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Experimental studies and physical and mathematical modeling of the influence of the inhomogeneity of the temperature field along a carbon particle on the characteristics of its ignition, burning and extinction

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This work is devoted to experimental studies and physico-mathematical modeling of high-temperature heat and mass transfer and chemical transformation of carbon particles, accounting for internal thermal conductivity. The relevance of the study is driven by the need to improve the accuracy of predicting the ignition, combustion, and extinction characteristics of solid fuels in thermotechnical processes. Most theoretical approaches utilize an isothermal particle approximation, which can lead to errors in determining the induction period and burnout time, particularly for particles in the submillimeter and millimeter range.

A non-isothermal model is proposed, incorporating internal thermal conductivity within the particle, oxidation reactions, and heat exchange via convection and radiation. Numerical calculations were performed for a diameter range of 100–1000 μm, with an analysis of temperature fields and gradients during the ignition and extinction stages. It is shown that as the particle diameter increases, the temperature differential between the surface and the center grows, while the radial temperature gradient decreases due to the spatial expansion of the temperature field and the increase in transient thermal time. Experimental studies with millimeter-sized particles revealed significant temperature gradients at the ignition stage and identified the moment of ignition by the maximum value of the time derivative of the particle's surface temperature.

A comparison of calculations using isothermal and non-isothermal models demonstrated a systematic overestimation of ignition and burning time when internal thermal conductivity is neglected. It is shown that in the range of small particle sizes, failing to account for internal thermal conductivity leads to a predicted absence of ignition. The results obtained confirm the necessity of a non-isothermal description for the correct prediction of combustion characteristics for carbon particles larger than 200 μm.

Keywords: carbon particles, ignition, combustion, extinction, temperature gradient, internal thermal conductivity, induction period, burning time.

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Introduction

The processes of ignition and combustion of disperse carbon particles in a high-temperature gas medium play a key role in power engineering, pulverized coal combustion, solid fuel gasification, and a variety of high-temperature technological processes [1-4]. The characteristics of ignition, combustion, and extinction of these particles determine not only the efficiency of energy processes but also issues of technical safety, environmental performance, and operational reliability of equipment [5-7]. In the practice of coal utilization in the power industry, there is an increasing need for an accurate prediction of the temporal characteristics of ignition (induction period) and burnout for particles of various sizes and structures. This is due to the fact that the transition from the quasi-isothermal behavior of fine particles to a pronounced thermal gradient in large particles significantly affects the combustion process and can lead to erroneous estimates of key characteristics if such a gradient is ignored.

The ignition and combustion characteristics of coal particles strongly depend on the properties of the carbon matrix and the gas, the particle size, and the conditions of their interaction with the oxidizer. In particular, the analysis of high-temperature heat and mass transfer for single carbon particles and in gas suspensions has shown that the influence of the initial particle diameter and the ambient gas temperature on the induction period, combustion time, and critical parameters of ignition and extinction is decisive for describing the behavior of such systems [8-11]. Experimental studies of the ignition of coal particles and their mixtures with biomass [12] have established a significant effect of particle size on ignition delay and the stability of subsequent combustion, confirming the importance of accounting for real thermal regimes and the physical properties of both fuel and oxidizer.

In a large number of theoretical works, the description of the particle's thermal state is based on the isothermal approximation, within which the temperature of the solid phase is considered uniform throughout the volume. This approach substantially simplifies the mathematical model and, in several cases, yields satisfactory results for small particles or weak thermal effects. However, it fails to account for the finite rate of conductive heating of the solid phase and the possible formation of a temperature gradient inside the particle. This can be particularly relevant for millimeter-sized particles.

An analysis of thermophysical scales shows that the internal thermal state of a particle in a transient process is primarily determined by the characteristic time of thermal diffusion (temperature equalization), which increases quadratically with an increase in particle size. Even at small values of the Biot number (Bi), this can lead to a significant lag of the temperature in the central regions behind the surface temperature during induction heating, thereby resulting in internal non-isothermality.

In some theoretical works dedicated to the physical and mathematical modeling of high-temperature regimes in disperse carbon systems, the non-isothermality of the solid phase is taken into account [13-16], allowing for a more accurate interpretation of the results. It was established in [14] that the influence of non-isothermality on combustion characteristics increases with rising gas temperature. Experimental work [8] also draws attention to the role of internal non-isothermality for large particle sizes.

Despite the existence of individual studies focused on the non-isothermal heating of particles, a consistent physical explanation of the role of internal thermal conductivity at various stages of the process–from ignition to complete burnout–remains insufficiently formulated. The aim of this work is to establish the patterns of internal non-isothermality formation in carbon particles within a high-temperature gas medium and to determine its impact on the induction period of ignition, burnout duration, and extinction conditions, accounting for the transient thermal conductivity of the solid phase. To achieve this goal, it is necessary to: analyze the characteristic thermophysical time scales of the process; investigate the effect of particle size on the temperature differential between its surface and center; and establish the domains of applicability for isothermal and non-isothermal descriptions.

