Journal of Engineering Physics and Thermophysics, Vol. 71, No. 6, 1998

INFLUENCE OF NATURAL AND FORCED CONVECTION ON THE CHARACTERISTICS OF HETEROGENEOUS COMBUSTION OF A CARBON PARTICLE

V. V. Kalinchak, S. G. Orlovskaya,
Yu. V. Prudnikova, and Ibrahim Ganui

UDC 536.46:662.612

The little-studied problem of the effect of natural and forced convection on the stationary (combustion) and critical (ignition and extinction) high-temperature states of a carbon particle with account for radiative heat exchange with the cold walls of the processing setup is considered. The effect of molecular and convective heat and mass exchange of a carbon particle with a gas on the critical diameter of the particle d_e at which the particle is spontaneously extinguished (a jumpwise transition from combustion to oxidation) is analyzed.

Chemical conversions of carbon particles in torch or circulating fluidized bed furnaces occur with intense heat and mass exchange (HME) with a gas phase. The role of convective heat and mass exchange in the processes of heterogeneous ignition, combustion, and extinction of carbon particles has virtually not been revealed in the specialized and educational literature. The rate of convective HME can increase and decrease with change in the diameter and relative velocity of the particle. In [1] the existence of upper and lower limits of the size of motionless carbon particles that bound regions of stationary heterogeneous combustion of them is shown. It is found that the upper limits are related to the heat exchange of the particle with the cold walls of the processing setup.

In what follows, the effect of the relative velocity on the stationary and critical modes of heat and mass exchange of a moving particle is studied. With account for the parallel heterogenous chemical reactions $C + O_2 \rightarrow CO_2$ (I) and $2C + O_2 \rightarrow 2CO$ (II) for Bi << 1 the equation of heat balance of a particle has the form

$$\frac{1}{6} c_1 \rho_1 d \frac{dT_1}{dt} = q_{\text{ch}} - q_{\text{m.c}} - q_{\text{r}} , \quad T_1 (t = 0) = T_{\text{beg}} , \tag{1}$$

where

$$q_{\text{ch}} = \left(\sum_{i=1}^{2} k_i Q_i \right) \rho_2 n_{\text{ox}} \left(\frac{\sum_{i=1}^{2} k_i}{\beta} + 1 \right)^{-1} ; \quad k_i = k_{0i} \exp \left(- E_i/(RT_1) \right) ;$$

$$\beta = D \, \text{Nu}/d ; \quad D = \lambda_2/(c_2 \rho_2) ;$$

$$\text{Nu} = 2 + b \sqrt{\text{Re}} \, \text{Pr}^{1/3} , \quad b = 0.55 \ [2] , \quad \text{Re} = Ud/\nu_2 , \quad \nu_2 = \text{Pr} \, D ;$$

$$q_{\text{m.c}} = \alpha (T_1 - T_2) ; \quad \alpha = \frac{\lambda_2 \, \text{Nu}}{d} ; \quad q_{\text{r}} = \varepsilon \sigma (T_1^4 - T_{\text{w}}^4) .$$

The particle diameter d (the particle is taken to be spherical) decreases with time as a result of chemical conversions whose rate depends on the mass transfer of the oxidant to the particle surface:

I. I. Mechnikov Odessa State University. Translated from Inzhenerno-Fizicheskii Zhurnal, Vol. 71, No. 6, pp. 1050-1055, November-December, 1998. Original article submitted January 10, 1997; revision submitted August 20, 1997.

