

electron and hole current density vectors; A , coefficient of asymmetry in narrowing; ΔV_g , total narrowing of the forbidden bandwidth; γ_n , γ_p , degree of electron and hole degeneration; φ_T , temperature potential; ϕ_n , ϕ_p , electron and hole Fermi quasilevels; n_{in} , n_{ip} , effective proper electron and hole concentrations equal to $n_i \gamma_n \exp(A \Delta V_g / \varphi_T)$ and $n_i \gamma_p \exp[(1 - A) \Delta V_g / \varphi_T]$, respectively; R , excess of the recombination velocity above the generation velocity; ϵ , dielectric permittivity of the material; $B_{i,j}$, value of the variable B at the node of the spatial discretization mesh with the subscripts i, j ; $|\delta \psi^1|_{\max}$, maximal value of $\{|\delta \psi_{i,j}^1|\}$ in the first Newton iteration; V_i , V_e , V_b , V_c , ohmic contact potentials of the injector, emitter, base, and collector, respectively; and N_{it} , number of complete iterations of the method.

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HEAT AND MASS TRANSFER IN SKIN FORMATION

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A mathematical model of the heat conduction and diffusion on heating an oxidizing metal is presented, together with a numerical method of calculation.

On heating ingots and semifinished articles in furnaces, their outer surface is oxidized, which leads to significant loss of material. The skin layer formed on oxidation has relatively low heat conduction and a high specific volume, and consequently this layer appears as a heat-insulating coating [1-3], which must be taken into account in optimizing the heating of metallic bodies.

It has been established that, in the skin layer, diffusion of metal to the outer surface occurs, and it is mainly oxidized at this surface [4]. The concentration distribution of the components in the oxide has apparently not previously been considered. Skin formation on heating a body of arbitrary form may be described mathematically as follows. Suppose that W_1 and W_2 are regions of space (x, y, z) occupied by the metal and its skin; Γ_1 is the boundary between the metal and the skin; Γ_2 is the external boundary of the skin; t_1 and t_2 are temperature functions for the metal and the skin; C is the concentration of unoxidized metal in

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the skin. The regions W_1 and W_2 in the space (x, y, z, τ) , where $0 < \tau < \tau_{cr}$, correspond to cylinders $R_1 = \{W_1 \times [0, \tau_{cr}]\}$ and $R_2 = \{W_2 \times [0, \tau_{cr}]\}$ with surfaces $F_1 = \{\Gamma_1 \times [0, \tau_{cr}]\}$ and $F_2 = \{\Gamma_2 \times [0, \tau_{cr}]\}$. A heat conduction equation holds for the metal and skin

$$c_j \rho_j \frac{\partial t_j}{\partial \tau} = \text{div}(\lambda_j \text{grad } t_j) + \Pi_j, (x, y, z, \tau) \in R_j, j = 1, 2. \quad (1)$$

Here c_j and λ_j are the specific heat and thermal conductivity; ρ_j is the density; Π_j is the power of the heat sources. The concentration C of metal in the skin is described by the diffusion equation

$$\frac{\partial C}{\partial \tau} = \text{div}(D \text{grad } C) + \Pi_M, (x, y, z, \tau) \in R_2, \quad (2)$$

where Π_M is the density function of mass sinks of unoxidized metal in the skin.

For the initial instant ($\tau = 0$), values of the functions are specified

$$\begin{aligned} t_j(x, y, z, 0) &= t_{j0}(x, y, z), C(x, y, z, 0) = C_0(x, y, z), \\ F_j(x, y, z, 0) &= F_{j0}(x, y, z). \end{aligned} \quad (3)$$

At the metal-skin boundary F_1

$$t_1(P_1) = t_2(P_1) = T, \quad (4)$$

$$\lambda_1 \frac{\partial t_1(P_1)}{\partial v} - \lambda_2 \frac{\partial t_2(P_1)}{\partial v} = \frac{HD}{\rho_1} \frac{\partial C(P_1)}{\partial v}, \quad (5)$$

$$v(P_1) = \frac{D}{\rho_1} \frac{\partial C(P_1)}{\partial v}, \quad (6)$$

$$C(P_1) = C_S(T). \quad (7)$$

Here P_1 is a point belonging to the surface F_1 ; H is the specific heat of phase transition of the metal in the skin; v is the component of the velocity vector of a boundary point P_1 along the normal v ; C_S is a specified function of the temperature.