I. Experimental Studies

From the conducted literature review, it follows that many experimental studies are specifically devoted to determining the particle temperature during ignition and combustion. This is because temperature is a key element for determining the combustion reaction rate, as well as convective and radiative heat fluxes. Furthermore, temperature correlates with investigated parameters such as particle diameter, mass loss, and burnout time. Experimental studies in this work were conducted in this specific direction. The experiments were carried out using carbon particles with diameters of 4–8 mm, which were spherical in shape and mechanically fabricated from coal material. Experimental investigations of the ignition and combustion of these particles were performed on a setup, the block diagram of which is presented in Fig. 1.

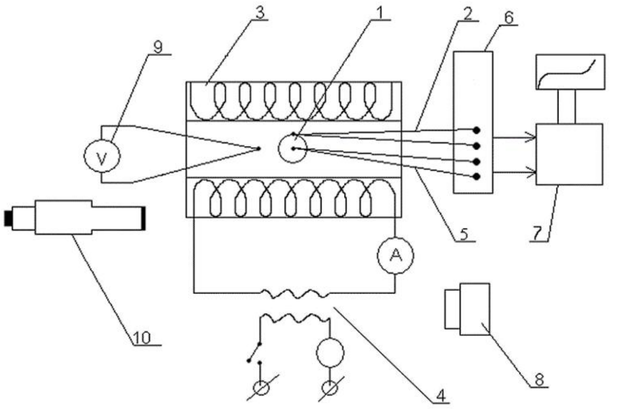


Fig. 1. Block diagram of the experimental setup:
1 – carbon particle; 2, 5, 9 – thermocouples; 3 – high-temperature furnace; 4 – autotransformer; 6 – analog-to-digital converter (ADC); 7 – personal computer;
8 – digital camera; 10 – brightness pyrometer.

The carbon particle (1) was introduced into a high-temperature furnace (3) using a thermocouple (5). The surface temperature of the particle was monitored by a chromel-alumel thermocouple (type K) (2), which was tightly pressed against the surface. The furnace was heated by applying voltage via an autotransformer (4). The temperature of the heated air inside the furnace was controlled by another chromel-alumel thermocouple (9). The temperature variations at the surface and the center of the particle were recorded by an analog-to-digital converter (6). The signals were then transmitted to a personal computer (7), where data processing was performed, including the calculation of the particle's temperature time derivatives (dT/dt). Additionally, the temperature of the carbon particles during the high-temperature oxidation process was measured using a brightness pyrometer (10). Simultaneously, video recording of the particle was conducted with a digital camera (8) to monitor the oxidation process and determine the particle diameter in real-time.

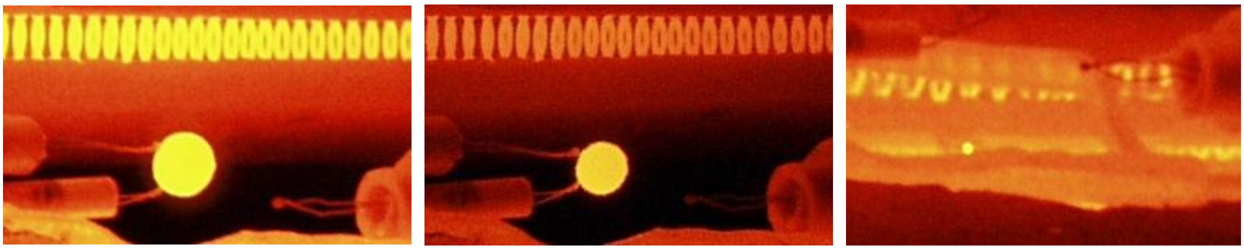
Fig. 2 shows images of the high-temperature oxidation of a carbon particle with a diameter of $d_b = 5.1$ mm in a furnace at a temperature of 1140 K. Due to the reduction in particle size during burnout, the particle eventually falls onto a quartz substrate. On this substrate, at the same gas temperature, further oxidation continued and was recorded in real-time by a digital camera until the moment of extinction.

The results of the experimental data processing are presented in Fig. 3 as time-dependent profiles of the temperatures at the particle center and surface, the time derivatives of temperature (dT/dt), and the particle diameter. Figs. 3a and 3c specifically highlight the initial stages of heating and ignition.

Based on the obtained time dependencies of the surface and center temperatures, as well as their rates of change, the following stages of high-temperature particle oxidation are clearly distinguishable:

1. Inert heating: The section of the curves up to point I', where the derivative dT/dt is at its minimum.
2. Chemical heating stage: The interval I'–I, during which the particle heats up due to the heat released by self-accelerating exothermic chemical reactions. At the end of this stage, the particle ignites (point I), and the derivative dT/dt reaches its maximum.
3. Quasi-steady high-temperature oxidation stage: The section of the curves following point I.

It is observed that during the inert heating stage, the surface temperature of the particle exceeds the temperature at its center. The behavior of the dT/dt curves is similar for both, with the center lagging by approximately 10 seconds. Twenty seconds after ignition, the surface and center temperatures equalize. Subsequently, throughout the entire high-temperature



t = 23 s   t = 144 s   t = 780 s

Fig. 2. Images of a particle undergoing oxidation in a heated furnace on a thermocouple and subsequently on a substrate at a temperature of 1140 K.

