NOTATION

Q, energy; q, energy flux density; C, capacitance; U, voltage; R_{ef}, effective resistance of plasma; t, time; d, vacuum gap between electrodes; l, size of microparticles; q*, total charge of ions; m, mass; n_z, density of z-fold ionized ions; n, density of plasma atoms; η, charge ratio.

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HEAT AND MASS TRANSFER IN THE SORPTION OF HYDROGEN BY INTERMETALLIC COMPOUNDS

S. V. Svinarev and S. N. Trushevskii

UDC 536.242

The heat and mass transfer in the sorption of hydrogen by intermetallic compounds in a steady plane layer is calculated, taking account of heat liberation and filtration, by finite-difference and approximate integral methods.

Intermetallic compounds (IMC), which reversibly absorb hydrogen, are currently the subject of numerous investigations in connection with the possibility of their use in hydrogen accumulators, thermal machines, thermal pumps and accumulators, sorptional compressors, etc. The dynamics of hydrogen sorption in IMC must be investigated for the analysis and design of the above-noted devices. Trends in such investigations may now be distinguished: the study of the true chemical kinetics of sorption [1]; and the investigation of the sorption dynamics in extended IMC layers of dimensions characteristic for practical applications [2]. In the first case, attempts are made to minimize the layer thickness so that the influence of heat liberation and filtrational resistance may be neglected. In the second, as assumed in these works, the rate of sorption is completely determined by the rate of heat transfer inside the IMC layer. However, these works do not give criteria by which the experimental conditions may be chosen, and often the conditions themselves are not completely described.

In connection with this, calculations of the sorption process in which the heat liberation and filtration of hydrogen through the IMC layer are taken into account are of interest both for practical applications and for the elucidation of the conditions in which the process may be regarded as purely kinetic or controlled by the heat and mass transfer in the layer.

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To elucidate the basic features in the formulation of the mathematical problem, the conditions chosen are the simplest that are at the same time close to reality. It is assumed that IMC powder is arranged in the form of an infinitely plane layer of thickness L, so that the problem may be regarded as one-dimensional. One boundary of the layer is thermally insulated, and hydrogen is supplied here, at a pressure that remains constant. The other boundary is maintained at constant temperature and is impermeable to gas. Since there is no single view on the true reaction mechanism and the form of the equation for its velocity at present, an equation qualitatively transmitting the basic features known from experimental works is used

$$\frac{d\alpha}{d\tau} = \pm K \exp\left(-\frac{E}{RT}\right)\left[\frac{P - P_D(T)}{P_D(T)}\right](1-\alpha). \tag{1}$$

It is assumed that the gas flow in the layer conforms to Darcy's law. It is assumed that all the thermophysical and filtrational characteristics do not depend on T, P, and α.

Complete description of the system requires the addition to Eq. (1) of the filtration and heat-conduction equations [3]

$$\frac{\varepsilon}{R}\frac{\partial}{\partial\tau}\left(\frac{P}{T}\right) = \frac{\partial}{\partial\tilde{x}}\left(\frac{k}{\mu}\frac{P}{RT}\frac{\partial P}{\partial\tilde{x}}\right) \mp G, \tag{2}$$

$$(1-\varepsilon)C\rho\frac{\partial T}{\partial\tau} = \lambda\frac{\partial^2 T}{\partial\tilde{x}^2} - \varepsilon C_H\frac{\partial}{\partial\tilde{x}}(\rho_H v T) \pm \Delta H G, \tag{3}$$

$$v = -\frac{k}{\mu}\frac{\partial P}{\partial\tilde{x}}, \tag{4}$$

$$P = \frac{\rho_H R T}{M_H}. \tag{5}$$

The upper sign preceding the terms including G corresponds to absorption and the lower sign to desorption. Analysis of Eqs. (2) and (3) shows that, in calculating the filtration, the nonisothermal layer may be neglected, and the convective term makes a small contribution in the heat-conduction equation. Taking these simplifications into account, the system in Eqs. (1)-(3) are solved by the finite-difference method with the following initial and boundary conditions

$$\begin{gathered} P(0,\tilde{x}) = P_D(T_0),\quad T(0,\tilde{x}) = T_0,\quad P(\tau,0) = P_0,\quad T(\tau,L) = T_0, \\ \frac{\partial P}{\partial\tilde{x}}(\tau,L) = 0,\quad \frac{\partial T}{\partial\tilde{x}}(\tau,0) = 0,\quad \alpha(0,\tilde{x}) = 0, \end{gathered} \tag{6}$$

and also taking into account that

$$G = \frac{n\rho}{M}\frac{d\alpha}{d\tau}, \tag{7}$$

where n is the maximum number of moles of H_2 per formal unit of IMC (the plateau width). A purely implicit two-layer difference scheme with simple iterations at each time step is used [4].

