INFLUENCE OF STEFAN FLOW AND CONVECTION ON THE KINETICS OF CHEMICAL REACTIONS AND HEAT AND MASS EXCHANGE OF CARBON PARTICLES WITH GASES

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The problem of the heat and mass transfer and the kinetics of chemical transformation of a carbon particle $(C + O_2 \rightarrow CO_2 (I), 2C + O_2 \rightarrow 2CO (II), C + CO_2 \rightarrow 2CO (III))$ is solved within the framework of the model of a reduced film with account for the Stefan flow and natural and forced convection. Analytical expressions are obtained for the velocity of the Stefan flow, the rates of chemical reactions, the concentrations of gaseous components, the densities of the heat and mass fluxes, and the density of chemical heat release on the surface of the carbon particle.

The mutual effect of the heat and mass transfer and the kinetics of chemical reactions with account for the Stefan flow on the surface of a motionless particle of solid carbon was considered in [1, 2] in the exothermic parallel chemical reactions $C + O_2 \rightarrow CO_2$ (I) and $2C + O_2 \rightarrow 2CO$ (II) without account for the endothermic reaction $C + CO_2 \rightarrow 2CO$ (III) and the homogeneous reaction $2CO + O_2 \rightarrow 2CO_2$ (IV). Neglect of the chemical reaction (III), as is shown by a comparison of calculations and experiments [3], leads to erroneous results for the rate of chemical transformation of carbon at high temperatures of the particle. In [4], a mechanism of the effect of the relative velocity of motion of a carbon particle on the characteristics of its combustion without account for the Stefan flow in reactions (I) and (II) is found. It should be noted that under certain conditions where the Damköhler number [5, 6] or the Semenov number [7, 8] are smaller than a certain value, one can disregard the effect of the homogeneous reaction $2CO + O_2 \rightarrow 2CO_2$. This is possible when [5]

Se =
$$\sqrt{\frac{k_4 d^2}{D(Nu)^2}} < 0.4$$
, $k_4 = k_{04} \exp{\frac{-E_4}{RT_g}}$

Under the conditions described in [3] (air at room temperature and with velocity V = 0.6 m/sec blows over a motionless carbon particle of diameter $d \approx 1.2$ cm heated to a high temperature), the Semenov number is of about 10⁻⁴. The small value of Se is determined by the low temperature of the gas. Reaction (IV) can be disregarded for a small size of the particle as well, althrough the gas temperatures can be high.

In this work, we consider the kinetics of the chemical reactions (I), (II), and (III) and of the heat and mass transfer of a carbon particle with account for the Stefan flow and for forced and natural convection. Analytical expressions are derived for the velocity of the Stefan flow, the densities of the heat and mass fluxes, the density of chemical heat release, the concentration of gaseous components, and the rates of chemical reactions on the surface of the carbon particle.

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On the particle surface, the heat and mass of gaseous components are transferred by heat conduction, concentration diffusion, and Stefan flow, which is determined by the chemical transformation of solid carbon to gaseous components as a result of reactions (I)–(III). Since the molar masses of the gaseous components are close, heat transfer by diffusion heat conduction and mass transfer by thermal diffusion can be disregarded [7, 8]. In this case, the expressions for the densities of the heat and mass fluxes on the surface of a spherical particle with account for the Stefan flow are

$$q_{\rm gs} = -\lambda_{\rm g} \left. \frac{\partial T_{\rm g}}{\partial r} \right|_{\rm s} + c_{\rm g} \left(\rho_{\rm g} U \right)_{\rm s} T_{\rm gs} \,, \quad T_{\rm gs} > T_{\rm g\infty} \,, \tag{1}$$

$$j_{js} = -D\rho_g \left. \frac{\partial C_j}{\partial r} \right|_s + (\rho_g U)_s C_{js}, \quad C_{js} > C_{j\infty}, \qquad (2)$$

where j = 1 for O₂, 2 for CO₂, 3 for CO, and 4 for N₂.