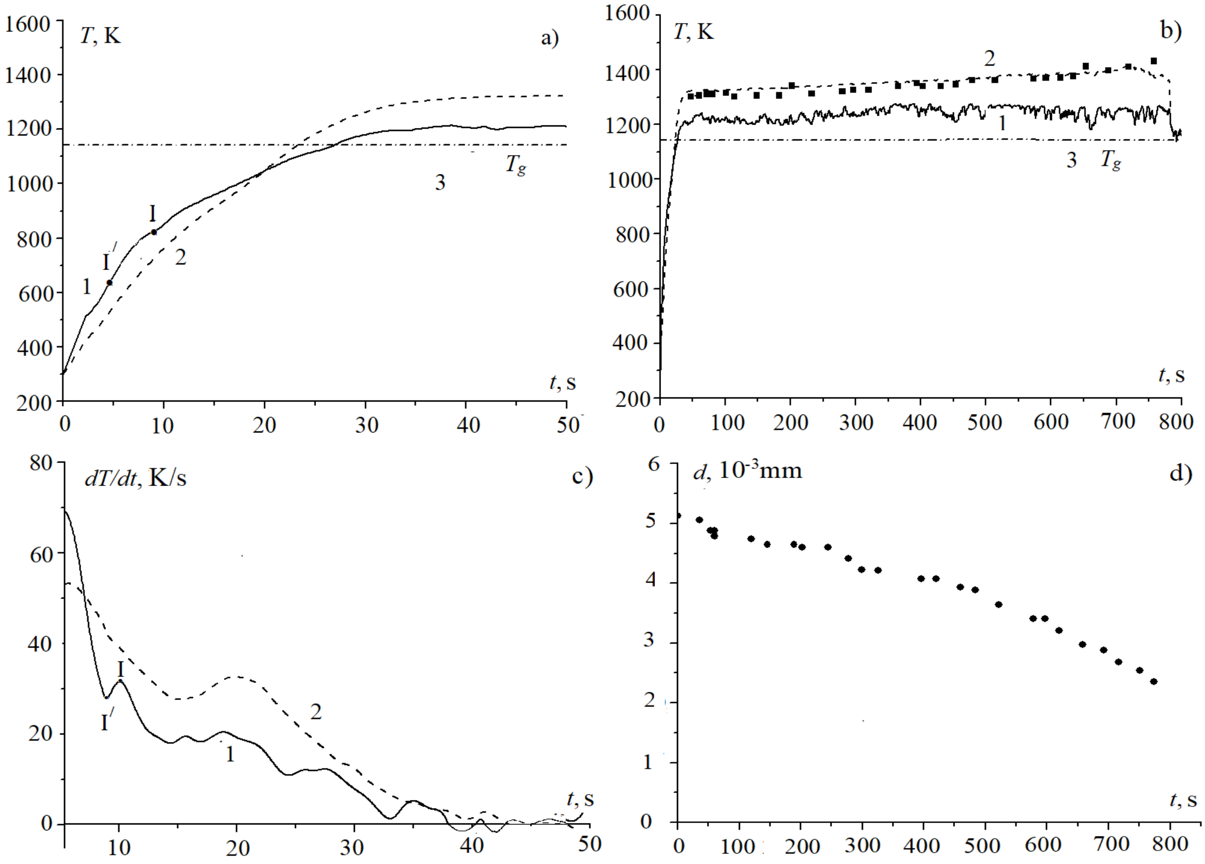


Fig. 3. Experimental time dependencies**:** a) and c) temperatures and their derivatives during the ignition stage: (1) – measurements at the particle surface, (2) – measurements at its center; b) and d) during the entire experiment: b) (1) – surface temperature Ts, (2) – center temperature Tc, (3) – furnace air temperature Tg, ■ – temperature measured by the brightness pyrometer; d) instantaneous particle diameter. $d_b = 5.1$ mm, Tg = 1140 K.

oxidation stage, the thermocouple at the center of the particle records a higher temperature than the thermocouple on the surface.

One of the reasons for the underestimation of the temperature is the higher heat losses via convection and radiation from the surface of the external thermocouple. Furthermore, shortly after ignition, the contact between the thermocouple and the particle is disrupted due to the reduction in particle diameter during burnout. The moment of loss of tight contact between the external thermocouple and the particle was monitored using high-speed film of the oxidation process. Therefore, the surface temperature values can be considered reliable only during the heating and ignition periods, as well as at the initial stage of the high-temperature regime. Subsequently, this thermocouple recorded the gas temperature near the particle surface. Fluctuations in the time dependencies of the surface temperature and its derivative (dT/dt) during the high-temperature stage (Fig. 3b, c) arise as a result of convective heat fluxes from the particle. The particle temperature measured by the brightness pyrometer during the oxidation process is in good agreement with the temperature measured by the internal thermocouple.

After the transition to the high-temperature state, the particle diameter begins to decrease intensively (Fig. 3d), but its measurements are interrupted at a value of 2.5 mm due to the particle falling from the thermocouple onto the quartz substrate. Processing the time dependence of the instantaneous particle diameter in $d^2 = f(t)$ coordinates indicated a diffusion-controlled combustion regime for all studied diameters of the carbon fuel.