At the external boundary, the following conditions hold

$$\lambda_2 \frac{\partial t_2(P_2)}{\partial v} = \sigma \varepsilon [t_c^4 - t_2^4(P_2)] + \alpha [t_c - t_2(P_2)] + H_2 D \frac{\partial C(P_2)}{\partial v}; \quad (8)$$

$$C(P_2) = 0; v_2(P_2) = \frac{D}{\rho_2} \frac{\partial C(P_2)}{\partial v} \frac{\mu_2}{\mu_1}, P_2 \in F_2. \quad (9)$$

Here $\sigma = 5.67 \cdot 10^{-8} \text{ W/m}^2 \cdot \text{K}^4$; H_2 is the heat of chemical transformation of 1 kg of metal in the skin; v_2 is the component of the velocity vector of boundary point P_2 along the normal v . The condition in Eq. (9) holds when the rate of chemical reaction of the metal with atmospheric oxygen at the external boundary of the skin is sufficiently large. Otherwise, Eq. (9) may be replaced by a condition of the form

$$D \frac{\partial C(P_2)}{\partial v} = B_2 \exp\left(-\frac{\beta_2}{t_2(P_2)}\right),$$

where B_2 and β_2 are constants characterizing the rate of this chemical reaction.

In the skin layer, as well as diffusion of the metal to the external surface, there may be diffusion of oxygen to the metal-skin interface. In this case, the concentration function of oxygen at internal points of the skin satisfies a diffusion equation analogous to Eq. (2). On account of chemical reaction of the metal and oxygen inside the skin, the source terms Π_M in Eq. (2) and Π_k in the diffusion equation for oxygen and also in heat-conduction Eq. (1) for the skin layer are nonzero. They are functions of the metal and oxygen concentrations and also of the temperature.

There has been insufficient study of the transition of metal atoms to the skin. According to experimental data [4], the velocity of motion of the metal boundary on account of ox-

idation is inversely proportional to the thickness of the skin layer L and is often written in the form [1, 5-7]

$$v = \frac{B}{L} \exp\left(-\frac{\beta}{T}\right). \quad (10)$$

The velocity v is relatively small and, taking into account Eq. (9), may be expressed approximately in terms of the concentration at the metal-skin boundary

$$v = \frac{D}{\rho_1} \frac{\partial C(P_1)}{dx} \approx \frac{D}{\rho_1} \frac{C(P_1) - C(P_2)}{L} = \frac{D}{\rho_1} \frac{C(P_1)}{L}. \quad (11)$$

It follows from Eqs. (10) and (11) that

$$C(P_1) = \frac{\rho_1 B}{D} \exp\left(-\frac{\beta}{T}\right), \quad (12)$$

i.e., the concentration is a function of the temperature. In accordance with this, the exponential temperature dependence of the concentration $C(P_1)$ may be explained on the basis of the Clapeyron-Clausius equation or the Arrhenius law.

Investigating skin formation on the basis of the given mathematical model entails solving the heat- and mass-transfer problem in a system with moving boundaries [8]. The peculiarity of this problem is the significant change in density of the material in the chemical transformation of the metal in the skin. In [7], an algorithm was proposed for numerical solution of the problem of skin formation on a plane plate, disregarding the density change on transformation of metal in the skin and the accompanying diffusional process, on the basis of an implicit scheme with a relatively low order of approximation $O(\Delta x + \Delta \tau + \Delta \tau / \Delta x)$.

Without any simplifying assumptions, Eqs. (1)-(11) may be solved on the basis of a difference method with explicit separation of the phase boundaries [9] and the use of a three-layer difference scheme [10]. This difference scheme is distinguished by simplicity, which is characteristic of explicit difference schemes, and is also no less economical than implicit schemes for the solution of systems of parabolic equations realized by matrix fitting.