The effect of the relative velocity of motion of the particle on the kinetics of chemical reactions and on heat and mass transfer is allowed for by the notion of a reduced film on the surface of which the parameters of an undisturbed flow are specified [7]. In the absence of forced and natural convection (the particle is motionless relative to the gas), the radius of the reduced film r_{∞} is equal to infinity. It decreases with increase in the intensity of natural and forced convection, thus approaching the particle radius r_s . The dependence of the dimensionless radius of the reduced film on the Nusselt number (Nu), which, in turn, is determined by the effective Reynolds number (Re_{ef}), is represented in the form

$$\frac{r_{\infty}}{r_{\rm s}} = \left(1 - \frac{2}{\rm Nu}\right)^{-1},\tag{3}$$

where

Nu = 2 + A Re_{ef}^{1/2} Pr^{1/3}, A = 0.55 [3],

or

$$Nu = 0.56 \sqrt{Re_{ef}} / [1 - \exp(-0.28 \sqrt{Re_{ef}})] [3], \quad Nu = 2 + 0.16 Re_{ef}^{2/3} [8],$$

$$Re_{ef} = Re_V + Re_G, \quad Re_V = \frac{Vd}{v_g}, \quad Re_G = \sqrt{0.5Gr},$$

$$Gr = \frac{gd^3 (T - T_{g\infty})}{273v_g^2}, \quad v_g = \Pr a_g, \quad a_g = \frac{\lambda_g}{c_g \rho_g}, \quad \beta = \frac{D Nu}{d}, \quad \alpha = \frac{\lambda_g Nu}{d}.$$
(4)

For a motionless particle Nu = 2, $\beta = 2D/d$, $\alpha = 2\lambda_g/d$, and $r_{\infty} = \infty$.

The coefficients of heat and mass transfer in explicit form do not depend on time, since the characteristic time of establishment of the stationary fields of concentrations and temperatures in the gas phase is smaller than the time of change in the particle temperature. The coefficients of heat and mass transfer change with time as a result of the change in the temperature of the particle and the decrease in its diameter:

$$\frac{1}{6}c\rho d\frac{\partial T}{\partial t} = q_{\rm ch} - q_{\rm h}, \quad T(t=0) = T_{\rm b}, \quad -\frac{1}{2}\rho\frac{\partial d}{\partial t} = W_{\rm C}, \quad d(t=0) = d_{\rm b},$$

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$$W_{\rm C} = \frac{M_{\rm C}}{M_{\rm O_2}} \left(k_1 + 2k_2\right) \rho_{\rm gs} C_{\rm O_2,s} + \frac{M_{\rm C}}{M_{\rm CO_2}} k_3 \,\rho_{\rm gs} C_{\rm CO_2,s}\,,\tag{5}$$

$$q_{\rm ch} = (k_1 Q_1 + k_2 Q_2) \rho_{\rm gs} C_{\rm O_2,s} - k_3 Q_3 \rho_{\rm gs} C_{\rm CO_2,s},$$

$$k_1 = k_{01} \exp\left(-\frac{E_1}{RT}\right), \quad k_2 = k_{02} \exp\left(-\frac{E_2}{RT}\right), \quad k_3 = k_{03} \exp\left(-\frac{E_3}{RT}\right), \quad q_h = q_g + q_w, \quad q_w = \varepsilon \sigma \left(T^4 - T^4_w\right).$$
(6)

The relative mass concentrations of oxygen $C_{O_2,s}$, carbon dioxide $C_{CO_2,s}$, carbon monoxide $C_{CO,s}$, and nitrogen $C_{N_2,s}$ and also the velocity of the Stefan flow U_s are found from the equalities of the densities of the mass fluxes of O_2 , CO_2 , CO, and N_2 , written with account for the Stefan flow, to the rates of chemical reactions for the corresponding components:

$$j_{O_{2},s} = D\rho_{g} \frac{\partial C_{O_{2}}}{\partial r} \bigg|_{s} - (\rho_{g}U)_{s} C_{O_{2},s} = (k_{1} + k_{2}) \rho_{gs}C_{O_{2},s} ,$$

