DOI: 10.6060/ivkkt.20206307.6206

УДК: 536.2.02

ТЕОРЕТИЧЕСКОЕ ИССЛЕДОВАНИЕ ТЕПЛОПРОВОДНОСТИ В МНОГОСЛОЙНОМ СФЕРИЧЕСКОМ ТЕЛЕ С ФАЗОВЫМИ ПЕРЕХОДАМИ В СЛОЯХ

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Целью исследования является построение простой, но информативной математической модели, которая описывает теплопроводность в многослойном сферическом теле с фазовыми переходами в слоях. Для численного решения этой задачи предложена численная схема, базирующаяся на теории цепей Маркова. Радиальный сектор тела разделен на конечное число ячеек идеального перемешивания различного объема, которые формируют цепь ячеек. Теплообмен между ячейками описан матрицей теплопроводности, элементы которой зависят от локальных теплофизических свойств материала в ячейках (коэффициент теплопроводности, плотность, удельная теплоемкость). Эти свойства могут изменяться от одной ячейки к другой и с течением времени. Внешняя ячейка цепи может обмениваться теплотой с окружающей средой, температура которой может меняться во времени. Состояние процесса наблюдается в дискретные моменты времени, разделенные малой, но конечной продолжительностью перехода. Если температура в ячейке достигает величины, при которой начинается фазовый переход, эволюция термического и фазового состояния ячейки описывается соответствующим кинетическим уравнением фазового перехода. Для качественной верификации модели в качестве примера рассмотрен процесс плавления-отвердевания в слоях тела. Приведены графики изменения распределения температуры и фазового состояния в сферическом многослойном теле. Полученные результаты по эволюции термического и фазового состояния шара не противоречат физическому смыслу процесса. Предложенный алгоритм требует незначительных затрат машинного времени (1-3 мин для расчета одного режима). Другие процессы фазовых переходов могут быть легко подключены к модели, например, сушка, экзотермические и эндотермические, химические реакции и другие.

Ключевые слова: теплопроводность, фазовый переход, многослойное сферическое тело, ячеечная модель, плавление, отвердевание, распределение температуры, распределение содержания фаз

Для цитирования:
Мизонов В.Е., Митрофанов А.В., Басова Е.В., Шуина Е.А., Tannous K. Теоретическое исследование теплопроводности в многослойном сферическом теле с фазовыми переходами в слоях. *Изв. вузов. Химия и хим. технология*. 2020. Т. 63. Вып. 7. С. 54–60

For citation:
Mizonov V.E., Mitrofanov A.V., Basova E.V., Shuina E.A., Tannous K. Theoretical study of heat conduction in multilayer spherical body with phase transformation in layers. *Izv. Vyssh. Uchebn. Zaved. Khim. Khim. Tekhnol*. [Russ. J. Chem. & Chem. Tech.]. 2020. V. 63. N 7. P. 54–60

THEORETICAL STUDY OF HEAT CONDUCTION IN MULTI-LAYER SPHERICAL BODY WITH PHASE TRANSFORMATION IN LAYERS

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The objective of the study is to build a simple yet informative mathematical model that describes the heat conduction in a spherical multi-layer body with phase transformation in the layers. The numerical scheme based on the theory of Markov chains is proposed to solve this problem numerically. The radial sector of the body is divided into finite number of spherical perfectly mixed cells of different volume, which form a chain of cells. The heat exchange between the cells is described with the heat conduction matrix, the entries of which depend on the local thermophysical properties of material in the cells (heat conduction coefficient, density, specific heat capacity). These properties can vary from one cell to another and with time. The outer cell of the chain can exchange with heat with outside environment, the temperature of which can vary with time. The state of the process is observed in discrete moments of time separated by small but finite transition duration. If the temperature of a cell reaches the value, the phase transformation begins at which, the evolution of the cell thermal and phase state is described with the corresponding kinetic equation of the phase transformation. The process of melting and solidification is used as the example to verify the qualitative predictability of the model. The graphs of temperature distribution evolution and diagrams of phase content distribution in a multi-layer spherical body are presented. The obtained results on the evolution of the thermal and phase state of the ball have no contradiction to the physical sense of the process. The proposed algorithm has very low computational time (1-3 min for one regime). The other processes of the phase transformation can be easily implemented in the model, for instance, drying, exothermic and endothermic chemical reactions, etc.