Thus, based on the research objectives and experimental results, the following can be concluded: 1) the transition to high-temperature oxidation of the particle (burning) occurs when the time derivative of its temperature reaches its maximum value. This reflects the maximum excess of heat release from chemical oxidation reactions over heat losses via convective, molecular, and radiative transfer; 2) upon ignition, the surface temperature of the particle leads the temperature at its center; therefore, the induction period calculated relative to the surface and the center of the particle has different values; 3) the high-temperature oxidation of carbon particles occurs in a diffusion-controlled regime.

II. Physical and mathematical modeling

We shall conduct physical and mathematical modeling of the high-temperature heat and mass transfer and chemical transformation of carbon fuel particles, accounting for the temperature gradient throughout the carbon matrix. Let us consider the problem of transient thermal conductivity for a spherical carbon particle placed in a gaseous oxidizing medium, the temperature of which (T_g) is significantly higher than the initial temperature of the particle (T_b). For a single particle, it can be assumed that the temperature of the gas medium (air) remains constant during the heating and oxidation process. The particle begins to heat up due to the molecular-convective heat exchange at its surface:

$$q_\alpha = \alpha(T - T_g), \qquad \alpha = \frac{\lambda_g Nu}{d}, \tag{1}$$

where q_α is the molecular-convective heat flux density; λ_g is the thermal conductivity coefficient of the gas; α is the heat transfer coefficient; Nu is the Nusselt number; T_W is the temperature of the chamber walls; T_g is the gas temperature.

As the surface temperature increases, chemical oxidation reactions begin to occur. The primary chemical reactions taking place on the surface of a carbon particle in dry air are those that form carbon dioxide and carbon monoxide [17]:

$$C + O_2 = CO_2 + Q_1 \tag{I}$$

$$2C + O_2 = 2CO + Q_2 \tag{II}$$

where Q_1, Q_2 are the thermal effects (enthalpies) of the reactions. These reactions are exothermic. The total chemical heat release can be calculated using the law of mass action and the Arrhenius law:

$$q_{ch} = \sum_{i=1}^{2} Q_i W_{chi} \,,$$

$$W_{chi} = C_{O_2 s} \cdot k_i, \;\; k_i = k_{0i} exp(-E/RT). \tag{2}$$

In these equations: q_{ch} is the heat release density due to chemical reactions; W_{chi} is the rate of the chemical reaction: ρ_g is the gas density; $C_{O_2 s}$ is the oxygen concentration at the particle surface; k_i is the reaction rate constant; k_{0i}, E_i are the pre-exponential factor and the activation energy of the reaction, respectively.

The oxygen concentration at the particle surface is determined by both the kinetics of chemical reactions and the diffusion of oxygen to the surface:

$$C_{O2s} = C_{O2\infty} \left(\frac{\sum_{i=1}^{2} k_i}{\beta} + 1 \right)^{-1}, \tag{3}$$

where $\beta = DSh/d$ is the mass transfer coefficient, D is the diffusion coefficient, Sh is the Sherwood number, $n_{O2\infty}$ is the relative concentration of oxygen in the air.

The radiative heat exchange between the particle surface and the walls of the experimental setup is governed by the Stefan-Boltzmann law:

$$q_w = \varepsilon\sigma(T^4 - T_w^4), \tag{4}$$

where q_w is the radiative heat flux density, T_w is the temperature of the chamber walls, ε is the emissivity of the fuel, $\sigma$is the Stefan-Boltzmann constant.

The differential heat conduction equation for a spherical particle without internal heat sources is written as:

$$\rho C \frac{\partial T}{\partial t} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(\lambda r^2 \frac{\partial T}{\partial r}\right) \,, \tag{5}$$

where: λ, ρ and C - are the thermal conductivity, density, and specific heat capacity of the fuel particle, respectively; the radial coordinate r varies within $0 \le r \le r_s, r_s = d/2$, where r_s and d are the radius and diameter of the particle.