$$j_{CO_{2},s} = -D\rho_{g} \frac{\partial C_{CO_{2}}}{\partial r} \bigg|_{s} + (\rho_{g}U)_{s} C_{CO_{2},s} = \frac{M_{CO_{2}}}{M_{O_{2}}} k_{1} \rho_{gs}C_{O_{2},s} - k_{3} \rho_{gs}C_{CO_{2},s} ,$$

$$j_{CO,s} = -D\rho_{g} \frac{\partial C_{CO}}{\partial r} \bigg|_{s} + (\rho_{g}U)_{s} C_{CO,s} = \frac{2M_{CO}}{M_{O_{2}}} k_{2} \rho_{gs}C_{O_{2},s} + \frac{2M_{CO}}{M_{CO_{2}}} k_{3} \rho_{gs}C_{CO_{2},s} ,$$

$$j_{N_{2},s} = D\rho_{g} \frac{\partial C_{N_{2}}}{\partial r} \bigg|_{s} - (\rho_{g}U)_{s} C_{N_{2},s} = 0 .$$
(7)

In writing (7), we assumed that the coefficients of diffusion of the components of the gas mixture are $D = D_{O_2} = D_{CO_2} = D_{CO} = D_{N_2}$. To calculate them, we use the simple exponential formula

$$D = D_0 \left(\frac{P_0}{P}\right) \left(\frac{T_g}{T_0}\right)^{n+1}, \quad n = 0.5 - 1,$$

where D_0 is the coefficient of diffusion for the pressure $P = P_0$ and the temperature of the gas $T_g = T_0$ [8].

The density of the gas mixture is found from the isobaricity condition (P = const) in the form

$$P = \rho_{g\infty} T_{g\infty} \sum_{j=1}^{4} \frac{C_{j\infty}}{M_j} = \rho_{gs} T_{gs} \sum_{j=1}^{4} \frac{C_{js}}{M_j} = \rho_g T_g \sum_{j=1}^{4} \frac{C_j}{M_j},$$

where M_j is the molar mass of the *j*th component.

As the first approximation we can take

$$\rho_{\rm g} = \rho_{\rm g0} \left(\frac{P}{P_0} \right) \left(\frac{T_0}{T_{\rm g}} \right). \tag{8}$$

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Using the condition $C_{O_2} + C_{CO_2} + C_{CO} + C_{N_2} = 1$, we obtain from (7) that the mass velocity of the Stefan flow on the particle surface is determined by the algebraic sum of the densities of the mass fluxes of the components of the gas mixture:

$$(\rho_g U)_s = j_{CO_2,s} + j_{CO,s} - j_{N_2,s} - j_{O_2,s} = \frac{M_C}{M_{O_2}} (k_1 + 2k_2) \rho_{gs} C_{O_2,s} + \frac{M_C}{M_{CO_2}} k_3 \rho_{gs} C_{CO_2,s} .$$
(9)

Comparing (9) and (5), we see that the mass velocity of the Stefan flow on the surface of a carbon particle is equal to the rate of its chemical transformation to gaseous components:

$$(\rho_{\rm g}U)_{\rm s} = W_{\rm C} = -\frac{1}{2}\rho \frac{\partial d}{\partial t}.$$

The dependences $C_{O_2}(r)$, $C_{CO_2}(r)$, $C_{N_2}(r)$, and $T_g(r)$ for $r_s < r < r_{\infty}$ are found from the solution of the equations of heat conduction, diffusion, and continuity:

$$\frac{\partial}{\partial r} \left(r^2 \lambda_{\rm g} \frac{\partial T_{\rm g}}{\partial r} \right) = \frac{\partial}{\partial r} \left(c_{\rm g} \rho_{\rm g} T_{\rm g} U r^2 \right), \quad \frac{\partial}{\partial r} \left(r^2 \rho_{\rm g} D \frac{\partial C_j}{\partial r} \right) = \frac{\partial}{\partial r} \left(C_j \rho_{\rm g} U r^2 \right), \quad \rho_{\rm g} U r^2 = \rho_{\rm gs} U_{\rm s} r_{\rm s}^2. \tag{10}$$