Key words: heat conduction, phase transformation, multi-layer spherical body, cell model, melting, solidification, temperature distribution, phase content distribution

INTRODUCTION

The problem of non-linear heat conduction arises in many technologies connected with thermal treatment of metals, particulate solids, or construction materials. Very often physicochemical processes inside the medium complicate such problems where heat conduction occurs. In general, it is a problem of heat conduction in a composite domain of complex boundaries and temperature-dependent thermophysical properties of the media inside it. It is not realistic to obtain an analytical solution to the problem. All attempts to do that require far-going assumptions that do not fit the case in question.

A new analytical method is presented in [1], which provides close-formed solutions for both transient indoor and outdoor temperature changes in buildings. Time-dependent boundary temperature is presented as Fourier series. Applying the periodic properties of the boundary condition, an approximate analytical solution for heat transfer is obtained. However, the method is valid only for one-dimensional heat transfer in a plane wall that does not allow taking into account non-homogeneity of the wall in principle. The paper [2] proposes a new strategy for fine time resolution on the calculation of the response factors through Laplace's method considering a comparison with the performance of the State Space method when used to calculate conduction transfer functions. It was emphasized in [3] that as a rule, the exterior layers of building envelope usually experience seasonal freezing/thawing in winter that can reduce the thermal resistance about 7% and more, and it is inadequate to keep thermo-physical parameters constant in modeling.

It was emphasized in [4, 5] that any non-homogeneity in a building envelop structure forms a so-called thermal bridges. The paper [4] is concerned with minimizing thermal bridging through typical window systems in buildings of hot regions. The approach to modeling used is based on an integrated 3D dynamic simulation. It is found that the thermal bridging through typical window systems is significant and should be taken into account in buildings design. It is obvious that a simple but effective mathematical tool is required to estimate the heat loss caused by such bridges. The method of the equivalent thermal wall employed for modeling the transient response of high-inertial thermal bridges was reported in [5]. It was shown that if the thermal bridge was not considered, an underestimation of 25% in the heat flux across the bridge was predicted. However, the approach does not take into account the possible variation of thermophysical properties of a wall material due to moisture freezing/thawing and deals with two types of the bridge topology only. The paper [6] shows a new method for implementing bi-dimensional and three-dimensional heat transfer in dynamic energy simulation software. It allows modeling heat flows in a multi-dimensional structured wall due to discontinuities in both materials and geometry. According to our viewpoint, presentation of a thermal process in the state space is a very interesting and fruitful approach. However, the phase transformation of moisture inside a wall material is not taken into account in this work.

An interesting method for semi-analytical solution of different variants of heat conduction equation was proposed in [7-10]. The method is based on an analytical solution of the heat conduction equation with respect to a spatial co-ordinate that changes from one time step to another. It allows taking into account variation of time and temperature dependent properties of a heated medium during the process. However, the method was used for a single layer medium only. The papers [11-13] describe application of the method of cellular automata to solve such problems. The presented examples of its application to solve several particular problems show that this tool is effective. However, it does not follow from the examples how the method can be used for the problem in question.

According to the authors' viewpoint, one of the most effective tools to solve such problems is the theory of Markov chain. The fundamentals of its application in chemical engineering are described in [14]. It was successfully applied to solve various problems of heat and mass conduction: numerical study of melting a rod by a periodically moving local heat source [15], theoretical study of the thermal state of building envelop in the neighborhood of embedded item [16], modeling the heat state of a cross section of heat insulated pipeline [17], modeling the moisture content distribution in a rotating porous cylinder [18], modeling the heat conduction in a rink domain with non-stationary boundary conditions [19], modeling the phase transformation in a spherical droplet at cooling [20].

