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ON THE PROBLEM OF MODELING TEMPERATURE FIELDS IN BODIES WITH VARIABLE BOUNDARIES*

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Abstract. **Introduction.** When melting, solidifying and oxidizing a metal, the problem arises of calculating the temperature field in areas with time-varying boundaries. Usually, to solve the heat equation in such cases, the method of catching the boundary into a node of a spatial grid is used, which necessitates the use of a variable time step in calculations, in addition, the number of spatial nodes will also be variable. All this leads to a change in the amount of computational work. However, in many cases the method of grids with moving nodes may be more preferable, in this case there is no need to change the number of spatial nodes and the time step. **Purpose of the study.** Develop an algorithm for approximating the convective boundary condition for grids with moving nodes. **Materials and methods.** The analysis and generalization of literature data on the problem is carried out. It has been established that the direct replacement of derivatives in the boundary condition by finite differences leads to a large error in calculating the surface temperature and, as a result, the entire temperature field of the body. When using a grid with a constant spatial step for a finite-difference approximation of the boundary condition, one can use the Beck formula. There is no formula similar to the Beck formula in the literature for meshes with moving nodes, so the problem arises of determining such a formula. To solve the stated problem of approximation, the method of heat balance for an elementary cell near the surface of the body is applied. **Results.** An analogue of the Beck formula for grids with moving nodes is found. The obtained finite-difference formula was tested, including with the help of a computational experiment. **Conclusion.** The obtained formula for approximating the convective boundary condition for grids with moving nodes can be a kind of addition to the theoretical foundations of the method of grids with moving nodes used in practice for calculating temperature fields in areas with variable boundaries; its application makes it possible to increase the accuracy of calculating the temperature field of a body.

Keywords: finite-difference scheme, convective boundary condition, the grid method with mobile nodes, computational domain with moving boundaries, temperature field approximation

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К ЗАДАЧЕ МОДЕЛИРОВАНИЯ ТЕМПЕРАТУРНЫХ ПОЛЕЙ В ТЕЛАХ С ПЕРЕМЕННЫМИ ГРАНИЦАМИ*

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Аннотация. **Введение.** При плавлении, затвердевании и окислении металла возникает задача расчета температурного поля в областях с переменными во времени границами. Обычно для решения уравнения теплопроводности в таких случаях применяют метод ловли границы в узел пространственной сетки, это обуславливает необходимость использования при расчетах переменного шага по времени, кроме того, переменным будет и число пространственных узлов. Все это приводит, как правило, к увеличению объема вычислительной работы. Однако во многих случаях более предпочтительным является метод сеток с подвижными узлами, в этом случае нет необходимости в изменении числа пространственных узлов и шага по времени. **Цель исследования.** Разработать алгоритм аппроксимации конвективного граничного условия для сеток с подвижными узлами. **Материалы и методы.** Выполнен анализ и обобщение литературных данных по проблеме. Установлено, что непосредственная замена производных в граничном условии конечными разностями приводит к большой погрешности вычисления температуры поверхности и, вследствие этого, и всего температурного поля тела. При использовании сетки с постоянным шагом по пространству с целью повышения точности расчетов для конечно-разностной аппроксимации граничного условия можно использовать формулу Бека. В литературе для сеток с подвижными узлами формулы, аналогичной формуле Бека, нет, поэтому возникает задача по определению такой формулы. Для решения поставленной задачи аппроксимации применен метод теплового баланса для элементарной ячейки у поверхности тела. **Результаты.** Найден аналог формулы Бека для сеток с подвижными узлами. Выполнена апробация полученной конечно-разностной формулы, в том числе и с помощью вычислительного эксперимента. **Заключение.** Полученная формула аппроксимации конвективного граничного условия для сеток с подвижными узлами может быть неким дополнением к теоретическим основам используемого в практике вычислений температурных полей в областях с переменными границами метода сеток с подвижными узлами, ее применение позволяет повысить точность расчета температурного поля тела.