In addition, an attempt is made to obtain an approximate solution of Eqs. (1)-(3) in analytic form, using the integral method of [5]. Analytical dependences may be used for rough calculations, and also to estimate the influence of different parameters on the behavior of the system. The results of machine calculations are used, on the one hand, as a guide in choosing the profiles of T and α and, on the other, to estimate the error in the approximate solutions. In Eq. (2), the term including $(\partial P/\partial\tilde{x})^2$ is neglected. The system is brought to dimensionless form using the following relations

$$x = \frac{\tilde{x}}{L},\quad t = \frac{a\tau}{L^2},\quad \Pi = \frac{P - P_D(T_0)}{P_0 - P_D(T_0)},\quad \Theta = \frac{T - T_0}{T_R - T_0}, \tag{8}$$

where

$$a = \frac{\lambda}{C\rho(1-\varepsilon)};\quad T_R = T_0\left[1 - \frac{RT_0}{\Delta H}\ln\frac{P_0}{P_D(T_0)}\right]^{-1};$$

T_R is the retardation temperature of sorption, i.e., $P_0 = P_D(T_R)$. If, in addition, $\Theta_R = (T_R - T_0)/T_R \ll 1$, Eqs. (1)-(3) are written in the form

$$\frac{\partial\Theta}{\partial t} = \frac{\partial^2\Theta}{\partial x^2} + H\frac{d\alpha}{dt}, \tag{3'}$$

$$V\left(\frac{\partial\Pi}{\partial t} - \frac{1+\Pi\Pi_0}{1+\Theta\Theta_R}\,\frac{\Theta_R}{\Pi_0}\,\frac{\partial\Theta}{\partial t}\right) = \frac{\partial^2\Pi}{\partial x^2} - S\frac{d\alpha}{dt}, \tag{2'}$$

$$\frac{d\alpha}{dt} = \pm\frac{1}{\tau_0}\,\frac{[1+\Pi\Pi_0 - \exp(B\Theta)]}{\Pi_0}\,(1-\alpha)\exp[(A-B)\Theta], \tag{1'}$$

where

$$\Pi_0 = \left|\frac{P_0 - P_D(T_0)}{P_0}\right|; \quad H = \frac{\Delta H n}{CT_0|\Theta_R|M};$$

$$V = \frac{2\varepsilon\mu a}{k[P_0 + P_D(T_0)]}; \quad \tau_0 = \frac{a}{L^2 K\Pi_0\exp(-E/RT_0)};$$

$$S = \frac{2\mu a R T_0 n\rho}{k|P_0^2 - P_D^2(T_0)|M}; \quad A = \frac{E}{RT_0}\Theta_R, \quad B = \frac{\Delta H}{RT_0}\Theta_R.$$

Since there are no literature data on the permeability of IMC layers, the following equation is used [6]

$$k = \frac{\varepsilon^3}{(1-\varepsilon)^2}\,\frac{d^2}{180}. \tag{9}$$

The system is considered for values of Π_0 at which temperature increase results in slowing of the reaction, i.e., at $\Pi_0 \leqslant B/(A-B)$. This is the significant difference between this problem and the problem of filtrational combustion [7].

The parameters H, V, τ_0, S determining the behavior of the system are estimated for $LaNi_5$, the most-studied IMC, at $T_0 = 300$°K, $\Pi_0 = 4$, d = 2 μm, L = 2.5 cm. The values of the reaction rate constants are taken from [1]. It is found that $H = 9.3$; $V = 1.3\cdot10^{-3}$; $\tau_0 = 0.1$; $S = 0.24$. The result of the smallness of V is that the left-hand side of Eq. (2') may be neglected for approximate analysis. Only at the beginning of the process, when $\partial\Pi/\partial t$ is large, this is not so, and it may be approximately assumed that the pressure relaxes to a "quasisteady" profile with a characteristic time $\tau_S = V\tau_a/S$. Since τ_S is small, Eq. (2') may be replaced by the equation