Nevertheless, the demonstrated examples do not cover all aspects of the problem in question, and additional investigation is needed to solve the problem as it was formulated.

THEORY

Fig. 1 shows schematically the cell structure of the model. The process is supposed spherically symmetrical. Fig. 1a shows the spherical sector of the body. It contains several layers of different thermophysical properties (3 layers are shown as an example). The sector is divided into m perfectly mixed cells of identical radial length $\Delta r = R/m$. The volumes of the cells are different and can be calculated by the following formula

$$V_j = \left(\frac{r_j}{R}\right)^z S_R \Delta r \qquad (1)$$

where S_R is the area of the outside surface of the sector. It is taken equal to 1 in further modeling. The power z allows adjusting this formula to different co-ordinate systems: z = 2 for the spherical co-ordinates, z = 1 for the cylindrical ones, and z = 0 for the plane one-dimensional one.

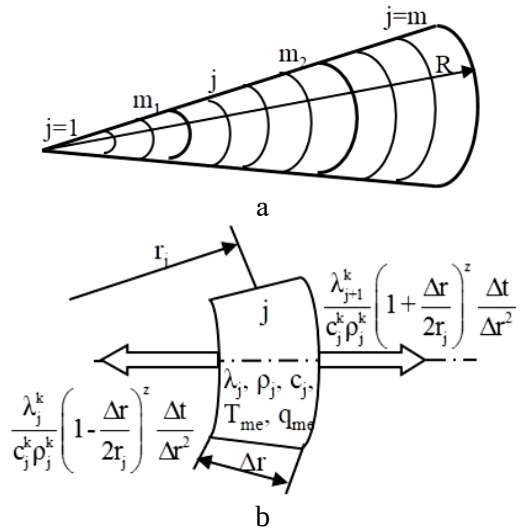

Fig. 1. Computational scheme of the model: a – division of spherical sector into the chain of cells, b – heat transfer from the j-th cell during a single time transition

Рис. 1. Расчетная схема модели: a – разделение сферического сектора на цепь ячеек, b – перенос теплоты из j-ой ячейки в течение одного временного перехода

Fig. 1b shows a separate cell: its dimensions and the amount of heat that transits to the neighboring cells j+1 and j-1 during the single time transition Δt. Using Δt, the current time of the process can be calculated as $t_k = (k-1)\Delta t$ where k is the number of the current time transition (the discrete analogue of time). The material properties and the process parameters are arranged as the column vectors of the size m×1. For example, **λ**, **ρ** and **c** are the vectors of the heat conduction coefficients, densities and specific heat capacities of the cells, **Q** and **T** are the vectors of the heat and temperature in the cells, **V** and **M** are the vectors of the cells volume and their mass. It allows writing the computational formulas in compact notation. For instance, the correlation between heat and temperature can be written in the following form:

$$\mathbf{Q = T.*\rho.*V.*c},$$

where the symbol «**.***» means the element by element multiplication of vectors.

The properties of the material and process parameters vary with time. During the single time transition Δt, the state k transits into the state k+1. The first stage of the process modeling is to describe the vector **Q** evolution due to pure heat conduction without taking into account the external and internal heat sources. This evolution can be describes by the recurrent formula

$$\mathbf{Q^{k+1} = P^k Q^k} \qquad (2)$$

where $\mathbf{P^k}$ is the matrix of heat conduction (the matrix of transition probabilities in terms of the Markov chains theory) that depends on the thermal state of the chain in its state k. It is a tri-diagonal matrix, the rules of its entries constructing are described in details in [15-20]. The formulas are listed below:

$$P^k_{j,j+1} = \frac{\lambda^k_{j+1}}{c^k_{j+1}\rho^k_{j+1}}\left(1 - \frac{\Delta r}{2r_{j+1}}\right)^2 \frac{\Delta\tau}{\Delta r^2},\ j = 1,..,\ m\text{-}1 \qquad (3)$$