The boundary conditions for the temperature of the gas and for the relative mass concentrations of the gaseous components on the particle surface $(r = r_s)$ and on the surface of the reduced film $(r = r_{\infty})$ are

$$T_{g}(r=r_{s}) = T_{gs} = T$$
, $C_{j}(r=r_{s}) = C_{js}$, $T_{g}(r=r_{\infty}) = T_{g\infty}$, $C_{j}(r=r_{\infty}) = C_{j\infty}$.

we assume that $\lambda_g/(c_g \rho_g) = D$, and introduce dimensionless variables and quantities

$$\theta = \frac{C_j - C_{j_s}}{C_{j_{\infty}} - C_{j_s}} = \frac{T_g - T_{g_s}}{T_{g_{\infty}} - T_{g_s}}, \quad \xi = \frac{U_s r_s}{D} \left(1 - \frac{r_s}{r}\right), \quad \xi_{\infty} = \frac{U_s r_s}{D} \left(1 - \frac{r_s}{r_{\infty}}\right).$$

With account for (3) and (9), we obtain that the dimensionless velocity of the Stefan flow is

$$\xi_{\infty} = \frac{U_{\rm s}}{\beta} = \frac{M_{\rm C}}{M_{\rm O_2}} \frac{(k_1 + 2k_2)}{\beta} C_{\rm O_2, s} + \frac{M_{\rm C}}{M_{\rm CO_2}} \frac{k_3}{\beta} C_{\rm CO_2, s} \,. \tag{11}$$

This makes it possible to reduce the system of equations (10) to one equation:

$$\frac{\partial^2 \theta}{\partial \xi^2} = \frac{\partial \theta}{\partial \xi}, \quad \theta \ (\xi = 0) = 0, \quad \theta \ (\xi = \xi_{\infty}) = 1,$$

whose solution has the form

$$\frac{C_j - C_{j_{\rm S}}}{C_{j_{\infty}} - C_{j_{\rm S}}} = \frac{T_{\rm g} - T_{\rm g_{\rm S}}}{T_{\rm g_{\infty}} - T_{\rm g_{\rm S}}} = \frac{\exp\left(\xi\right) - 1}{\exp\left(\xi_{\infty}\right) - 1} \,. \tag{12}$$

Having substituted (12) into (1), with account for (4), we find the density of the heat flux which characterizes the heat exchange between the particle surface and the gas:

$$q_{\rm g} = \alpha \left[(T - T_{\rm gw}) \frac{\xi_{\infty} \exp\left(-\xi_{\infty}\right)}{1 - \exp\left(-\xi_{\infty}\right)} + \xi_{\infty}T \right]. \tag{13}$$

Assuming that $\xi_{\infty} \ll 1$ and substituting exp $(-\xi_{\infty}) = 1 - \xi_{\infty} + \frac{1}{2}\xi_{\infty}^2$ into (13), we obtain that q_g is determined by the sum of the densities of the heat fluxes:

$$q_{\rm g} = \alpha \left[(T - T_{\rm g\infty}) + \frac{\xi_{\infty}}{2} (T + T_{\rm g\infty}) \right].$$

To find ξ_{∞} , $C_{O_2,s}$, $C_{CO_2,s}$, $C_{CO_3,s}$ and $C_{N_2,s}$, we substitute (12) into the left-hand sides of Eqs. (7). As a result, we obtain the system of equations

$$j_{O_{2},s} = \beta \rho_{g} \frac{\left[C_{O_{2}^{\infty}} \exp\left(-\xi_{\infty}\right) - C_{O_{2},s}\right] \xi_{\infty}}{1 - \exp\left(-\xi_{\infty}\right)} = (k_{1} + k_{2}) \rho_{gs} C_{O_{2},s} ,$$

$$j_{CO_{2},s} = \beta \rho_{g} \frac{\left[C_{CO_{2},s} - C_{CO_{2}^{\infty}} \exp\left(-\xi_{\infty}\right)\right] \xi_{\infty}}{1 - \exp\left(-\xi_{\infty}\right)} = \frac{M_{CO_{2}}}{M_{O_{2}}} k_{1} \rho_{gs} C_{O_{2},s} - k_{3} \rho_{gs} C_{CO_{2},s} ,$$