$$\frac{\partial^2\Pi}{\partial x^2} - S\frac{d\alpha}{dt} = 0 \tag{10}$$

with the initial condition

$$\Pi(0, x) = \exp\left(-\sqrt{\frac{S}{\tau_0}}\,x\right). \tag{11}$$

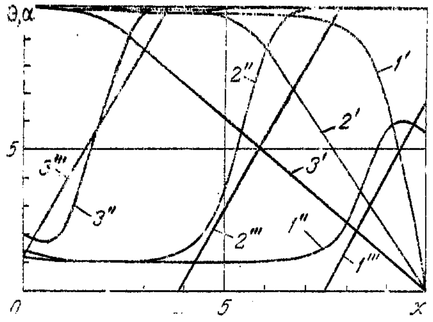
It is evident from Eq. (11) that, if $\sqrt{S/\tau_0} \ll 1$, then $\Pi \approx 1$ and the process occurs without filtrational complications from the very beginning. If not, then a pressure wave propagates through the layer.

Now consider a layer in which the pressure remains everywhere constant: $\Pi = 1$. The integral method of [5] is used to obtain an approximate solution of Eqs. (1') and (3'). The term $\partial\Theta/\partial t$ in Eq. (3') is neglected. It is known from experiments on sufficiently extended layers that initially the reaction occurs over the whole volume, as long as the temperature does not reach T_R. At T_R, a temperature difference is formed between the wall and the reaction zone and, as heat is supplied to the system, the reacton zone moves over the layer. It is assumed that the reaction zone is of width δ_0, and moves over the layer according to the law $\delta(t)$. The temperature profile in the layer is chosen in the form

$$\Theta(t, x) = \begin{cases} 1, & 0 \leqslant x < \delta, \\ 1 - [(x-\delta)/(1-\delta)]^m & \delta \leqslant x \leqslant 1, \end{cases} \tag{12}$$

and the degree of conversion in the form

$$\alpha(t, x) = \begin{cases} 0, & 0 \leqslant x \leqslant \delta, \\ (x-\delta)\,\delta_0, & \delta < x < \delta + \delta_0, \\ 1, & \delta + \delta_0 \leqslant x \leqslant 1. \end{cases} \tag{13}$$



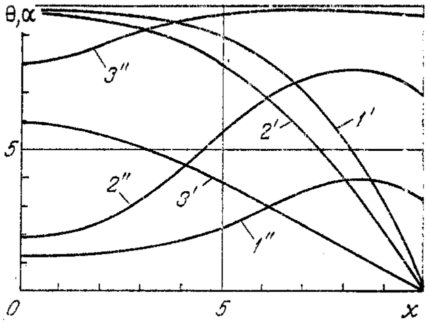


Fig. 1 Fig. 2

Fig. 1. Distribution of temperature and degree of conversion over the layer for times t = 0.1 (1), 1.0 (2), 3.0 (3); H = 9.3; τ_0 = 0.1; 1', 2', 3') Θ; 1", 2", 3") α from the finite-difference solution; 1"', 2"', 3"') from the approximate solution.

Fig. 2. Distribution of temperature and degree of conversion over the layer for times t = 0.5 (1), 1.5 (2), 4.5 (3); H = 9.3; τ_0 = 1.2; 1', 2', 3') Θ; 1", 2", 3") α (on the coordinate axes, 5 must be replaced by 0.5).

After integrating the heat-conduction Eq. (3'), in which Eqs. (12) and (13) are substituted, an ordinary differential equation is obtained for δ(t)

$$H(1-\delta)\frac{d\delta}{dt} = -m. \tag{14}$$

If the analogous procedure is undertaken with the linearized Eq. (1'), the following estimate is obtained

$$\delta_0 \approx \sqrt{m(m+1)(m+2)\tau_0/H}. \tag{15}$$

Essentially, m is a fitting parameter. Analysis of the temperature profile from the finite-difference solution gives $m \approx 1.5$. It is supposed that the model of a diffuse reaction front is valid when $\delta_0 < 1$. For $LaNi_5$, with the above-noted conditions, $\delta_0 = 0.4$. Equation (14) is valid for $0 < \delta < 1 - \delta_0$. If the integral method is applied to time segments when the reaction front intersects the boundary planes, the law of motion δ(t) may be found for the whole sorption process

$$\begin{aligned} &\delta = 1-(3m\delta_0 t/H)^{1/3}, \quad 0<t<t_1; \\ &\delta = 1-\sqrt{2m(t-t_1)/H+\delta_0^2}, \quad t_1<t<t_2; \\ &\delta = \sqrt{\delta_0^2+2m\delta_0(t_2-t)/H}-\delta_0, \quad t_2<t<t_3, \end{aligned} \tag{16}$$

where

$$t_1 = \frac{H\delta_0^2}{3m}; \quad t_2 = t_1 + \frac{(1-\delta_0^2)}{2}H; \quad t_3 = t_2 + \frac{H\delta_0}{2m};$$

t_3 is the total time of sorption; $t_3 = H/2m(1 + 3\delta_0/2 - \delta_0^2/3)$.