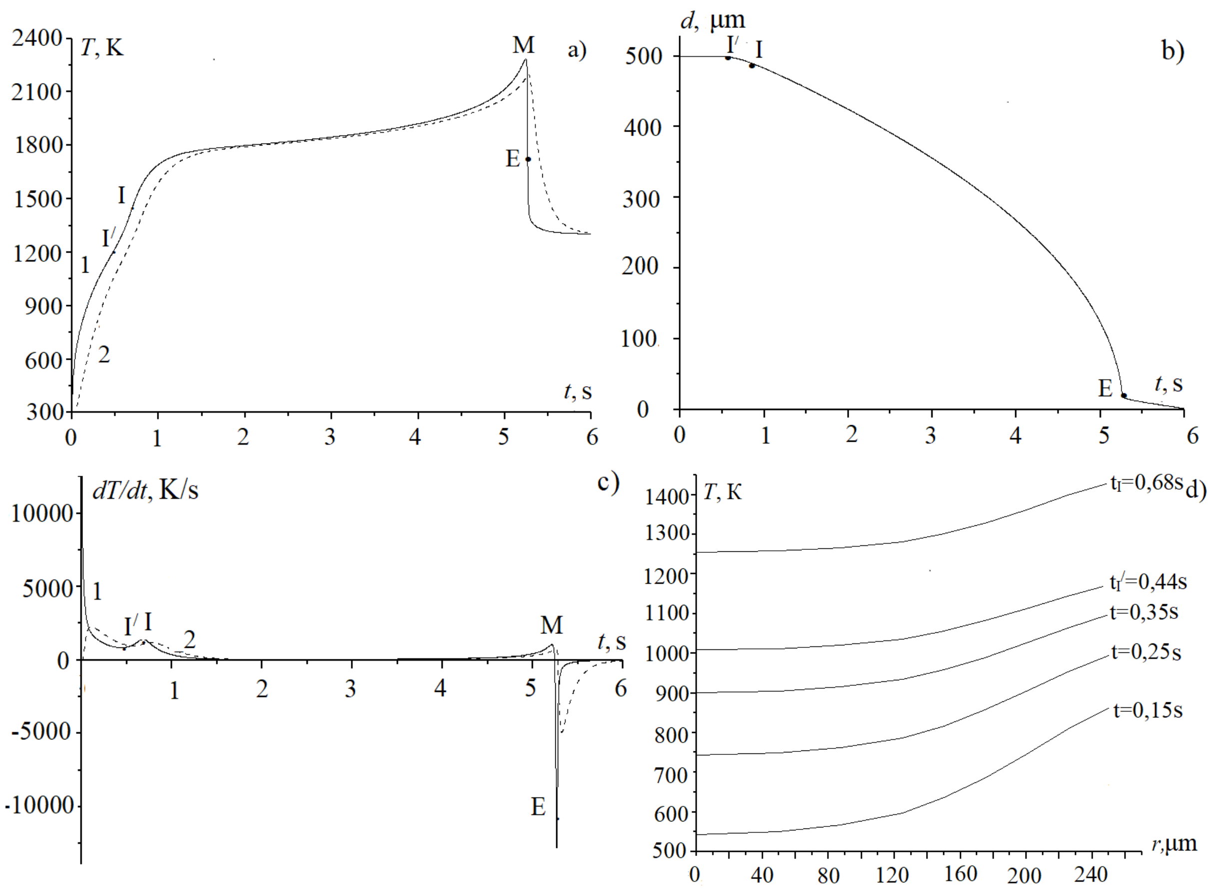


Fig. 4. Time dependencies of: a) temperature at the particle surface (1) and at the center (2); b) particle diameter; c) derivative dT/dt at the surface (1) and at the center (2) of the particle; d) temperature difference along the particle radius. d_b=500 μm (r_s=250 μm), T_g=1300 K, T_g=T_w.

The initial and boundary conditions for this problem are as follows.

Initial conditions:

$$t = 0 \quad \text{and} \quad 0 \le r \le r_s, \quad T = T_b \ . \qquad (6)$$

Boundary conditions at the center of the particle (r = 0):

$$\left|\frac{\partial T}{\partial r}\right|_{r=0} = 0. \qquad (7)$$

Boundary conditions at the surface of the particle (r = r_s):

$$\left|\frac{\partial T}{\partial r}\right|_{r=rs} = q_{ch} - q_{\alpha} - q_{w} \ . \qquad (8)$$

As a result of high-temperature oxidation, the diameter of the carbon particle decreases according to the mass balance equation:

$$-\frac{1}{2}\rho\frac{\partial d}{\partial t} = \frac{M_C}{M_{O_2}}(k_1 + 2k_2)C_{O_{2s}}, \quad d(t = 0) = d_b, \qquad (9)$$

where M_C, M_{O_2} are molar masses of carbon and oxygen.

In the absence of a temperature gradient across the particle, provided $\lambda_g << \lambda$ (hence Bi<1), the heat balance equation for the particle can be written as:

$$\frac{1}{6}c\rho d\frac{\partial T}{\partial t} = q_{ch} - q_{\alpha} - q_{w}, \ T(t = 0) = T_b, \qquad (10)$$

The equation (1)–(9) was solved numerically using the finite difference method. During the computer simulation, an analysis was conducted to determine the influence of the radial temperature gradient on the characteristics of particle ignition, combustion, and extinction in heated air. To identify the particle sizes for which accounting for the temperature gradient is necessary, simulations were performed over a wide range of diameters: 100–1000 μm.

Figure 4 presents the calculation results for a carbon particle with a diameter of d_b = 500 μm, oxidizing in air heated to a temperature of T_g = 1300 K. A clear analogy is observed between the calculated and experimental time dependencies of the surface and center temperatures, as well as their respective derivatives dT/dt. The extrema of the surface temperature derivative dT/dt mark the moments of ignition (point I) and extinction (point E). The induction period (t_{ind}) consists of two successive stages: inert heating (up to point I') and chemical heating (up to point I). In the first stage, the particle temperature increases due to molecular-convective heat exchange with the gas; in the second stage, it increases due to the heat from exothermic oxidation reactions. During the ignition stage, large temperature gradients are observed both at the beginning of heating and at the moment of ignition (Fig. 4d), which affects the accuracy of determining the induction period.