$$j_{CO_{3},s} = \beta \rho_{g} \frac{\left[C_{CO,s} - C_{CO_{\infty}} \exp\left(-\xi_{\infty}\right)\right] \xi_{\infty}}{1 - \exp\left(-\xi_{\infty}\right)} = \frac{2M_{CO}}{M_{O_{2}}} k_{2} \rho_{gs} C_{O_{2},s} + \frac{2M_{CO}}{M_{CO_{2}}} k_{3} \rho_{gs} C_{CO_{2},s} ,$$

$$j_{N_{2},s} = \beta \rho_{g} \frac{\left[C_{N_{2}^{\infty}} \exp\left(-\xi_{\infty}\right) - C_{N_{2},s}\right] \xi_{\infty}}{1 - \exp\left(-\xi_{\infty}\right)} = 0 .$$
(14)

From (14) we express the surface concentrations of the components in terms of ξ_{∞} :

$$C_{O_2,s} = C_{O_2^{\infty}} \frac{\beta (1 - \xi_{\infty} F)}{\beta + (k_1 + k_2)F}, \quad F = (1 - \exp(-\xi_{\infty}))/\xi_{\infty},$$
(15)

$$C_{\text{CO}_{2},\text{s}} = C_{\text{CO}_{2}^{\infty}} \frac{\beta \left(1 - \xi_{\infty}F\right)}{\beta + k_{3}F} + C_{\text{O}_{2},\text{s}} \frac{M_{\text{CO}_{2}}}{M_{\text{O}_{2}}} \frac{k_{1}F}{(\beta + k_{3}F)},$$
(16)

$$C_{\rm CO,s} = C_{\rm CO\infty} \left(1 - \xi_{\infty} F\right) + \frac{2M_{\rm CO}}{M_{\rm O_2}\beta} C_{\rm O_2,s} F\left(k_2 + k_3 \frac{M_{\rm O_2}}{M_{\rm CO_2}} \frac{C_{\rm CO_2,s}}{C_{\rm O_2,s}}\right),\tag{17}$$

$$C_{N_2,s} = C_{N_2^{\infty}} \exp(-\xi_{\infty}).$$
 (18)

Substituting (15) and (16) into (11), we obtain the transcendental equation for determination of the dimensionless velocity of the Stefan flow on the particle surface:

$$\xi_{\infty} = C_{O_{2^{\infty}}} \frac{(1 - \xi_{\infty}F)}{[\beta + (k_{1} + k_{2})F]} \frac{M_{C}}{M_{O_{2}}} \left(k_{1} + 2k_{2} + \frac{k_{1}k_{3}F}{\beta + k_{3}F}\right) + \frac{M_{C}}{M_{CO_{2}}} C_{CO_{2^{\infty}}} \frac{k_{3}(1 - \xi_{\infty}F)}{\beta + k_{3}F}.$$
(19)

Numerical calculations show that $\xi_{\infty} \ll 1$. For the approximation exp $(-\xi_{\infty}) = 1 - \xi_{\infty}$, assuming that $C_{CO_{2^{\infty}}} = 0$, from (19) we obtain

$$\xi_{\infty} = P_{\rm sf} \left[1 + \frac{\beta}{k_1 + k_2} + P_{\rm sf} \right]^{-1}, \tag{20}$$

$$P_{\rm sf} = \frac{M_{\rm C}}{M_{\rm O_2}} \left[1 + \frac{k_2}{k_1 + k_2} + \frac{k_1}{(k_1 + k_2)} \frac{k_3}{(k_3 + \beta)} \right] C_{\rm O_2^{\infty}} \,. \tag{21}$$

Substituting (20) into (15) at F = 1, we have the relation between $C_{O_2,s}$ and $C_{O_2,s}$ in explicit form:

$$C_{O_2,s} = C_{O_2,\infty} \left(\frac{(k_1 + k_2) (1 + P_{sf})}{\beta} + 1 \right)^{-1}.$$
(22)