Ключевые слова: конечно-разностная схема, конвективное граничное условие, метод сеток с подвижными узлами, расчетная область с подвижными границами, температурное поле, аппроксимация

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Introduction

During melting, solidification and oxidation of metal, in case of emergency freezing of water in heat pipelines and in water supply systems, when calculating the process of cooling and freezing of a moving front of a heat carrier during filling of an empty pipeline when starting up in winter conditions, when wet soil freezes, including in the presence of snow cover with variable thickness and in other cases, the problem of calculating temperature fields in regions with time-varying boundaries arises [1–7]. In the finite-difference solution of such a problem, as a rule, the method of catching the boundary in a node of the spatial grid is used [7, 8], which necessitates the use of a variable time step in the calculations, in addition, the number of spatial nodes will also be variable. Here, the method of grids with movable nodes may be more preferable [9–12]. This makes it possible, in particular, to avoid changing the number of nodes of the computational grid and, therefore, the dimension of the used information arrays, as well as the time step, which can be quite attractive, for example, when developing software. However, it should be borne in mind that in any case, both in numerical calculations with constant sizes of steps in spatial coordinates, and with variable sizes of such steps, a finite-difference approximation of the boundary conditions is necessary, which describe the features of heat transfer of the solid body under study with the environment. Moreover, it is known that the solution of this problem by direct replacement of derivatives by finite differences can lead to large computational errors. Therefore, it is necessary to develop special approaches and solutions to this issue.

The relevance of the issue under study

According to the data of [1, 5–7], the relevance of the problem of calculating temperature fields in regions with time-varying boundaries for the present time is very significant, the literature notes the insufficient development and validity of some approaches and techniques, in particular, the method of grids with moving nodes. Therefore, the study and identification of all aspects and features of the method of meshes with moving nodes is of great importance.

Statement of the research problem

Most often, heat transfer at the boundary is described by a boundary condition of the third kind, which has the form:

$$-\lambda \frac{\partial t}{\partial N}\bigg|_G = \alpha\left(t_C - t\big|_G\right), \tag{1}$$

where $t = t(M, \tau)$ – body temperature at point M at the moment τ; N – normal to border G (body surface); λ, α – respectively, the coefficients of thermal conductivity and heat transfer; $t_C, t|_G$ – respectively ambient temperature and body surface temperature (body temperature at the border).

It is known that equation (1) is usually approximated by the following finite-difference scheme:

$$\lambda \frac{t_n^k - t_{n-1}^k}{h} = \alpha\left(t_C^k - t_n^k\right), \tag{2}$$

where t_n^k – body surface temperature (in the node n) at the moment $k \cdot \Delta\tau$; t_{n-1}^k – body temperature in an adjacent node $n-1$, remote from the surface node by the size of the space step h, at the same time $k \cdot \Delta\tau$; t_C^k – temperature of the medium at time $k \cdot \Delta\tau$; $\Delta\tau$ – size of the calculated time step. It is assumed here that the size of the computational domain in the normal direction N divided by n parts (steps h).

It is also known [13] that the approximation of the boundary condition (1) by the finite-difference scheme (2) gives a noticeable error in determining the temperature of the body surface if

$$\frac{\alpha h}{\lambda} < 1. \tag{3}$$

In this case, in order to increase the accuracy of determining the surface temperature and, therefore, the entire temperature field of the body when calculating by the method of grids with a constant step along the spatial coordinate h one can use the approximation formula proposed by Beck [14]. According to [13 and others], Beck's formula has been successfully tested in computational practice.

If the method of grids with movable nodes is used to calculate the temperature field [9–12], then, naturally, the question arises: what form will have a formula similar to Beck's formula, but for grids with movable nodes. This work provides an answer to this question.

The theoretical part of the study

When deriving the approximation formula in [14], a fairly well-known technique was used: to obtain a difference solution that well describes the real temperature field, it is advisable to fulfill the energy conservation law for the difference scheme itself [15, 16]. This method is often called the finite control volume method [16] or the heat balance method for elementary volumes [8, 16]. It should be noted that, in contrast to [14], when deriving a formula for approximating the boundary condition for grids with moving nodes, we will use averaging not temperatures over the time interval $\Delta\tau$, and heat flux densities.