The burning time was defined as the duration of high-temperature oxidation from the moment of ignition to the moment of extinction: $t_{bur} = t_E - t_{ind}$. At the end of the high-temperature stage, a sharp increase in the particle temperature occurs. An analysis of the heat fluxes showed that this is related to the decrease in radiative heat loss from the particle as its diameter–and consequently its emitting surface area-decreases. However, molecular-convective heat losses increase simultaneously (according to equation (1)). The surface temperature reaches its maximum value (point M) and then begins to decrease.

Calculations showed that during the high-temperature oxidation stage, the temperatures of the surface and the center are practically identical (Fig. 4a), meaning that the temperature gradients along the particle radius are negligible. Oxidation at this stage occurs in the diffusion-controlled regime and is therefore limited by the rate of oxygen diffusion to the particle surface. The intensive change in diameter at this stage follows the $d^2= K_{bur}$=const, which is consistent with the experimental data. When the particle diameter and temperature reach critical values (point E), a spontaneous transition from the high-temperature heat exchange regime to the low-temperature one occurs. A kink appears on the d (t) curve at point E, characterizing the transition to the regime of slow chemical reactions. While the center temperature lags behind the surface temperature during ignition, the opposite occurs during extinction: the surface temperature is significantly lower than the temperature at the center (Fig. 4).

To analyze the calculation results, we introduce the concept of the average radial temperature gradient, which is defined as the ratio of the temperature difference between the surface and the center of the particle to its radius: $\langle dT/dr\rangle=(T_s-T_c)/r_s$. Such an estimate is meaningful if the heating or cooling regime is transient (which is the case in our study). The transient nature of the process is caused by the exothermic chemical reactions occurring on the surface of the carbon particle.

Table 1 presents the calculated temperature differences and radial temperature gradients during the ignition and extinction of carbon particles of various diameters.

The internal temperature drop between the surface and the center of the particle, $\Delta T=Ts - Tc$, directly reflects the balance between the heat release of the surface reaction and the heat transfer within the solid phase. This makes it an informative parameter for analyzing the critical regimes of ignition and extinction.

From the presented data, it can be seen that during ignition, as the diameter increases, the temperature difference between the surface and the center also increases, whereas the average radial temperature gradient decreases. The increase in ΔT is caused by the growth of the characteristic linear dimension of the system (the particle radius). Specifically, the characteristic heat transfer length increases, leading to an increase in internal thermal resistance and, consequently, the formation of a larger temperature drop.

Let us estimate the time required for temperature equalization along the particle radius. The characteristic time scale of internal thermal equalization is determined by heat transfer from the surface and follows from the solution of the transient heat conduction equation. For a spherical particle, it scales as $\tau\sim r_s^2/a$, where a is the thermal diffusivity of the material (carbon particle) [18]. The calculation results are shown in Table 2. As the particle radius increases, the temperature equalization time grows as r_s^2; therefore, the internal region remains cold for a longer period, and the temperature difference between the surface and the center increases (Table 1).

As shown in Table 1, although the temperature difference increases with diameter, the average radial gradient $\Delta T/r_s$ decreases. Let us evaluate the growth rate of ΔT as r_s increases, based on the data in Table 1.

Let $\Delta T \propto r_s^{\ n}$, then $\left(\frac{\Delta T}{r_s}\right) \propto r_s^{n-1}$. If n < 1 – the gradient decreases, n = 1 - constant, n > 1 - increases. The estimate of n, using the data in Table 1, gives the value n = 0.33. Then for the average radial gradient we have: $\frac{\Delta T}{r_s} \propto r_s^{-0.67}$, i.e. the average radial gradient decreases with increasing particle radius even despite the increase in the temperature difference itself as $\Delta T \propto r_s^{0.33}$.

The experimentally determined exponent n = 0.33 reflects the chemical reaction regime at the moment of ignition. In a purely kinetic regime, the reaction rate is determined solely by the temperature dependence according to Arrhenius' law, while the oxygen concentration at the surface remains constant and equals $C_{O2,s}\approx C_{O2\infty}$. In this case, the chemical heat release density (2) is independent of the particle size and is determined only by the surface temperature:

Table 1.

Temperature difference between the surface and the center ΔT, and average radial gradients during ignition (point I) and extinction (point E) of carbon particles. (where $\Delta T=Ts - Tc$, subscripts s and c denote surface and center, respectively). d_E = 18 μm is the critical diameter at which the particle undergoes extinction at the given temperature T_g=1300 K.

$d_b=2r_s$, μm		200	500	800	1000
Ignition	ΔT, K	145.1	174.8	213.4	245.7
	$\Delta T/r_s$, K/m	$1.45*10^6$	$6.9*10^5$	$5.3*10^5$	$4.9*10^5$
Extinction	ΔT, K	-426.7	-413.3	-415.5	-502.2
	$\Delta T/r_E$, K/m	$-4.74*10^7$	$-4.59*10^7$	$-4.62*10^7$	$-5.58*10^7$

Table 2.