$$P^k_{j+1,j} = \frac{\lambda^k_{j+1}}{c^k_j\rho^k_j}\left(1 + \frac{\Delta r}{2r_j}\right)^2 \frac{\Delta\tau}{\Delta r^2},\ j = 1,..,\ m\text{-}1 \qquad (4)$$

$$P^k_{j,j} = 1 - P^k_{j+1,j} - P^k_{j\text{-}1,j},\ j = 1,..,\ m \qquad (5)$$

The multiplies in parentheses play the role of Lamé coefficients for the generalized co-ordinate system. As it was mentioned above, the power z allows adjusting these formulas to different co-ordinate systems: z = 2 for the spherical co-ordinate (the case in question), z = 1 for the cylindrical one, and z = 0 for the plane one-dimensional one. Thus, Eqs. (3,4) can be used for any system of co-ordinate that makes the model more universal.

After calculating the heat distribution over the cells due to heat conduction, the temperature distribution can be calculated as follows:

$$\mathbf{T^{k+1} = Q^{k+1}./\rho./V./c}, \qquad (6)$$

where the symbol «**./**» means element by element division of vectors.

The next step of modeling is taking into account heat sources acting in the process during Δt. The heat exchange of the body with environment brings correction into the vector $\mathbf{Q^{k+1}}$:

$$\mathbf{Q_m^{k+1} := Q_m^{k+1} + \alpha(T_{out} - T_m^k)\Delta t}, \qquad (7)$$

where «:=» is the operator of assignment, α is the heat transfer coefficient. After that, it is necessary to renew the temperature distribution using Eq.(6).

The further step connected with the phase transformation is more complicated. For the sake of determinacy, suppose that the phase transformation occurs due to melting of a low-melt material in the intermediate layer surrounded by the layers of high-melting materials (see Fig. 1). It means that the low-melt material occupies the body from the cell j = m_1+1 to the cell j = m_2. It is supposed that at the initial moment of time all the layers are in the solid state, and the vector of solid mass in the cells can be calculated as $\mathbf{M_s = V.*\rho}$. Respectively, the vector of liquid mass $\mathbf{M_L}$ is the zero column vector.

At every time state, the cells of the low-melt layer between j = m_1+1 and m_2 are checked for their thermal and phase state. If $T_j^{k+1} > T_j^k$ (the process of heating the body) and $T_j^{k+1} > T_{me}$ but $M_{Lj}^{k+1} = M_{Sj}$ (melting in the cell is over), the temperature T_j^{k+1} remains the same. Otherwise, melting begins or continues. The heat that is absorbed for melting during Δt is

$$\Delta Q^{k+1}_{me} = (T^{k+1}_j - T_{me})c^k_j\rho^k_j V_j \qquad (8)$$

that leads to appearing of the liquid mass

$$\Delta M^{k+1}_{Lj} = \Delta Q^{k+1}_{me}/q_{me} \qquad (9)$$

The new state of the cell becomes

$$Q^{k+1}_{me} := Q^{k+1}_{me} - \Delta Q^{k+1}_{me} \qquad (10)$$

$$M^{k+1}_{Lj} := M^{k+1}_{Lj} + \Delta M^{k+1}_{Lj} \qquad (11)$$

$$T_j^{k+1} = T_{me} \qquad (12)$$

$$M_{Lj}^{k+1} = M_{Sj},\ \text{if}\ M_{Lj}^{k+1} > M_{Sj} \qquad (13)$$

If $T_j^{k+1} < T_j^k$ (the process of cooling the body), the sign at the right hand part of Eq.(8) becomes negative, and Eqs. (8)-(13) describe the process of the low-melt material solidification.

Thus, the model allows describing the process in multi-layer ball with melting/solidification of the layers.