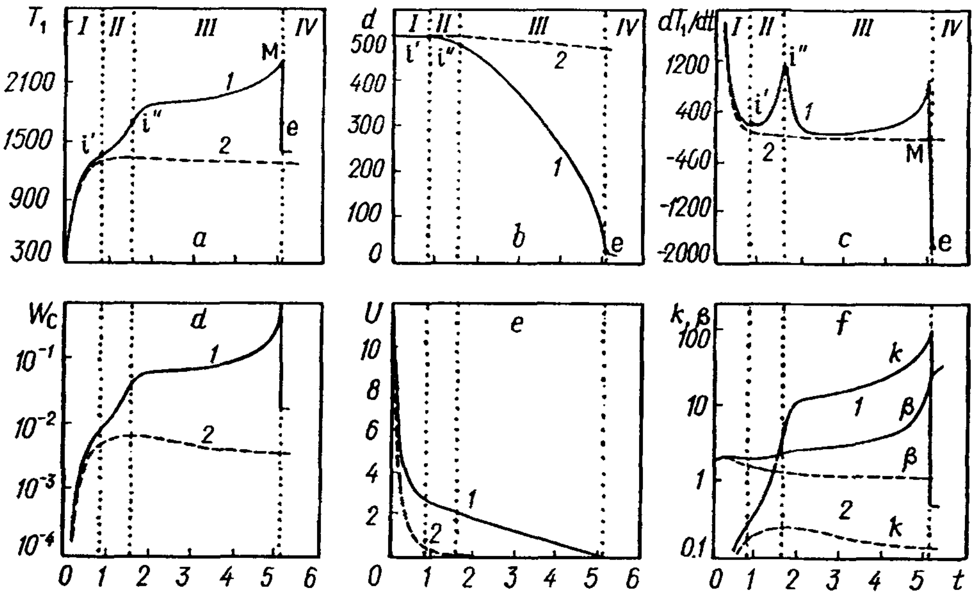

Fig. 1. Time dependences of T_1, d, dT_1/dt, W_C, U, k, and β for a particle with $d_{beg} = 505\ \mu m$, $U_{beg} = 11$ m/sec, $T_2 = 1400$ K, $T_w = 500$ K: 1) $F_g \neq 0$, 2) 0. T_1, K; d, μm; dT_1/dt, K/sec; W_C, kg/(m^2·sec); U, k, β, m/sec; t, sec.

$$\frac{d(d)}{dt} = -\frac{2\rho_2}{\rho_1}\left(\sum_{i=1}^{2} k_i \Omega_i\right) n_{ox} \left(\frac{\sum\limits_{i=1}^{2} k_i}{\beta} + 1\right)^{-1}, \quad d(t=0) = d_{beg}. \qquad (2)$$

The relative velocity of the particle U is found from the equation of motion

$$\frac{1}{6}\pi d^3 \rho_1 \frac{dU}{dt} = F_g - F_{fl} - F_{fr}$$

or

$$\rho_1 \frac{dU}{dt} = (\rho_1 - \rho_2) g - \frac{3}{4d}\psi \rho_2 U^2, \quad U(t=0) = U_{beg}, \qquad (3)$$

where F_g, F_{fl}, F_{fr} are the force of gravity, the Archimedes force, and the force of friction, respectively; U_{beg} is the initial velocity of the particle; the coefficient of head resistance of the particle ψ depends on the Reynolds number, and within the range $1 < \mathrm{Re} < 400$ it is found by the Klyachko formula [3]

$$\psi = \frac{24}{\mathrm{Re}} + \frac{4}{\sqrt[3]{\mathrm{Re}}}. \qquad (4)$$

Numerical solution of Eqs. (1)-(3) with account for (4) and their analysis allow one to find the laws governing the occurrence of stationary high- and low-temperature states as a function of the velocity of motion and the diameter of the particle. The calculations were conducted for the following parameters: $E_1 = 140.03$ kJ/mole; $E_2 = 154$ kJ/mole; $k_{01} = 45{,}000$ m/sec; $k_{02} = 130{,}000$ m/sec; $Q_1 = 10{,}125$ kJ/(kg O_2); $Q_2 = 6843.75$ kJ/(kg O_2); $n_{ox} = 0.23$; $\varepsilon = 0.78$ [3]. The study of the stability of the stationary modes of HME ($dT_1/dt = 0$) makes it possible to determine the critical values of the velocity of motion of a particle and its diameter (and, correspondingly, α_{cr} and β_{cr}), which characterize transitions from stationary low-temperature to high-temperature states and conversely.

Figure 1 presents time dependences of the temperature (a), particle diameter (b), derivative dT_1/dt (c), rate of chemical conversion of a particle with respect to carbon $W_C = -(1/2)\rho_1 d(d)/dt$ (d), relative velocity of particle motion (e), and rate constants of the chemical reactions and the coefficient of mass transfer (f) for two

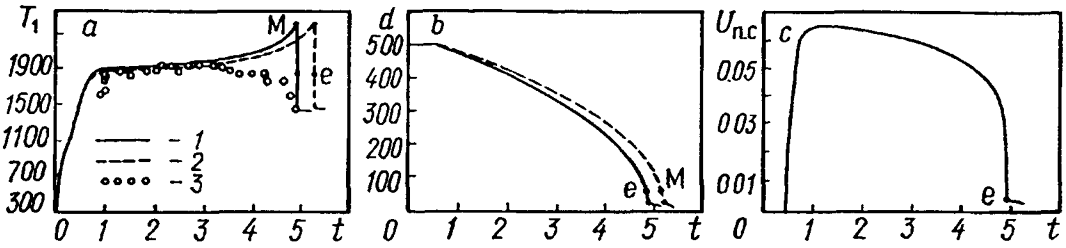

Fig. 2. Dependences $T_1(t)$, $d(t)$, $U_{n.c}(t)$ with (1) and without (2) account for natural convection for d_{beg} = 505 μm, T_2 = 1400 K, T_w = 500 K; 3) experimental data [4]. $U_{n.c}$, m/sec.