Characteristic thermal equalization time τ due to thermal conductivity. $r_s= d_b/2$.

r_s, μm	50	100	250	400	500
$\tau\sim r_s^2/a$, s	0.003	0.01	0.07	0.18	0.28

$q_{ch} = (\sum_{i=1}^{2} k_i Q_i) C_{O2\infty}$. Due to thermal conductivity, this heat propagates into the depth of the carbon mass. In this case, the dependence of the temperature difference ΔT on the radius is linear, i.e., n = 1.

$$\Delta T = T_s - T_c = q_{ch} r_s / \lambda. \qquad (11)$$

In the diffusion-controlled regime of the reaction, the reaction rate is limited by the rate of oxidant supply to the particle surface. It then follows from (2) and (3) that

$$q_{ch} = \frac{\sum_{i=1}^{2} k_i Q_i}{\sum_{i=1}^{2} k_i} C_{O2\infty}\, \beta \ . \qquad (12)$$

Since the mass transfer coefficient is inversely proportional to the radius, then $q_{ch} \propto \frac{1}{r_s}$.

Taking this into account in the temperature difference (11), we have: $\Delta T \propto (1/rs)\ rs = 1$ or $\Delta T \propto rs^0$, then n = 0 – for a purely diffusion region.

Thus, based on the experimental ignition data, we found that $0 < n \approx 0.33 < 1$. This indicates that during ignition, the chemical reaction occurs in the transition regime, which is consistent with the calculation results [10].

An analysis of the results from Table 1 regarding extinction was conducted. Much larger values of temperature differences and average radial temperature gradients are observed compared to ignition: temperature differences ΔT and gradients $\Delta T/r_s$ are more than twice as high, while the average radial gradient $\Delta T/r_E$, calculated relative to the extinction radius, is 30–100 times greater. While particle ignition occurs at diameters close to the initial d_b, extinction happens upon reaching a critical value d_E (Fig. 2, b). Since $d_E << d_b$, the radial gradients at the moment of extinction are sufficiently large. The core temperature is much higher than the surface temperature. The surface cools down rapidly due to molecular-convective heat transfer with the gas (q_α) when the particle diameter reaches the critical value d_E. Radiation heat losses (q_w) are significantly lower due to the reduction in the particle surface area. At extinction, no clear dependence of the temperature difference and the average radial gradient on the initial particle diameter is observed. This occurs because the critical extinction diameter d_E is independent of the initial particle size and is determined by the gas characteristics (gas temperature, oxidant concentration). Therefore, the temperature differences and radial temperature gradients for all initial diameters differ insignificantly at the moment of extinction.

We shall compare the characteristics of ignition, combustion, and extinction considering the temperature gradient across the particle (non-isothermal model, equations (1)-(9)) and without it (isothermal model, equations (9)-(10)), i.e., assuming instantaneous heating of the carbon mass to the surface temperature $T_{s.}$. The results of this analysis are presented in Table 3.

It is evident that neglecting internal thermal conductivity into the depth of the carbon mass (isothermal model) leads to overestimated values for ignition, combustion, and extinction characteristics. This is particularly significant for the induction period. For a particle with a uniform temperature, the induction period across the entire studied range of initial diameters is 50% longer than when considering the temperature distribution across the particle radius. For the combustion time, this error is smaller and increases with particle size (from 7% for d_b = 200 μm to 17% for d_b = 1 mm. Furthermore, the isothermal approach slightly alters the critical ignition conditions: a particle with diameter d_b = 100 μm at T_g = 1300 K does not ignite, whereas the non-isothermal model shows stable ignition and combustion (Table 3).

Thus, accounting for the radial non-isothermality of the particle leads to heat accumulation in the near-surface region and a reduction in the effective heated volume of the particle compared to its total volume. This results in a shorter ignition time (t_{ind}) compared to the isothermal model. In other words, the localization of heat at the surface accelerates ignition.

During combustion, a lesser effect of non-isothermality is observed, as the temperatures of the surface and the core are nearly identical (Fig. 4, a). Combustion occurs in the diffusion regime, and the reaction rate (and consequently, heat release) is determined by the mass transfer coefficient (Equation 12), which is inversely proportional to the particle radius. Therefore, the internal radial gradient has a weaker influence on the burning time (t_{bur}), and the difference between the models is significantly smaller. The maximum combustion temperature in the case of neglecting temperature non-uniformity across the carbon mass is nearly 100 degrees higher for all studied diameters.

The isothermal approach also leads to an increase in the critical extinction diameter (Table 3), as significant radial gradients exist during extinction: the particle core is maximally overheated relative to the surface. The maximum temperature values, as well as the critical extinction diameters, are independent of the initial particle diameter and are determined by the parameters of the air medium. Thus, neglecting the radial temperature gradient across the particle leads to erroneous estimates of the key ignition, combustion, and extinction characteristics of carbon fuel.

Table 3.

Ignition, combustion, and extinction characteristics of a carbon particle with ($dT/dr \neq 0$) and without ($dT/dr = 0$) accounting for the radial temperature gradient at a gas temperature T_g = 1300 K.