On the assumption that $C_{CO_{2}\infty} = 0$, $C_{CO_{\infty}} = 0$, and $C_{N_{2}\infty} = 1 - C_{O_{2}\infty}$, in a similar fashion from formulas (16)–(18) we find the surface concentrations of CO₂, CO, and N₂:

$$C_{\text{CO}_2,\text{s}} = C_{\text{O}_2,\text{s}} \frac{M_{\text{CO}_2}}{M_{\text{O}_2}} \frac{k_1}{(\beta + k_3)}, \quad C_{\text{CO},\text{s}} = C_{\text{O}_2,\text{s}} \frac{2M_{\text{CO}}}{M_{\text{O}_2}\beta} \left(k_2 + \frac{k_1k_3}{\beta + k_3}\right), \quad C_{\text{N}_2,\text{s}} = (1 - C_{\text{O}_2^{\infty}})(1 - \xi_{\infty}).$$
(23)

Using formulas (22) and (23), we analyze the effect of the temperature, the diameter, and the relative velocity of motion of a particle on $C_{O_2,s}$, $C_{CO_2,s}$, $C_{CO_3,s}$ and $C_{N_2,s}$ and consequently on q_{ch} and W_C . At low temperatures (T < 1600 K), the chemical reactions occur in the kinetic region, for which

$$\frac{\left(k_1 + k_2\right)\left(1 + P_{\rm sf}\right)}{\beta} << 1 \;, \;\; \frac{k_3}{\beta} << 1 \;.$$

It follows from (5), (6), and (15)-(17) that

$$W_{\rm C} = -\frac{1}{2} \rho \frac{\partial d}{\partial t} = \frac{M_{\rm C}}{M_{\rm O_2}} (k_1 + 2k_2) \rho_{\rm gs} C_{\rm O_2^{\infty}}, \quad q_{\rm ch} = (k_1 Q_1 + k_2 Q_2) \rho_{\rm g} C_{\rm O_2^{\infty}},$$

i.e., q_{ch} and W_C increase with increase in the temperature according to the Arrhenius dependence and are not related to the diameter and the relative velocity of motion of a particle. In this case, the chemical reaction (III) can be disregarded.

In the region of intermediate temperatures (1600 K < T < 2400 K), the increase in the temperature leads to the involvement of the processes of mass transfer and the endothermic reaction (III), which shifts the kinetics of the chemical reactions to the transition region

$$\frac{\left(k_1+k_2\right)\left(1+P_{\rm sf}\right)}{\beta}\approx 1 \ , \ \ \frac{k_3}{\beta}\approx 1 \ . \label{eq:kappa}$$

An analysis shows that in this region of temperatures q_{ch} decreases as the temperature increases due to the effect of the endothermic reaction (III) within a certain range of particle sizes.

A further increase in the temperature (T > 2400 K) leads to a shift of the kinetics of the chemical reactions to the diffusion region, where the following conditions are fulfilled:

$$\frac{(k_1 + k_2) (1 + P_{\rm sf})}{\beta} >> 1 , \ \frac{k_3}{\beta} >> 1 ,$$

using which at high temperatures, from (21)-(23) we obtain the asymptotic expressions

$$P_{\rm sf}^* = \frac{2M_{\rm C}}{M_{\rm O_2}} C_{\rm O_{2^{\infty}}}, \quad C_{\rm O_{2^{N}}} = C_{\rm O_{2^{\infty}}} \frac{\beta}{(k_1 + k_2) (1 + P_{\rm sf}^*)}, \quad C_{\rm CO_{2^{N}}} = C_{\rm O_{2^{N}}} \frac{M_{\rm CO_{2}}}{M_{\rm O_{2}}} \frac{k_1}{k_3},$$

$$C_{\rm CO,s} = C_{\rm O_{2^{N}}} \frac{2M_{\rm CO}}{M_{\rm O_{2}}} \frac{(k_1 + k_2)}{\beta}, \quad C_{\rm N_{2^{N}}} = (1 - C_{\rm O_{2^{\infty}}}) \frac{1}{1 + P_{\rm sf}^*}.$$
(24)

