resistors, which are responsible for the thermal resistance, and one capacitor, which is responsible for the heat capacity of the plate.

The verification of the adequacy of such a model was carried out by comparing the simulation results with the results obtained by direct finite-element (FE) analysis. Fig. 9 shows the dependence of the cold side of the thermoelectric module on time at an applied alternating current.

Numerical study of the super-cooling effect for a model of one thermoelectric element. Let us turn to the study of the possibilities of modeling essentially non-stationary thermoelectric processes using the proposed compact model, presented in Fig. 10.



Fig. 8. An effective scheme of the module TB 31-1.0-2.5 in Simulink



Fig. 9. Dependence of the temperature of the cold side of the TEM on time with an applied alternating electric current (--) - FULL FEM; (-) - RC-model



Fig. 10. Geometric model of thermoelectric element

In the present example, the case is considered when the lower conductor is maintained at a constant temperature $T_0 = 300$ K, while a constant electric current $J_0 = 0.7 \frac{\text{MA}}{\text{m}^2}$ is set on the cross section of the upper conductor.

A non-stationary process in a thermocouple is modeled both by the finite element method in a two-sided coupled thermoelectric formulation, and using a compact model.

The material parameters in the constructed effective model are functions of the operating temperature, and correspond to the material parameters for the full FE model. When simulating the effect of overcooling, a stepped current pulse with an amplitude of $2.5I_{max}$ and a duration of 2 sec was used. Fig. 11 shows a comparison of the simulation of the effect using a compact model of thermoelectric element, as well as a



Fig. 11. Dependence of the thermoelement temperature on the cold side as a function of time, with an applied impulse current (- - -) – Simulink; (- - -) – COMSOL

complete FE. The two models predict almost the same dynamic characteristics of the temperature of the cold side of the thermoelement, which indicates that this compact model can be used to simulate substantially unsteady thermoelectric processes.

As can be seen from the coincidence of the curves, the compact model adequately describes the complete FE model of the TE. The constructed compact model can be used for quick calculations of non-stationary processes in an object with varying values of controlled parameters, as well as for forming a high-level system (for example, a high-precision measuring device as a thermal model of the device design + thermoelectric models of Peltier elements). The model also considers the dependence of material properties on temperature. The advantage of the presented compact model is that it requires much less time for numerical integration (1–5 minutes) than direct finite element analysis, the calculation of which can take within 2–5 hours (for a FE model containing about 30,000 elements).

Numerical methods of algebraic reduction of systems of large dimension

The exact modeling of dynamic systems almost always leads to a large number of differential equations and state variables ($n \ge 10^4$) which describe the behavior of the system over time. For example, when discretizing partial differential equations on a spatial grid, or when modeling systems with a large number of components, such as integrated circuits. The applications in which large-scale models emerge are numerous and cover different areas: space industry, various MEMS devices, and even simulation of biochemical systems.

Such models, especially in control theory, are often formulated in the state space representation (20), where the state vector $x \in \mathbb{R}^n$ describes the state of the system at each moment of time:

$$\dot{x} = Ax + Bu,$$

$$y = Cx + Du,$$
(20)

or in an alternative form:

$$M_c \dot{x} = M_c A x + M_c B u,$$

$$y = C x + D u.$$
(21)

Form (21) is more suitable for large systems because the matrices M_C and M_CA tend to become sparser than A. With ever-increasing modeling requirements, the order of the model can become excessively large $(n \ge 10^4)$. This creates big problems for the numerical processing of such models, primarily due to storage limitations. In fact, even in the simpler but common case of linear systems, maintaining a matrix of this size can become a difficult task.

The problem is that it takes too much memory to store all the elements of the matrix, which is impossible on a standard computer. In [12], a set of tools Sparse State-Space and Model Order Reduction (sssMOR) is presented, which overcomes this disadvantage by defining sparse objects of state space, that is, dynamical systems defined using sparse matrices. This allows both to store large-scale models with hundreds of millions of state variables and to use the sparsity of system matrices to reduce the computational load of their analysis.

In order to reduce computational resources in large-scale models, it is convenient to use Reduced Order Model (ROMs) of a much smaller order $q \ll n$, which fix the corresponding dynamics. Using the sssMOR module makes it possible to analyze dynamical systems with a state-space dimension greater than $n = 10^4$, which is usually the limit for Matlab built-in functions. It is also shown in [12] that the use of sss and sssMOR is very beneficial in terms of memory and computational resource requirements, even for medium-sized tasks ($n \approx 10^3$), and allows you to analyze models that otherwise would be unavailable.

Consider the following heat conduction problem for a rectangular region. The finite element model and boundary conditions are shown in Fig. 12.