An algorithm for calculating heat and mass transfer in skin formation for a plane plate of thickness $2X$ is outlined below. In connection with the significant difference in density of the metal and skin, the approximate values t_i^n of the temperature $t_1(x_i, \tau_n)$ in the metal and t_m^n and C_m^n of the skin temperature $t_2(x_m, \tau_n)$ and concentration $C(x_m, \tau_n)$ of the metal in the skin layer are determined in autonomous difference schemes

$$\begin{aligned} \tau_n &= n\Delta\tau, \quad n = 0, 1, \dots, \quad \Delta\tau = \text{const}; \quad x_i = i\Delta x_1, \quad i = 0, 1, \dots, I^n - 1, \\ x_j^n &= X_1^n, \quad X_1^n - x_{j-1}^n < \Delta x_1, \quad \Delta x_1 = \text{const}; \\ x_m &= m\Delta x_2, \quad m = 0, 1, \dots, M^n - 1, \quad x_M^n = X_2^n, \quad \Delta x_2 = \text{const}. \end{aligned}$$

Here the integers I^n and M^n are determined from the conditions

$$0 < X_1^n - (I^n - 1)\Delta x_1 \leq \Delta x_1, \quad 0 < X_2^n - (M^n - 1)\Delta x_2 \leq x_2.$$

The difference scheme for solving this problem of skin formation takes the form

$$t_i^0 = t_{10}(x_i); \quad t_m^0 = t_{20}(x_m); \quad C_m^0 = C_0(x_m); \quad X_1^0 = X; \quad X_2^0 = X_0; \quad M^0 = 0; \quad (13)$$

$$\delta_\tau X_1^n = D\delta_x C_m^n; \quad \delta_\tau X_2^n = \frac{\rho_1 \mu_2}{\rho_2 \mu_1} D\delta_x C_m^n; \quad (14)$$

$$\delta_\tau t_i^n (1 + \theta_1) - \delta_\tau t_i^{n-1} \theta_1 = \frac{1}{c_1 \rho_1} \delta_x (\lambda_1 \delta_x t_i^n), \quad i = 0, 1, \dots, I^n - 2; \quad (15)$$

$$\delta_\tau t_i^n = \frac{1}{c_1 \rho_1} \delta_x (\lambda_1 \delta_x t_i^{n+1}), \quad i = I^n - 1; \quad (16)$$

$$(1 + \theta_2) \delta_\tau t_m^n - \theta_2 \delta_\tau t_m^{n-1} = \frac{1}{c_2 \rho_2} \delta_x (\lambda_2 \delta_x t_m^n), \quad m = 0, 1, \dots, M^n - 2; \quad (17)$$

$$\delta_{\tau} t_m^n = \frac{1}{C_2 t_2^n} \delta_x (\lambda_2 \delta_x t_m^{n+1}), \quad m = M^n - 1 \text{ и } X_2^n > 2\Delta x_2; \quad (18)$$

$$(1 + \theta_3) \delta_{\tau} C_m^n - \theta_3 \delta_{\tau} C_m^{n-1} = \delta_x (D \delta_x C_m^n), \quad m = 1, 2, \dots, M^n - 2; \quad (19)$$

$$\delta_{\tau} C_m^n = \delta_x (D \delta_x C_m^{n+1}); \quad m = M^n - 1; \quad (20)$$

$$C_0^{n+1} = B \exp\left(-\frac{\beta}{t_I^{n+1}}\right), \quad C_M^{n+1} = 0; \quad (21)$$

$$t_I^{n+1} = t_{m=0}^{n+1}, \quad \lambda_1 \delta_x t_I^{n+1} - \lambda_2 \delta_x t_{m=0}^{n+1} = H D \delta_x C_0^{n+1}; \quad (22)$$

$$\lambda_2 \delta_x t_M^{n+1} = \{\sigma \varepsilon [t_c^2 + (t_M^n)^2] (t_c + t_M^n) + \alpha\} (t_c - t_M^{n+1}) + H_2 D \delta_x C_M^{n+1}; \quad (23)$$

$$I^{n+1} = \begin{cases} I^n & \text{when } \frac{X_1^{n+1}}{\Delta x_1} - I^n + 1 > 0, \\ I^n - 1 & \text{when } \frac{X_1^{n+1}}{\Delta x_1} - I^n + 1 \leq 0, \end{cases}$$

$$M^{n+1} = \begin{cases} M^n & \text{when } \frac{X_2^{n+1}}{\Delta x_2} - M^n + 1 > 0, \\ M^n + 1 & \text{when } \frac{X_2^{n+1}}{\Delta x_2} - M^n + 1 \leq 0; \end{cases} \quad (24)$$

$$t_{m-1}^{n+1} = t_m^{n+1} - (t_m^{n+1} - t_{m-2}^{n+1}) \frac{X_2^{n+1} - m \Delta x_2}{X_2^{n+1} - (m-1) \Delta x_2} \text{ when } m = M^{n+1} = M^n + 1.$$