cases: 1) the gravity force F_g and the force of friction F_{fr} affect the particle; 2) only the friction force affects the particle. In the first case ($F_g \neq 0$), in some time that is characteristic for isothermal motion the velocity of the particle should become stationary, and in the second case, ($F_g = 0$) it should become close to zero. Heat losses by radiation with weak heating by heat conduction do not allow the particle to ignite when $F_g = 0$ (dashed lines in Fig. 1). The velocity of the particle tends to zero with time.

When $F_g \neq 0$, the particle ignites (stages I and II), burns (stage III), and is extinguished and oxidized (stage IV) (Fig. 1, solid lines; in the figure characteristic stages are separated by vertical dashed lines). The onset of self-acceleration of a chemical reaction is determined by point i′ ($dT_1/dt > 0$, $d^2T_1/dt^2 = 0$, $d^3T_1/dt^3 > 0$), which is characterized by the course of the chemical reaction in the kinetic region ($k = k_1 + k_2 << \beta$) (Fig. 1f). Then the rate of chemical conversion of the particle increases (Fig. 1d), and dT_1/dt increases and attains a maximum at point i″ (Fig. 1c) as a result of process retardation due to mass transfer of the oxidant ($dT_1/dt > 0$, $d^2T_1/dt^2 = 0$, $d^3T_1/dt^3 < 0$). At this point the resultant constant $k \approx \beta$. The duration of first two stages (up to point i″) is called the period of induction t_{ind}.

At the third stage (III) with a duration t_{bur} a high-temperature quasistationary mode ($dT_1/dt \approx 0$) – particle burning – occurs, during which T_1 attains a maximum value $T_{1.M}$ (point M, Fig. 1a, c). Here the particle diameter decreases at a high rate (Fig. 1b), and at point e at the instant of time t_e, when the diameter has a critical value d_e, a jumpwise transition to a low-temperature mode occurs. At point e the conditions $dT_1/dt < 0$, $d^2T_1/dt^2 = 0$, $d^3T_1/dt^3 > 0$ are valid for the particle temperature.

The fourth stage (IV) is characterized by the transition of HME processes and chemical reactions to the low-temperature mode and by a slow decrease in the diameter of the particle.

The velocity of the particle as a function of time for $F_g \neq 0$ has a nontrivial character (Fig. 1e). Soon after the moment of particle injection into the air flow the velocity of the particle is established, and it changes weakly with time (stage II). This is the so-called velocity of particle floating. In this portion the particle diameter is practically constant (Fig. 1b). Then, the increase in the temperature of the particle and the decrease in its diameter due to chemical conversions lead to sharp growth of F_{fr}, thus causing a fall of U to zero.

Figure 2 illustrates the effect of natural convection on $T_1(t)$ and $d(t)$ of a motionless particle. The relative gas velocity was determined in terms of the Grashof number Gr in the form

$$U_{n.c} = \frac{\nu_2}{d}\sqrt{0.5\,\mathrm{Gr}}, \quad \mathrm{Gr} = \frac{gd^3(T_1 - T_2)}{273\nu_2^2}.$$

Account for natural convection gives the most satisfactory agreement between calculated and experimental data of [4] on the total time of burning. The deviation with respect to T_1 in the region of the maximum temperature (Fig. 2a, point M) is likely due to heat removal through the suspension to which the particle was fixed. The effective velocity of air motion due to natural convection facilitates enhancement of mass transfer, thus leading to an increase in the rate of combustion and, consequently, to a decrease in the time of particle burning. Both the critical diameter determining extinction of the particle and natural convection do not affect the period of induction, since the chemical reactions take place in the kinetic region (see Table 1). The effect of natural convection is strongest at large initial diameters of the particle.