The results both of numerical calculation and from Eqs. (12), (13), (15), and (16) are shown in Fig. 1. It is clear that the approximation of a sharp reaction front which is sometimes employed [8], while typical of problems with phase conversion, is only valid when $\delta_0 \ll 1$. Numerical calculation of the initial equations when $H/\tau_0 = 1500$ in fact gives a sharp reaction front, but the finite-difference scheme is stable here for a time step of less than 10^{-5} and hence is not very effective. The results of numerical calculation of the system in Eqs. (1)-(3), when $H/\tau_0 = 7.9$ ($\delta_0 = 1.3$) are shown in Fig. 2. It is evident that the reaction front is spread out over the whole width of the layer.

It is obvious that the other limiting case $\delta_0 \gg 1$ corresponds to a sorption process which is controlled by the true chemical kinetics, in accordance with Eq. (1), for example. For the approximate calculation, it is assumed that

$$\alpha(t, x) = \varphi(t), \quad \Theta(t, x) = (1-x^2)\psi(t), \tag{17}$$

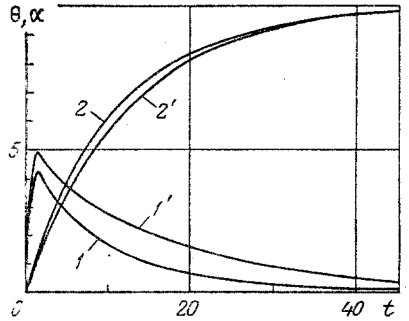


Fig. 3

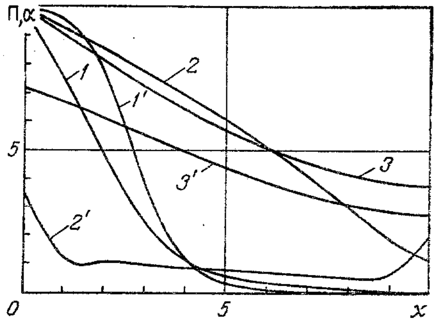


Fig. 4

Fig. 3. Dependence of the maximum temperature in the layer $\Theta(t, 0)$ (1, 1') and integral mean degree of conversion $\bar{\alpha}(t)$ (2, 2') on the time; 1, 2) finite-difference solution; 1', 2') Eqs. (19) and (20).

Fig. 4. Distribution of the pressure and the degree of conversion over the layer: 1, 2, 3) Π; 1', 2', 3') α (on the coordinate axes, 5 must be replaced by 0.5).

and the integral method is used, leading to a system of ordinary differential equations

$$\dot{\varphi} = \left(1 - \frac{2}{3}\psi - \varphi + \frac{2}{3}\psi\varphi\right)/\tau_0,$$
$$\dot{\psi} = -3\psi + \frac{3H}{2\tau_0}\left(1 - \frac{2}{3}\psi - \varphi + \frac{2}{3}\psi\varphi\right), \tag{18}$$
$$\varphi(0) = 0,\ \psi(0) = 0.$$

In the first approximation, the product $\psi\varphi$ may be neglected, and the solutions φ_0 and ψ_0 obtained. To obtain the next approximation, the known function $\psi\varphi$ is substituted into Eq. (18) in place of $\psi_0\varphi_0$. The approximate solutions φ_1 and ψ_1 are written in the form

$$\varphi_1 = 1 - \left[1 - \frac{q}{(1+q)^2}\frac{t}{\tau_0}\right]\exp\left[-\frac{t}{\tau_0(1+q)}\right], \tag{19}$$

$$\psi_1 = \frac{1.5q}{(1+q)}\left[\left(\frac{1+3q}{1+q} + \frac{q}{(1+q)^2}\frac{t}{\tau_0}\right)\exp\left[-\frac{t}{\tau_0(1+q)}\right] - \exp\left[-3(1+q)t\right]\right], \tag{20}$$

where $q = (H + 1)/3\tau_0$.