Here the initial values of the functions t_{10} , t_{20} , C_0 , X , X_0 and also the physical characteristics of the bodies ρ_1 , ρ_2 , c_1 , c_2 , λ_1 , λ_2 , μ_1 , μ_2 , B , β , H , H_2 , σ , ε , D are assumed to be specified: $\theta_j > 0$, $j = 1, 2, 3$;

$$\begin{aligned} \delta_x C_0^n &= \frac{C_1^n - C_0^n}{\Delta x_2} \text{ when } X_2 > \Delta x_2, \quad \delta_x C_0^n = \frac{C_M^n - C_0^n}{X_2} \text{ when } X_2 < \Delta x_2; \\ \delta_x C_M^n &= \frac{C_M^n - C_{M-1}^n}{X_2^n - (M^n - 1) \Delta x_2} \text{ when } X_2 \geq \Delta x_2, \\ \delta_x C_M^n &= \frac{C_M^n - C_0^n}{X_2^n} \text{ when } X_2^n < \Delta x_2; \\ \delta_{\tau} \varphi^n &= \frac{\varphi^{n+1} - \varphi^n}{\Delta \tau}, \quad \varphi = X_1, X_2, t_i, t_m, C_m; \end{aligned} \quad (25)$$

$$\delta_x (\xi \delta_x \varphi_j^n) = \frac{1}{2\Delta x_{\gamma}^2} [(\xi_{j+1}^n + \xi_j^n) (t_{j+1}^n - t_j^n) - (\xi_j^n + \xi_{j-1}^n) (t_j^n - t_{j-1}^n)],$$

$$\begin{aligned} \delta_x (\xi \delta_x \varphi_j^{n+1}) &= \frac{1}{\Delta x_{\gamma} + \Delta \bar{x}_{\gamma}} \left[(\xi_{j+1}^n + \xi_j^n) \frac{\varphi_{j+1}^{n+1} - \varphi_j^{n+1}}{\Delta \bar{x}_{\gamma}} - \right. \\ &\left. - (\xi_j^n + \xi_{j-1}^n) \frac{\varphi_j^{n+1} - \varphi_{j-1}^{n+1}}{\Delta \bar{x}_{\gamma}} \right], \quad \xi = \lambda_1, \lambda_2, D; \quad j = i, m; \quad \gamma = 1, 2; \end{aligned}$$

$$\Delta \bar{x}_1 = X_1^{n+1} - (I^n - 1) \Delta x_1 \text{ when } \varphi_j = t_{I-1};$$

$$\Delta \bar{x}_2 = X_2^{n+1} - (M^n - 1) \Delta x_2 \text{ when } \varphi_j = t_{M-1}, C_{M-1}.$$

The stability conditions for Eqs. (15), (17), and (19)

$$\Delta\tau \leq \min \left\{ \frac{c_j \rho_j (1 + 2\theta_j)}{2\lambda_j \Delta x_j^2}, \frac{1 + 2\theta_3}{2D \Delta x_2^2} \right\}, j = 1, 2,$$

allow any difference-scheme step to be chosen by varying the parameter θ , as for implicit difference equations; however, since the approximation error of Eqs. (15), (17), and (19) is of order $O(\Delta x_j^2 + \Delta\tau)$, it is inexpedient to choose a step that is too large. The values of the grid functions t_i^{n+1} , t_m^{n+1} for the initial instant ($n = 0$) are determined from the relation

$$\varphi^0 - \varphi^{-1} = \theta_0 (\varphi^1 - \varphi^0), \quad \varphi = t_i, t_m, C_m, \quad 0 \leq \theta_0 \leq 1. \quad (26)$$