Characteristics		t_{ind}, s		t_{bur}, s		d_E, μm		T_{max}s, K	
dT/dr		≠0	=0	≠0	=0	≠0	=0	≠0	=0
d_b, μm	100	0.1	-	0.17	-	18	-	2304	-
	200	0.21	0.34	0.69	0.74	18	22.8	2298	2393
	500	0.68	1.05	4.58	5.12	18	22.8	2289	2393
	800	1.17	1.73	12.23	14.18	18	22.8	2280	2393
	1000	1.47	2.13	19.43	22.8	18	22.8	2278	2393

Conclusions

Physical and mathematical modeling of high-temperature heat and mass transfer and chemical transformation of carbon particles, accounting for internal thermal conductivity, demonstrated that during the ignition and extinction of particles with initial diameters d_b=100-1000 μm, a temperature difference ΔT and a corresponding radial temperature gradient $\Delta T/r_s$ are formed between the surface and the core. This indicates the non-isothermal nature of the solid phase thermal state.

It was established that as the initial particle diameter increases, the temperature difference between the surface and the core grows due to the slowing of internal thermal equalization, the characteristic time of which scales as the ratio of the square of the particle radius to the thermal diffusivity coefficient ($\tau \sim r_s^2/a$). Simultaneously, this difference is distributed over a larger spatial distance; therefore, the radial temperature gradient decreases. Consequently, the simultaneous increase in ΔT and decrease in the gradient $\Delta T/r_s$ is a direct consequence of transient thermal conductivity in larger particles.

Experimental studies conducted with millimeter-sized particles confirmed a significant lag of the core temperature relative to the surface temperature at the moment of ignition, i.e., the existence of a temperature difference and a radial gradient. Furthermore, it was experimentally confirmed that at the moment of ignition, the time derivative of the particle temperature reaches its maximum value, which serves as a criterion for determining the induction period of carbon particles. The diffusion-controlled combustion regime $d^2(t)=K_{bur}$=const of the particles was also confirmed.

Calculations established that during extinction, the temperature difference and radial gradients are significantly higher than during ignition; they are independent of the initial particle diameter and are determined by the critical extinction diameter. The increase in the temperature difference is caused by a sharp deceleration of the chemical reaction at the surface amid rising molecular-convective heat losses. Due to finite internal thermal conductivity, the core temperature significantly exceeds the surface temperature. Thus, neglecting the thermal inertia of the particle volume leads to an incorrect determination of the combustion time.

It is shown that using an isothermal model for the diameter range of 100-1000 μm results in overestimated values for the induction period, combustion time and temperature, and critical extinction diameter. The error is up to 50% for the ignition time (induction period), 7 % to 17% for the combustion time, and 26% for the critical extinction diameter. In the small-diameter range (100 μm), critical ignition conditions are not met for an isothermal particle. Consequently, the isothermal model systematically underestimates the characteristic time scales of the process.

The obtained results justify the necessity of a non-isothermal description even for particles in the submillimeter range. Accounting for radial thermal conductivity and the internal temperature gradient within the particle is essential for the correct prediction of high-temperature processes and their characteristics.

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С.Г. Орловська

Експериментальні дослідження та фізико-математичне моделювання впливу неоднорідності температурного поля по вуглецевій частинці на характеристики її займання, горіння і згасання

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Робота присвячена експериментальним дослідженням та фізико-математичному моделюванню високотемпературного тепломасообміну та хімічного перетворення вуглецевих частинок з урахуванням внутрішньої теплопровідності. Актуальність дослідження зумовлена необхідністю підвищення точності прогнозування характеристик займання, горіння та згасання твердих палив в теплотехнічних процесах. У більшості теоретичних підходів використовується ізотермічне наближення частинки, що може привести до похибок у визначенні періоду індукції і часу вигоряння, особливо для частинок субміліметрового та міліметрового діапазону.

Запропонована неізотермічна модель, що включає внутрішню теплопровідність в частинці, реакції окиснення, теплообмін конвекцією і випромінюванням. Проведено чисельні розрахунки для інтервалу діаметрів 100-1000 мкм з аналізом температурних полів та градієнтів на стадіях займання і згасання. Показано, що зі зростанням діаметра частинки збільшується температурний перепад між поверхнею і центром, тоді як радіальний температурний градієнт зменшується внаслідок просторового розтягнення температурного поля та зростання нестаціонарного теплового часу. Експериментальні дослідження з міліметровими частинками показали значні температурні градієнти на стадії займання і ідентифікували момент займання максимальним значенням часової похідної поверхневої температури частинки.

Порівняння розрахунків з використанням ізотермічної та неізотермічної моделей засвідчило систематичне підвищення часу займання і горіння частинки без врахування внутрішньої теплопровідності. Показано, що в області малих розмірів частинок неврахування внутрішньої теплопровідності призводить до відсутності займання. Отримані результати підтверджують необхідність неізотермічного опису для коректного прогнозування характеристик горіння вуглецевих частинок з розмірами більше 200 мкм.

Ключові слова: вуглецеві частинки, займання, горіння, згасання, температурний градієнт, внутрішня теплопровідність, період індукції, час горіння.