It is evident from Eq. (19) that the process occurs with a time content τ_0 only if $q \ll 1$, and hence the condition for investigation of the true chemical kinetics in the experiment is

$$\frac{H+1}{3\tau_0} \ll 1. \tag{21}$$

However, it is found that Eq. (19) is very close to the isothermal relation

$$\varphi_i = 1 - \exp(-t/\tau_0) \tag{22}$$

even when q is close to unity. For example, the slopes of the curves of Eqs. (19) and (22) in the coordinates ln $(1 - \varphi)$, t differ by 1.5% at $q = 0.3$ and by 10% at $q = 0.7$. Unexpectedly, it is found that Eq. (9) also provides a good description of the integral mean $\bar{\alpha}(t)$ at large q. For example, when $q = 3$, the difference of $\bar{\alpha}(t)$ from Eq. (19) is no more than 0.02, although α depends considerably on x, as is evident from Fig. 2. It is obvious that the condition in Eq. (21) must be satisfied with decrease in thermal effect of the reaction $|\Delta H|$. However, it is evident that, as $H \to 0$, Eq. (21) is not satisfied for all τ_0. This is because Eq. (18) is approximate. For $LaNi_5$, $H \geqslant 10$ for the whole of the pressure range which is of practical interest — $P_0/P_D(T_0) < 5$; therefore, this deficiency is insignificant. The results of numerical calculation of $\Theta(t, 0)$, $\bar{\alpha}(t)$ and the functions $\varphi_1(t)$ and $\psi_1(t)$ from Eqs. (19) and (20) for $q = 0.29$, $\tau_0 = 11.8$ are shown in Fig. 3.

Some further remarks may be made regarding the filtrational conditions. If the thermal effect is neglected ($H = 0$), and it is assumed that the "penetration depth" δ_1 for the pressure and the degree of conversion are the same, so that $\bar{\alpha} = \delta_1$, an estimate of the time for the pressure wave to pass over the layer, $\sim S$, may be obtained from Eq. (10). If this time is small in comparison with the characteristic sorption time τ_0, i.e., $S/\tau_0 \ll 1$, the process may be regarded as isobaric. However, if H/τ_0 is sufficiently large, a large part of the layer will rapidly reach the retardation temperature $\Theta = 1$, as is evident from Eqs. (12) and (15). Thereafter, sorption occurs in the layer with a characteristic time H, and hence the condition of isobaric sorption is $S/H \ll 1$.

In Fig. 4, curves of $\alpha(x)$ and $\Pi(x)$ obtained by solving Eqs. (1)-(3) for three different conditions are shown. In case 1, $S = 15$; $\tau_0 = 0.02$; $H = 0.37$, and hence $S/\tau_0 = 750$; $H/\tau_0 = 18$. In case 2, $S = 15$; $\tau_0 = 0.02$; $H = 9.3$; and $S/\tau_0 = 750$; $H/T_0 = 465$; $S/H = 1.3$. In case 3, $S = 0.75$; $\tau_0 = 0.02$; $H = 0.37$; and $S/\tau_0 = 37$; $H/\tau_0 = 18$; $S/H = 2$. It is evident that in cases 1 and 2, despite the identical values of $S/\tau_0 = 750 \gg 1$, filtrational and isobaric conditions, respectively, are established. In case 3, intermediate filtrational—kinetic conditions are seen. Thus, it may be assumed that filtrational conditions are realized when $S/\tau_0 \gg 10$, $H/\tau_0 \ll 10$ or $S/H \gg 1$, $H/\tau_0 \gg 10$. Under other conditions, sorption occurs at constant pressure.

Comparison of the results of calculation and experiment is complicated in that the values of the rate constants obtained by previous authors differ by two orders of magnitude [1, 9]. In [9], the sorption dynamics of H_2 in $LaNi_5$ at constant pressure and constant temperature of a copper substrate on which was applied an IMC layer of thickness $L = 0.15$ cm was investigated for $P_0/P_D = 2$, it is found that $H = 25$, $\tau_0 = 0.26$. Hence $H/\tau_0 = 95 \gg 13$ and $\delta_0 = 0.37$. Hence, even in such a thin layer, conditions with a smeared reaction front are realized and the sorption rate is limited by the heat transfer in the layer. According to Eq. (16), the total sorption time $t_3 = 10.9$ or $\tau_3 = L^2 t_3/a = 47$ sec. From the graph given in [9], it is evident that after this time the degree of conversion $\bar{\alpha}$ reaches ~ 0.9. Setting $\delta = 0.5$ in Eq. (14), the thermal conductivity of the IMC cover for this time may be calculated

$$\lambda = \frac{\Delta H n L \rho}{2m(T_T - T_0)M}\,\frac{d\delta}{d\tau}. \tag{23}$$