Let us denote the heat flux density by heat transfer at the beginning of the time interval $\Delta\tau$ through q_1^k, and at the end – through q_1^{k+1}, its average value – through $\overline{q}_1 = \left(q_1^k + q_1^{k+1}\right)/2$, and it is easy to see that

$$\overline{q}_1 = \alpha\left(\frac{t_C^k + t_C^{k+1}}{2} - \frac{t_n^k + t_n^{k+1}}{2}\right). \tag{4}$$

Further, the density of the heat flux by thermal conductivity in the surface layer of the body is denoted, respectively, at the beginning $\Delta\tau$ through q_2^k, and at the end – through q_2^{k+1}, its average value – through $\overline{q}_2 = \left(q_2^k + q_2^{k+1}\right)/2$, and it is easy to see that

$$\overline{q}_2 = \lambda\left(\frac{t_n^k - t_{n-1}^k}{2h^k} + \frac{t_n^{k+1} - t_{n-1}^{k+1}}{2h^{k+1}}\right). \qquad (5)$$

Here h^k and h^{k+1} – is the distance between the nodes of the computational grid at times $k \cdot \Delta\tau$ and $(k+1)\cdot\Delta\tau$ respectively.

Following [8, 14–16], let us assume that the size of the control volume (unit cell) for the surface is equal to the half-layer and estimate the heat content (enthalpy) of the half-layer on the surface at the beginning and at the end of the time step $\Delta\tau$: $c\rho t_n^k h^k/2$ and correspondingly $c\rho t_n^{k+1} h^{k+1}/2$. Here c, ρ – respectively, the specific heat and density of the substance; moreover, as in [14], it was assumed that the average temperature of the half-layer is equal to the temperature of the body surface.

The difference between the amount of heat supplied to the half-layer on the surface by heat transfer and the amount of heat removed from it during the time $\Delta\tau$ by thermal conductivity inside the body, according to the law of conservation of energy, it represents the stored amount of heat spent on changing the heat content (enthalpy) of the half-layer. Mathematically, it will be written like this:

$$\left(\overline{q}_1 - \overline{q}_2\right)\cdot\Delta\tau = c\rho\left(\frac{t_n^{k+1}h^{k+1}}{2} - \frac{t_n^k h^k}{2}\right). \qquad (6)$$

Transforming this equation accordingly, we obtain the required approximation formula:

$$t_n^{k+1} = \frac{t_n^k\left(\frac{\lambda h^k}{a\cdot\Delta\tau} - \alpha - \frac{\lambda}{h^k}\right) + \alpha\left(t_C^k + t_C^{k+1}\right) + \lambda\left(\frac{t_{n-1}^k}{h^k} + \frac{t_{n-1}^{k+1}}{h^{k+1}}\right)}{\frac{\lambda h^{k+1}}{a\cdot\Delta\tau} + \alpha + \frac{\lambda}{h^{k+1}}}. \qquad (7)$$

Here a – thermal diffusivity. Note also that if $h^k = h^{k+1} = h$, that is, if the interface between the media is motionless, then from (7) follows the Beck approximation formula [14], which in this case will have the form:

$$t_n^{k+1} = \frac{t_n^k\left(\frac{h^2}{a\cdot\Delta\tau} - \frac{\alpha h}{\lambda} - 1\right) + \frac{\alpha h}{\lambda}\left(t_C^k + t_C^{k+1}\right) + t_{n-1}^k + t_{n-1}^{k+1}}{\frac{h^2}{a\cdot\Delta\tau} + \frac{\alpha h}{\lambda} + 1}. \qquad (8)$$

Approbation of the approximation formula

It is shown in [13, 14] that the formula proposed by Beck for approximating the convective boundary condition together with the known methods [7, 15, 17] of the finite-difference replacement of the differential equation of heat conduction provides a fairly accurate description of heating (cooling) of massive bodies. This, to a certain extent, confirms its adequacy to real physical processes.

The adequacy of the approximation formula (7) obtained for grids with moving nodes, taking into account the above, is to a certain extent indicated by the fact that for $h^k = h^{k+1}$ from it a special case of the Beck approximation formula is obtained. In addition, in order to approbate formula (7), the following technique was used: the results of calculating the heating of a steel plate without and taking into account oxidation were compared, but under the assumption that the metal crumbles immediately after oxidation and does not affect heat transfer, i.e. oxidation only leads to a decrease in the thickness of the plate. This comparison is due to the fact that in the literature there are no accurate data on the temperature distribution in the scale and metal, taking into account the transfer of heat through the surface layer of the oxidized metal. In addition, a full-scale experiment to determine, for example, the temperature of a moving boundary is very difficult, in particular, due to the fact that in this case a movable temperature sensor is required.