Note that θ_0 has a pronounced influence on the value of the grid function only for the first few time steps. The solution of Eqs. (12)-(23) is undertaken as follows. Initially ($n = 0$), the values of the grid functions t_i^0 , t_m^0 , C_m^0 , X_1^0 , X_2^0 are specified. The initial temperature t_i^0 of a metallic plate of thickness X_1^0 fed into a furnace may be regarded as close. The skin thickness X_2^0 is close to zero here. In connection with this, without increasing the order of error of the difference-scheme approximation, it may be supposed that $X_2^0 \sim \Delta x_2^\gamma$, where $\gamma > 1$ and $M^0 = 1$. The concentrations C_0^0 and C_M^0 are determined from Eq. (21), and the temperature t_M^0 from Eq. (23), under the condition that $t_M^n = t_M^{n+1}$ when $n + 1 = 0$. Assume that the values of the grid functions t_i^k , t_m^k , C_m^k , X_1^k , X_2^k , $k = 1, 2, \dots, n$ have already been found, and their values for the layer $n + 1$ must be determined. First, the values of X_1^{n+1} and X_2^{n+1} are calculated from Eq. (14). Then, the grid function t_i^{n+1} is found from Eq. (15) at the internal grid points $i = 1, 2, \dots, I^n - 2$, which at times τ_i^n are at a distance of no less than the step Δx_j from the boundary surfaces X_j ($j = 1, 2$). Analogously, the functions t_m^{n+1} and C_m^{n+1} are found from Eqs. (17) and (19), when $m = 1, 2, \dots, M^n - 2$. The parameters θ_j^m ($j = 1, 2, 3$) appearing in difference Eqs. (15), (17), and (19) are then determined. First, for each of these equations, the maximum permissible (according to the stability condition) time step $\Delta\tau_j$ when $\theta_j = 0$ is calculated (for the case of an ordinary two-layer explicit difference equation)

$$\Delta\tau_1 = \frac{\Delta x_1^2 c_1 \rho_1}{2\lambda_1}, \quad \Delta\tau_2 = \frac{\Delta x_2^2 c_2 \rho_2}{2\lambda_2}, \quad \Delta\tau_3 = \frac{\Delta x_2^2}{2D}.$$

The final value of the time step $\Delta\tau$ is determined in terms of the minimal $\Delta\tau_{\min}$ of the steps $\Delta\tau_j$, $j = 1, 2, 3$ from the relation

$$\Delta\tau = \Delta\tau_{\min} (1 + 2\theta),$$

where θ is the maximum value of θ_j according to the condition that the error of the solution be within acceptable limits. Thanks to the significant difference in linear dimensions of the metal and the skin and also the monotonic dependence of the temperature on the coordinates and time, the error of the solution varies insignificantly up to $\theta = 50$, which corresponds to a 100-fold increase in the time step in comparison with the usual explicit scheme. The final values of θ_j are found from the condition

$$\theta_j = \begin{cases} 0 & \text{when } \Delta\tau \leq \Delta\tau_j, \\ (\Delta\tau - \Delta\tau_j) / (2 \times \Delta\tau_j) & \text{when } \Delta\tau > \Delta\tau_j, \end{cases}$$

which ensures stability of the solution of the corresponding difference equation.

The temperatures at boundary and adjacent points are determined as follows. In the initial stage, when the skin thickness $X_2^n \leq 2\Delta x_2$, the temperatures t_{I-1}^{n+1} , t_I^{n+1} , and t_M^{n+1} are found by simultaneous solution of Eqs. (16), (22), and (23), under the assumption that the temperature changes linearly in the skin layer. According to this hypothesis, when $X_2^{n+1} > \Delta x_2$ and $X_2^{n+1} > 2\Delta x_2$, the temperature t_m^{n+1} at the grid points $m = 1$ and $m = 2$ is calculated from Eq. (25). With a thickness of the skin layer $X_2^n > 2\Delta x_2$, the temperatures t_{I-1}^{n+1} and t_I^{n+1} are found from Eqs. (16) and (22) if $I^{n+1} = I^n$. If $I^{n+1} = I^n + 1$, the temperature t_i^{n+1} at the point $i = I^{n+1} - 1$ is determined from Eq. (15), and Eq. (22) is used to find t_I^{n+1} .

The temperatures $t_{M^n}^{n+1}$ and $t_{M^n-1}^{n+1}$ when $X_2^n > 2\Delta x_2$ are calculated from Eqs. (18) and (23). If $M^{n+1} = M^n + 1$, the temperature at the newly formed point $m = M^n + 1$ is determined by linear interpolation with respect to Eq. (25).