In [9], the formula used to calculate λ was equivalent to Eq. (23) with the substitution $m = 1$, which is the same as assuming that the temperature profile is linear. The result obtained in [9] was $\lambda = 1.32$ W/m·K, which is 20% higher than the known results, as the authors noted. It is evident that the use of the value $m = 1.5$ adopted here gives a result that is closer to the true conductivity. The same authors investigated the sorption dynamics of H_2 in FeTi by an analogous method in [10]. It was found that, when $P_0/P_D = 2$, the maximum temperature at $x = 0.5$ is $\Theta_m = 0.36$, while $H = 11.3$. It follows from Eq. (20) that this value of Θ_m corresponds to $\tau_0 = 7.1$. It may be found from Eq. (19) that the time to reach $\bar{\alpha} = 0.5$ is 18 sec, which is in good agreement with the experimental results. Thus, the method of approximate analysis proposed for the system in Eqs. (1)-(3) gives reasonable agreement with the results of experiment and of solving Eqs. (1)-(3) by a numerical finite-difference method. Analysis of the role of the various physical quantities appearing in the dimensionless complexes H, V, τ_0, and S shows that the quantities which have the greatest effect on the realization of particular conditions of sorption are L, $K(T_0)$, $P_D(T_0)$, and d.

NOTATION

$\tilde{x}$, coordinate, m; τ, time, sec; α, degree of conversion; T, temperature, K; P, pressure, Pa; K, rate constant, $\sec^{-1}$; E, activation energy, J/mole; R, universal gas constant, J/mole·K; P_D, equilibrium dissociation pressure, Pa; L, layer thickness, m; ε, porosity; k, permeability, m^2; μ, viscosity, Pa·sec; G, source power, mole H_2/m^3·sec; C, ρ, specific heat, J/kg·K, and density, kg/m^3, of IMC; λ, effective thermal conductivity of the layer, W/m·K; C_H, ρ_H, M_H, specific heat, J/kg·K, density, kg/m^3, and molecular mass, kg, of hydrogen; v, flow velocity of hydrogen, m/sec; ΔH, heat of sorption, J/mole; M, molecular mass of IMC, kg; d, characteristic dimension of particles in layer, m; x, t, Π, Θ, A, B, dimensionless coordinate, time, pressure, temperature, activation energy, and heat of sorption; δ, δ_0, dimensionless coordinate and sorption-zone width; H, S, V, τ_0, dimensionless numbers; m, parameter of temperature profile; φ, ψ, functions of t.

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PRINCIPLE OF LOCAL INFLUENCE IN THE METHOD OF STEP BY STEP MODELING

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UDC 536.2

The possibility of replacing spatially inhomogeneous effect on body boundaries by average effects is investigated. Error estimates are obtained for a temperature field computation.

The crux of the step-by-step modeling of the thermal mode of complex systems is the subsequent application of a number of mathematical models possessing a different degree of detailing in the description of temperature fields [1]. In the initial stages the thermal regime of the whole system is analyzed with minimally allowable detailing and the average values of the temperature and heat fluxes are determined. The following approach is used in computing the temperature field of a certain isolated domain of the system: the boundary conditions for the domain under consideration are compiled on the basis of values of the temperature and heat fluxes obtained in the preceding stages of the computation.

For a strict assignment of the boundary conditions it is necessary to know the spatial temperature distribution $T(x)$ or the heat flux density $q(x)$ on the boundary of the isolated domain, or in the case of boundary conditions of the third kind, the temperature distribution of the conditions medium $T_m(x)$. However, the models of the previous stages that possess a smaller degree of detailing permit the computation of just the temperature values $\langle T_k \rangle$ and $\langle q_k \rangle$ averaged over certain surfaces (or coordinates)

$$\langle T_k \rangle = \frac{1}{S_k} \int_{S_k} T(\mathbf{x})\, dS_k, \quad \langle q_k \rangle = \frac{1}{S_k} \int_{S_k} q(\mathbf{x})\, dS_k. \tag{1}$$

Hence, in the step-by-step modeling strict formulation of the boundary-value problem for an isolated domain of the system is replaced by an approximate formulation yielding the mean temperature on the sections Γ_k

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