Boundary condition on the lower face or Dirichlet condition:

$$T\Big|_{y=0} = T_0 = 273 \text{ K.}$$
 (22)

Heating F is supplied to the input, which is equal to

$$F = 1000 \frac{BT}{M^2}.$$
 (23)

We significantly refine the FE model mesh and extract the system in state variables using the parameter Q as the input variable and the temperature at the point of interest $T_1\left(\frac{a}{2}, \frac{b}{2}\right)$ as the output variable.

When using such a FE model, the system in state variables in full format can no longer be unloaded due to memory constraints, which means that it becomes necessary to use the sssMOR toolbox. To overcome the limitations of object storage, a sparse state space class is created. This class allows you to define sss objects, that is, state-space systems that are defined using sparse matrices.



Fig. 12. Finite element formulation of the problem



Fig. 13. Bode diagrams for the original and reduced systems (-) – sssSystem; (- -) – rkMetod; (- - -) – irkaMetod

We can obtain a reduced model of the system in state variables, with the help of reduction methods in a sparse form. Fig. 13 shows Bode diagrams for the original and reduced systems using 50 state variables. As can be seen from the comparison of the curves, the reduced model using only 50 variables provides

a good approximation of the original system over a wide frequency range.

Verification of methods for compact modeling of thermoelectric systems

The proposed technique for compact modeling of thermoelectric systems was tested on a model of some high-precision measuring device containing a thermostating system, shown in Fig. 14. The model is a simplified physical and geometric description of all components of the device, except for Peltier batteries. In this model, thermoelectric modules are replaced by the boundary conditions of heat fluxes at the contact areas. On radiators, the condition of convection with an environment with a fixed ambient temperature is applied.

For the constructed FE model, the system in state variables in a sparse format was extracted using the COMSOL LiveLink [™] for Matlab module. The inputs to this system in state variables are heat fluxes on



Fig. 14. Finite element model of sensor

the pads of thermoelectric modules and all external loads (ambient temperature), and the outputs are the temperatures of the corresponding pads, as well as the temperature value at the points of interest (locations of temperature sensors).

The reduced thermal model was integrated into the Simulink system and connected to an efficient thermoelectric module model. The resulting complete compact model in the Matlab Simulink system is shown in Fig. 15.

The following are the results of numerical simulation of controlled thermal processes in the device case when voltage is applied in manual mode in accordance with the graphs shown in Fig. 16.

Fig. 17 shows a graph of the temperature measured by the sensor during the experiment with changing the control voltage on the Peltier elements in manual mode.

The constructed system model allows simulating various scenarios of thermal loading of the sensor and the operation of the existing control algorithms for the temperature stabilization system.

The proposed approach allows solving such problems as: design optimization, selection of the optimal configuration of thermoelectric modules, synthesis of control algorithms for the thermostating system, considering the specific physical characteristics of the device of the required design.



Fig. 15. Compact thermoelectric model



Fig. 16. The graph of the change in the applied voltage to the Peltier elements



Fig. 17. The measured temperature on the sensors of the device when changing the control voltage on the Peltier elements in manual mode (-) - Sensor 1; (-) - Sensor 2

Conclusion

Based on the results of the accomplished work, we developed and verified a fairly general method of computationally efficient modeling of non-stationary thermoelectric processes in controlled systems. The paper describes the stages of building a model, boundary conditions for obtaining load vectors, and their application in the synthesis of a model in the state space. The reduction of the model is carried out and the transient processes to typical actions are studied. The proposed compact model has a number of advantages, namely: it requires much less time for numerical integration, it has the ability to consider the dependence of material properties on temperature, and allows simplified modeling of not only thermoelectric modules, but also the corresponding thermal FE models. The resulting compact model greatly simplifies the analysis of such systems, and also allows you to quickly and efficiently select the optimal control, which cannot be done in a conventional finite element calculation. Based on the results obtained, it can be concluded that the proposed method for constructing system models should find extensive application in the design and analysis of thermoelectric controlled processes.

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THE AUTHORS / СВЕДЕНИЯ ОБ АВТОРАХ

Zavorotneva Ekaterina V. Заворотнева Екатерина Владимировна E-mail: zavorotneva.ev@gmail.com

Indeitsev Dmitry A. Индейцев Дмитрий Анатольевич E-mail: Dmitry.indeitsev@gmail.com

Lukin Aleksei V. Лукин Алексей Вячеславович E-mail: lukin@compmechlab.com

Ророv Ivan A. Попов Иван Алексеевич E-mail: popov_ia@spbstu.ru **Udalov Pavel P.** Удалов Павел Павлович E-mail: pp_udalov@mail.ru

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