Substituting (24) into (6) and (5), we obtain that at high temperatures the density of chemical heat release is

$$q_{\rm ch} = Q_2 \frac{1}{1 + P_{\rm sf}^*} C_{\rm O_2^{\infty}} \left(\rho_{\rm g} D\right) \frac{\rm Nu}{d}, \qquad (25)$$

and the rate of chemical transformation of carbon is

$$W_{\rm C} = -\frac{1}{2} \rho \frac{\partial d}{\partial t} = \frac{2M_{\rm C}}{M_{\rm O_2}} \frac{1}{1 + P_{\rm sf}^*} C_{\rm O_2^{\infty}}(\rho_{\rm g} D) \frac{\rm Nu}{d},$$
(26)

i.e., q_{ch} and W_C increase with decrease in the diameter almost in inverse proportion, since Nu weakly depends on the diameter of the particle. As the temperature increases, q_{ch} and W_C increase similarly to the product $\rho_g D$. It is shown in [9] that $\rho_g D$ must be determined for the root-mean-square temperature of the particle and the gas. Taking n = 0.75 [7], we obtain that $q_{ch} \sim W_C \sim (D_0 \rho_0) [(T + T_g)/2T]^{0.75}$.

The increase in the relative velocity of motion of particles leads to a slight increase in the Nusselt criterion and consequently in q_{ch} and W_{C} .

It follows from formulas (25) and (26) that the rate of chemical transformation of a carbon particle in air at a high temperature is determined by the kinetics of the chemical reaction $2C + O_2 \rightarrow 2CO$ (II) occurring in the diffusion mode, which is confirmed by experimental data [3].

The expressions obtained allow one to analyze the high-temperature modes of heat and mass transfer and the kinetics of chemical transformation of carbon particles with account for the Stefan flow and for forced and natural convection.

NOTATION

T, temperature of the particle; T_g , temperature of the gas; $T_{g\infty}$, temperature of the gas on the surface of the reduced film; T_w , temperature of the walls of the chamber of the reaction unit; *P*, pressure of the gas; P_0 , atmospheric pressure; *V*, relative velocity of the particle; v_g , kinematic viscosity of the gas; *d*, diameter of the particle; a_g , thermal diffusivity; *c*, specific heat of the particle; ρ and ρ_g , density of the particle and the gas, respectively; *t*, time; q_{ch} , density of chemical heat release; q_h , density of the heat flux on the particle

surface; q_g , density of the heat flux characterizing the heat exchange between the particle and the gas (including the Stefan flow, heat conduction, and forced and natural convection); q_w , density of the radiative heat flux characterizing the heat exchange with the walls of the reaction unit; k_1 , k_2 , k_3 , and k_4 , rate constants of the chemical reactions (I), (II), (III), and (IV); M_C , M_{O_2} , M_{CO_2} , and M_{CO} , molar masses of carbon, oxygen, carbon dioxide, and carbon monoxide; C_{O_2} , C_{CO_2} , C_{CO} , and C_{N_2} , relative mass concentrations of O_2 , CO_2 , CO_3 , and N_2 ; Q_1 and Q_2 , thermal effects of the chemical reactions (I) and (II) calculated per unit mass of carbon dioxide; k_{01} , k_{02} , k_{03} , and k_{04} , preexponential factors; E_1 , E_2 , E_3 , and E_4 , activation energy of reactions (I), (II), (III), and (IV); ε , emissivity of the particle; σ , Stefan–Boltzmann constant; $D = D_{O_2} = D_{CO_2} = D_{CO} = D_{N_2}$, coefficients of diffusion of the components of the gas mixture; β , coefficient of mass transfer of the particle; U, velocity of the Stefan flow; r, radial coordinate; λ_g , thermal conductivity of the gas; c_g , specific heat of the gas; α , coefficient of heat transfer of the particle; Se, Nu, Gr, and Pr, Semenov, Nusselt, Grashof, and Prandtl numbers; Re_V, Re_G, and Re_{ef}, Reynolds numbers which determine forced, natural, and effective convection, respectively; D_0 , coefficient of diffusion for the pressure $P = P_0$ and the temperature of the gas $T_g = T_0$. Subscripts: g, gas; w, wall of the reaction unit; s, surface of the particle; ∞ , on the surface of the reduced film; b, initial value; C, carbon; ch, chemical; h, thermal; V, velocity; G (Gr), Grashof; ef, effective; sf, Stefan.

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