TABLE 1. Influence of Natural Convection on the Characteristics of Burning of Carbon Particles at $T_2 = T_w = 1400$ K

d_{beg}, μm	With (+), without (−) account for natural convection	t_{ind}, sec	t_{bur}, sec	t_e, sec	d_e, μm	$T_{l.M}$, K
100	−	0.069	0.17	0.239	21.3	2361
	+	0.067	0.16	0.236	21.5	2361
505	−	0.54	4.74	5.27	21.3	2361
	+	0.53	4.40	4.95	21.5	2361
800	−	0.99	12.23	12.43	21.4	2361
	+	0.83	11.58	11.68	21.3	2361

We find the dependence of the coefficients of heat and mass transfer, determining the stable and critical states of the particle, on the particle temperature from the stationarity condition $q_{ch} = q_{m.c} + q_r$. We obtain the quadratic equation

$$\bar{\beta}^2 - 2A\bar{\beta} + B = 0\,,$$

where $\bar{\beta}$ is the dimensionless coefficient of HME;

$$\bar{\beta} = \frac{\alpha (T_1 - T_2)}{\left(\sum_{i=1}^{2} k_i Q_i\right) \rho_2 n_{ox}} = \frac{\beta c_2 \rho_2 (T_1 - T_2)}{\left(\sum_{i=1}^{2} k_i Q_i\right) \rho_2 n_{ox}}\,; \tag{5}$$

$$A = 0.5\,(1 - A_1 - A_2)\,; \quad B = A_1 A_2\,;$$

$$A_1 = \frac{c_2 (T_1 - T_2) \sum_{i=1}^{2} k_i}{\left(\sum_{i=1}^{2} k_i Q_i\right) n_{ox}}\,; \quad A_2 = \frac{\varepsilon\sigma (T_1^4 - T_w^4)}{\left(\sum_{i=1}^{2} k_i Q_i\right) \rho_2 n_{ox}}\,.$$

The solution of the quadratic equation for β, α, and the complex $f = 2d/\mathrm{Nu}$ is presented in the form

$$\beta = \frac{\left(\sum_{i=1}^{2} k_i Q_i\right) \rho_2 n_{ox} (A \pm \sqrt{A^2 - B})}{c_2 \rho_2 (T_1 - T_2)}\,, \quad \alpha = \beta c_2 \rho_2\,,$$

$$f = \frac{2d}{\mathrm{Nu}} = \frac{2\lambda_2 (T_1 - T_2)}{\left(\sum_{i=1}^{2} k_i Q_i\right) \rho_2 n_{ox} (A \pm \sqrt{A^2 - B})}\,. \tag{6}$$

As follows from (6), for T_1 approaching T_2 the complex $f \to 0$; for T_1 approaching T_w, $f \to \infty$. In these two cases the power of the chemical heat release becomes negligibly small compared to $q_{m.c}$ in the first case and to q_r in the second case.

The complex $f = 2d/\mathrm{Nu}$ allows one to take into account the change in both the diameter of the particle and the velocity of its motion. Therefore, the results of the studies of $d(T_1)$ and $U(T_1)$ can be presented in the form of one generalized relation $f(T_1)$. This is illustrated in Fig. 3, where results of calculations by nonstationary and stationary models are presented. The solid line and the points (Fig. 3a) show the path of the complex f obtained numerically by the nonstationary model with and without account for natural convection. Natural convection increases the Nusselt number Nu, thus leading to some decrease in the complex f. Then, in particle burning, the

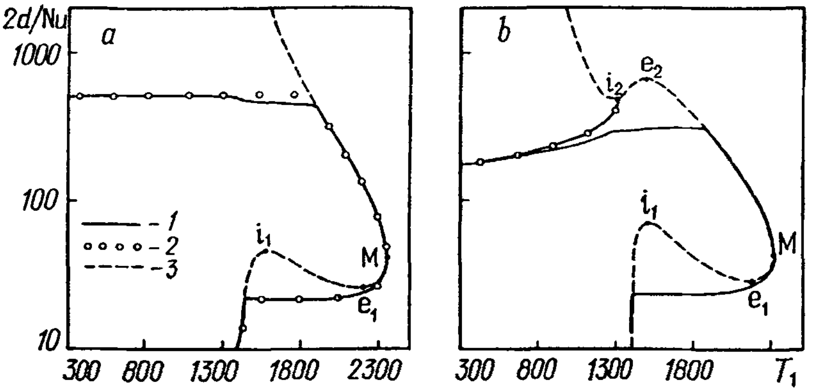

Fig. 3. Dependences of $2d/\mathrm{Nu}$ on the stationary temperature of a particle with $T_2 = 1400$ K: a) $T_w = 1400$ K; (with (1) and without (2) account for natural convection); b) $T_w = 500$ K [1) $F_g \neq 0$, 2) 0]; 1 and 2) calculation by the nonstationary model, $d_{\mathrm{beg}} = 505$ μm; 3) calculation by the stationary model. $2d/\mathrm{Nu}$, μm.

nonstationary and stationary dependences $f(T_1)$ coincide up to point e_1, and at this point a jumpwise transition to a low-temperature state occurs.