RESULTS AND DISCUSSION

The numerical analysis of the model described above was done for a tri-layer ball of the radius R = 0.1 m, divided into m = 20 cells of the radial length Δr = 0.005 m. The edge layers are supposed to be of the high-melting type, the middle layer being low-melt with the melting point T_{me} = 40 °C and the latent heat

of melting $q_{me} = 1 \cdot 10^5$ J/kg. It is also supposed that the density and specific heat capacity is identical for all of the layers and are 1000 kg/m^3 and 400 J/kg·°C respectively. The heat conduction coefficient of the edge layers is 0.8 W/m·°C; of the middle (low-melt) layer 0,2 W/m·°C. The initial temperature of the entire ball is $T_j^1 = 20$ °C. The external heat source with the temperature $T_{out}^k = 80$ °C and the heat transfer coefficient $\alpha = 20$ W/m^2 acts on the ball from outside. The calculations were done for $\Delta t = 3$ c.

The first example of modeling concerns the case when the low-melt layer reaches the center of the ball (in fact, it is a two-layer ball). This material occupies the cells j = 1,…,14, and the high-melting material occupies the cells j = 15,…,20.

The evolution of the temperature distribution over the ball radius is shown in Fig. 2. The first stage of the process is heating the ball until the temperature in the cell 14 reaches the melting point. After that, melting begins, which propagates to the ball center until the entire low-melt material becomes liquid. The temperature remains constant and equal to the melting point during this period. When the melting is over, heating the ball continues until it becomes heated up to the outside temperature.

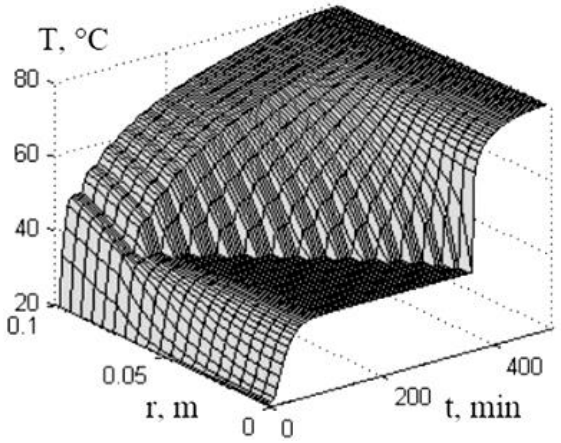

Fig. 2. Evolution of the temperature distribution over the ball radius in the two-layer ball

Рис. 2. Изменение распределения температуры по радиусу в двухслойном шаре

The evolution of the phase state of the ball is shown in Fig. 3 as a solid/liquid diagram. It corresponds to the graph shown in Fig. 2, and shows the propagation of the front of melting.

The next example concerns with the heating of a tri-layer ball with the low-melt layer in the middle. The layers are placed as follows: the high-melting layers occupy the cells j = 1,…,5 and j = 15,…,20, and the low-melt layer is placed in between. The external heat source begins to act at the beginning of the process and stops at t = 400 min. Fig. 4 illustrates the evolution of the temperature distribution during the process.

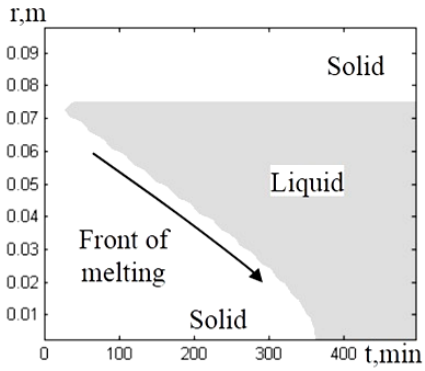

Fig. 3. The phase state diagram during heating the two-layer ball

Рис. 3. Диаграмма фазового состояния при нагреве двухслойного шара

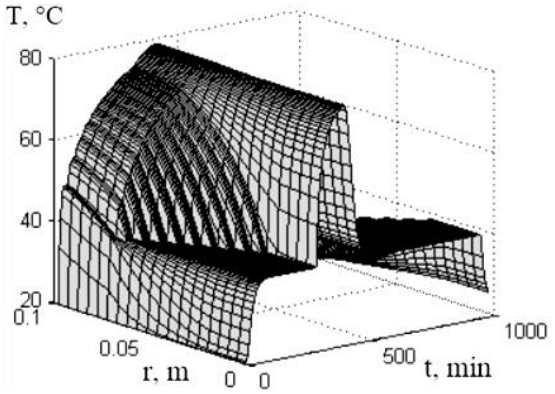

Fig. 4. Evolution of the temperature distribution over the ball radius in the tri-layer ball