When performing calculations in the first case, the boundary condition (1) was approximated by the Beck formula, and in the second, by the formula (7). The heat equation in all cases was approximated by an implicit difference scheme, which was solved by the sweep method. In the case of taking into account the oxidation of the metal, we used the scheme with movable nodes given in [10].

It is quite clear that a decrease in the geometric dimensions (thickness) of the plate due to oxidation in the calculations should lead to better heating of the metal. However, the temperature distributions in both cases should differ slightly from each other due to the relatively insignificant decrease in the thickness of the steel plate as a result of metal oxidation. This is confirmed by comparing the calculation results.

It is also of interest to compare the results of calculating the temperature fields for various methods of approximating the convective boundary condition for grids with a constant step in space: formula (2), obtained by simple replacement of the derivative by a finite difference, and Beck's formula.

The Table 1 shows the results of calculations of symmetric heating of a steel plate with a thickness $0{,}1$ m at $a = 0{,}02\ \text{m}^2/\text{h}$, $\lambda = 30{,}24$ W/(m·°C), $\alpha = 348{,}9$ W/(m^2·°C). In this case, it was assumed that at the initial moment of time the temperature at all points along the thickness of the plate is the same and equal to 700 °C (the so-called hot posad), heating medium temperature $t_C = 1300$ °C, and the oxidation of the metal is described by the following relationship:

$$\frac{\partial h_{OX}}{\partial \tau} = \frac{-39{,}4}{h_{OX}(\tau)} \cdot \exp\left[\frac{-7580}{t_{NM}(\tau)+273}\right] \cdot 10^{-4},\ \text{m/h},$$

obtained by approximating the experimental data. Here h_{OX} – dross thickness, and t_{NM} – surface temperature of unoxidized metal (under real conditions under the scale layer).

In Table 1: t_{SMi} and t_{Ci} – temperatures of the surface and center of the heated plate under the following conditions: $i=1$ – heating without taking into account oxidation when the boundary condition is approximated by formula (2); $i=2$ – the same, but when the boundary condition is approximated by the Beck formula; $i=3$ – heating taking into account oxidation, leading only to a decrease in the thickness of the plate (it is believed that the oxidized metal immediately crumbles), and the approximation of the boundary condition by formula (7). The half-thickness values given in the table are for case only $i=3$.

As can be seen from the Table 1, the discrepancy between the values t_{SM2} and t_{SM3}, as well as t_{C2} and t_{C3} is a relatively small value, which allows us to conclude that formula (7) provides a satisfactory description of the process and can be recommended for use in calculating temperature fields in regions with moving boundaries.

The practical significance of the results

The obtained formula for the approximation of the convective boundary condition for grids with movable nodes, as we see it, can be a kind of addition to the theoretical foundations of

Table 1

Plate surface and center temperature

Time, min	Temperature, °C						Half thickness unoxidized metal, m
	t_{SM1}	t_{SM2}	t_{SM3}	t_{C1}	t_{C2}	t_{C3}	
0	700	700	700	700	700	700	0,05
3	903,6	903,53	904,76	777,73	780,46	783,55	0,04897
6	976,77	967,26	969,27	870,46	867,48	872,20	0,04892
9	1035,45	1024,55	1027,67	948,22	941,22	946,99	0,04884
12	1083,4	1071,54	1075,43	1011,98	1002,45	1008,97	0,04872
15	1122,67	1110,54	1115,02	1064,19	1053,24	1060,29	0,04858
18	1154,81	1142,88	1147,79	1106,94	1095,36	1102,78	0,04842
21	1181,13	1169,70	1174,92	1141,93	1130,29	1137,94	0,04825
24	1202,68	1191,97	1197,36	1170,58	1159,26	1167,02	0,04807
27	1220,32	1210,38	1215,92	1194,04	1183,28	1191,04	0,04788
30	1234,76	1225,68	1231,24	1213,25	1203,20	1210,87	0,04770

the method of grids with movable nodes used in practice for calculating temperature fields in domains with variable boundaries.

Conclusions

The problem of approximation of the convective boundary condition for grids with moving nodes is considered. Using the law of conservation of energy for an elementary cell near the surface of a body, we obtained a formula for the numerical approximation of the boundary condition, which is similar to the Beck formula known in the literature. The approximation formula can be used to improve the accuracy of calculating the temperature field of a body with moving boundaries.

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