The calculation results for heating and skin formation with the following initial data are shown in Figs. 1 and 2 [3]: $\lambda_1 = 29.1$ W/m·K; $c_1 = 0.69$ kJ/kg·K; $\rho_1 = 7500$ kg/m³; $\lambda_2 = 0.872$ W/m·K; $c_2 = 1.047$ kJ/kg·K; $\rho_2 = 4000$ kg/m³; $X = 0.397$ m; $\sigma = 5.67 \cdot 10^{-8}$ W/m²·K⁴; $\epsilon = 1$;

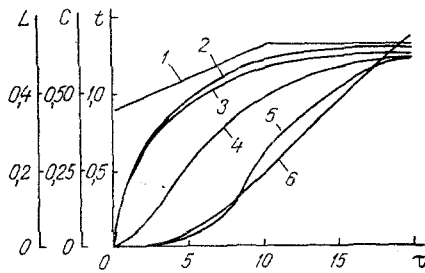


Fig. 1

Fig. 1. Variation in quantities characterizing the heating of an ingot: 1) furnace temperature; 2-4) temperatures at the external skin surface, at the metal-skin contact boundary, and at the center of the ingot; 5) concentration C of unoxidized metal in skin close to the metal-skin contact boundary; 6) thickness L of skin layer. t , 10^3 °C; C , 10^{-2} kg/m³; L , cm; τ , h.

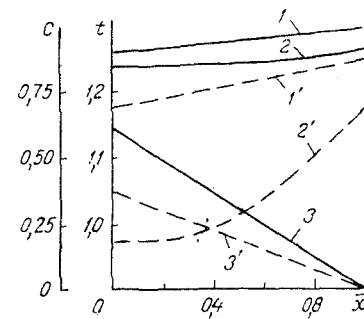


Fig. 2

Fig. 2. Temperature distribution over the thickness of the ingot (1, 1') and the skin (2, 2') and the concentration distribution of unoxidized metal over the skin thickness (3, 3'); the continuous curves correspond to the end of heating $\tau = 20.024$ and the dashed curves to $\tau = 10$ h.

$BD = 0.38$ m²/h; $b = 1.8 \cdot 10^4$ K; $\alpha = 0$; $D = 0.2 \cdot 10^{-6}$ m/sec. The dimensionless quantity \bar{x} in Fig. 2 determines the position of the point in the metal layer ($\bar{x} = x/X_1$) or skin ($\bar{x} = (x - X_1)/(X_2 - X_1)$). The temperature of the surrounding medium t_c , K (furnace temperature) varies over time τ , h, according to the law

$$t_c = \begin{cases} 1173 + 40\tau & \text{when } \tau < 10, \\ 1573 & \text{when } \tau > 10. \end{cases}$$

The duration of heating τ_{cr} is defined as the minimum time for which the following condition is satisfied [3]

$$\min t_1(x, \tau_{cr}) > 1513, \quad \frac{1}{X} \int_0^x t_1(x, \tau_{cr}) dx \geq 1523 \text{ K.}$$

In [3], diffusion processes in skin formation were not considered and no account was taken of the significant difference in velocities of the external and internal skin boundaries. On taking account of these factors, the theoretical heating time of the semifinished product is increased from 19.3 to 20.04 h. Reducing the diffusion coefficient D , while B and β remain unchanged, leads to increase in the concentration $C(X_1)$.

Note, in conclusion, that the method of calculation here developed is relatively simple, it requires little computer time for its realization, and it allows the influence of various factors on the heating of ingots to be taken more accurately into account. This latter attribute is necessary for optimization of the heating and elucidation of the laws of skin formation.

NOTATION

x, y, z , spatial coordinates; τ , time; λ, c, ρ , thermal conductivity, specific heat, density; t , temperature; Π, Π_M , density of heat and mass sources; D , diffusion coefficient; σ , Stefan-Boltzmann constant; ϵ , emissivity of skin surface; t_c , ambient temperatures; v , velocity of metal-boundary motion due to oxidation; X , thickness of layer of material; α , heat-transfer coefficient; μ , molecular weight. Indices: $j = 1, j = 2$, quantities relating to metal and skin; n , number of grid points with respect to time; i and m , number of grid points over the spatial coordinate in the metal layer and the skin.

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