Рис. 4. Изменение распределения температуры по радиусу в трехслойном шаре

The beginning of the process is similar to one shown in Fig. 2 but the melting propagates not to the ball center but to the external border of the internal layer. After the external heat source stops acting, cooling the ball begins. When the temperature of the cell j = 6 reaches the solidification temperature (which is equal to the melting point) the process of solidification begins, which propagates to the external border of the intermediate low-melt layer. After the solidification of the entire layer is over, the cooling of the ball continues up to the outside temperature.

The phase state diagram is shown in Fig. 5. It also corresponds to the data presented in Fig. 4. The propagation of the fronts of melting and cooling can be clear seen in the diagram. The completely melted layer exists between 300 and 440 min.

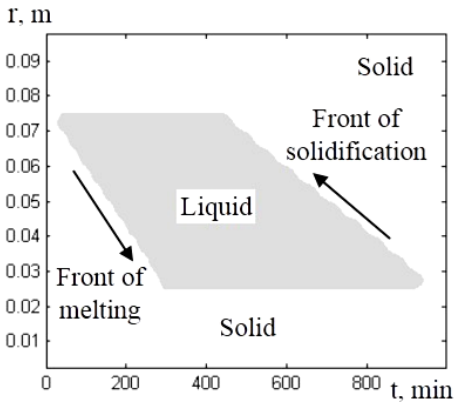

Fig. 5. The phase state diagram during heating and cooling the tri-layer ball

Рис. 5. Диаграмма фазового состояния при нагреве и охлаждении трехслойного шара

At last, Fig.6 shows the temperature variation of some particular cells. The dashed line 1 shows variation of the temperature of the external heat source. The lines 2 and 4 are related to the last and the first cell respectively. The line 3 concerns with the middle cell of the low-melt layer. All of the lines have no contradictions to the physical sense of the process.

CONCLUSIONS

The proposed mathematical model based on the theory of Markov chains allows describing the non-linear heat conduction in a multi-layer ball with phase transformation in the layers. The presented example of heating and cooling the tri-layer ball with melting and solidification of the intermediate layer approved predictability of the model, which allowed calculating the thermal and phase state evolution during the process with variable temperature of the external heat source. The obtained results on the evolution of the thermal and phase state of the ball have no contradiction to the physical sense of the process. The proposed algorithm has very low computational time (1-3 min for one regime). The other processes of the phase transformation can be easily implemented in the model, for instance, drying, exothermic and endothermic chemical reactions, etc.

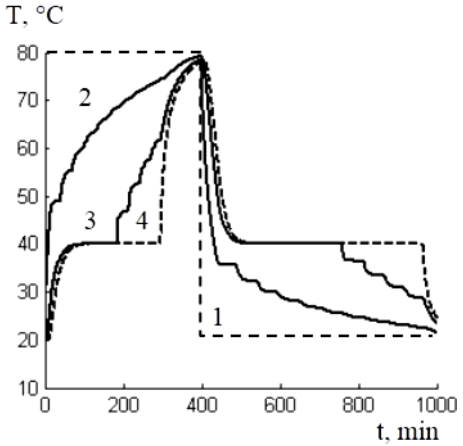

Fig. 6. Variation of the temperature of some cells: 1 – outside temperature, 2 – j=20, 3 – j=10, 4 – j=1

Рис.6. Изменение температуры некоторых ячеек: 1 – внешняя температура, 2 – j=20, 3 – j=10, 4 – j=1

ACKNOWLEDGEMENT

This work is supported by the Russian Foundation for Basic Research (project 18-08-00028).

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Поступила в редакцию 29.01.2020
Принята к опубликованию 05.03.2020

Received 29.01.2020
Accepted 05.03.2020