The extrem on the curves $f(T_1)$ determine the unstable stationary states of the particle: points i_1 and i_2 correspond to ignition, points e_1 and e_2 to extinction of the particle. The branches connecting points i_1 and e_1, i_2 and e_2 describe the effect of the initial temperature of the particle on its critical diameter characterizing ignition [1] (Fig. 3b).

Figure 3b presents results of calculations by the nonstationary model for two cases: 1) $F_g = 0$, 2) $F_g \neq 0$ at $d_{\mathrm{beg}} = 505$ μm and $U_{\mathrm{beg}} = 11$ m/sec. It is seen that at $F_g = 0$ there is no transition to a high-temperature mode of the particle with the assigned initial diameter due to a sharp decrease in the relative velocity of particle motion and a tendency to zero and, consequently, a decrease in the rate of heat exchange with the gas that heats the particle.

In the case $F_g \neq 0$ the particle is ignited as a result of its heating by convective heat exchange with the hot gas.

We note that a stationary velocity of motion, called the floating velocity, is peculiar to each diameter of the particle under the action of the combination of forces (F_g, F_{fl}, F_{fr}) on it. With the diameter of the particle and its floating velocity being known we can determine the feasibility of its ignition and the critical parameters characterizing spontaneous extinction of the particle, other conditions being assigned.

Thus, studies were conducted that made it possible to reveal the role of natural and forced convective heat and mass transfer and the kinetics of heterogeneous chemical conversions in the processes of realization of high-temperature stable quasistationary states of a moving carbon particle in air at atmospheric pressure.

It is found that the effect of the diameter and the velocity of motion on the characterictics of heterogeneous burning of the particle is allowed for by the ratio of its diameter to the Nusselt number (d/Nu).

It is shown that the motion and heterogeneous burning of a carbon particle are interrelated. It is found that neglect of convective HME can lead to the qualitatively incorrect conclusion of the impossibility of particle burning in the case where the temperature of the gas is much higher than that of the walls of the processing setup.

The authors are grateful to the International Foundation "Vidrodzhennya" within the framework of the Soros Program (ISSEP) for support (contract No. K6V100).

NOTATION

c_1, c_2, specific heat of the particle and the gas, respectively, J/(kg·K); D, coefficient of diffusion of oxygen in air, m^2/sec; d, d_{beg}, current and initial diameter of the particle, respectively, m; E_1, E_2, activation energy of the 1st and 2nd chemical reaction, respectively, J/mole; k_1, k_2, rate constants of the chemical reactions, m/sec;

k_{01}, k_{02}, preexponential factors, m/sec; n_{ox}, oxidant concentration in the medium; Bi, Biot number; Nu, Nusselt number; Pr, Prandtl number; Re, Reynolds number; Q_1, Q_2, energy releases of the chemical reactions, calculated per unit mass of oxygen, J/(kg O_2); q_{ch}, density of the chemical heat release, W/m^2; $q_{m.c}$, density of the heat flux by molecular convection, W/m^2; q_r, density of the heat flux by radiation, W/m^2; t, current time, sec; T_1, T_{beg}, $T_{1.M}$, current, initial, and maximum temperature of the particle, respectively, K; T_2, T_w, temperature of the gas and the walls of the processing setup, respectively, K; g, acceleration of gravity; α, α_{cr}, current and critical coefficients of heat transfer, W/(m^2·K); β, β_{cr}, current and critical coefficients of mass transfer, m/sec; ε, particle emissivity; λ_2, coefficient of thermal conductivity of the gas, W/(m·K); ν_2, coefficient of kinematic viscosity of the gas, m^2/sec; ρ_1, ρ_2, densities of the particle and the gas, kg/m^3; σ, Stefan–Boltzmann constant, W/(m^2·K^4); Ω_1, Ω_2, relative mass stoichiometric coefficients of the reactions. Subscripts: 1, particle; 2, gas (air); i = 1, reaction (I); i = 2, reaction (II); beg, initial; bur, burning; ch, chemical; cr, critical; fl, Archimedes force; fr, friction; g, force of gravity; ind, induction period; M, maximum (temperature); m.c, molecular-convective; n.c, natural convection; ox, oxidant; r, radiation; w, wall; points: e, extinction.

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