Comparison of Single Coal Char Particle Combustion at Different Conditions*

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Comparison of single coal char particle combustion at different operation modes is presented. Experiments were carried out applying a thermogravimetric method. During combustion of a single particle, time dependences of temperature inside the particle, around the particle, and the mass of particle were measured together with the internal porous structure of particles at different degrees of burnout. Obtained experimental results have shown that the mechanism of combustion is strongly dependent on the combustion conditions, especially on the initial temperature and oxygen content in the inlet gas. At temperatures below 500 ℃, the limiting factor was the oxygen concentration. Combustion using the inlet concentration of oxygen below 5 vol. % was governed by the reaction-diffusion mechanism. If the content of oxygen in the inlet gas exceeded 5 vol. %, combustion proceeded according to the shell progressive mechanism. At temperatures above 500 ℃, the shell progressive mechanism of coal particle combustion was supposed, independently of the oxygen concentration.

The problems related to mathematical modelling of the combustion of the single char particle under condition of reaction-diffusion mechanism are discussed.

Coal still belongs to one of the main energy sources throughout the world. Coal is the largest single energy source used for power production (Fig. 1) [1].

Increasing costs of high-grade coals and also the recognition of the need for environmental protection, prompt us to consume it more efficiently in coal processing technologies. A typical useful utilization of coal nowadays is combustion. So, the optimization of this process is really important in conjunction with the finity of coal resources. The relevance of coal as a resource of chemical compounds will increase in the future, too [2]. Obviously, the higher the concentration of carbon and the lower the amount of ash, the better fuel one has. Ideally, total combustion of carbon to CO_2 is expected, but very often the major reaction product is CO. As a consequence, much lower amount of heat is released from the coal by partial combustion. From the thermodynamic point of view, formation of CO is suppressed especially at low temperatures (less than 400 ℃) [3].

Combustion in the power plant combustors could proceed under nonstationary conditions, for example during the start-up of power plants, when the combustor works in a low output mode. Alternatively, during the operation time of plants, when the fluidized-bed combustor hydrodynamic conditions are changing, the so-called “cold corners” are formed. Low oxygen concentration in these places of the combustion chamber

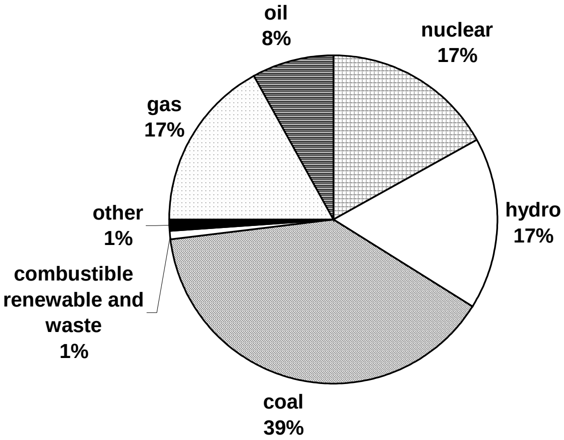

Fig. 1. Energy sources used for power generation [1].

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could cause sintering of coal, followed by shut-down of the combustor. This kind of situation could occur at temperatures below 530 ℃ when oxygen is not able to reach the whole surface of coal particles in the coal agglomerates.

Independently of the combustor type, coal combustion consists of several processes: drying, devolatilization, immediate combustion of volatiles, and finally char combustion. These processes proceed either consecutively or simultaneously, depending on the reaction conditions.

To propose an appropriate mathematical model of single coal particle combustion it is necessary to know the characteristics of coal as a heterogeneous substance at macroscopic and microscopic levels as well as the behaviour of components comprised in the particular coal during the combustion process. The amount of water, the amount and kind of volatile matters, and the content of carbon and other combustibles in the coal char play an important role in the combustion process and characterize the coal. In 1980, it was noted that the resurgence in coal science had not been accompanied in general by the molecular structure of coal. In many ways this still remains true a quarter of century later [4].

Previously, experimental study of the combustion of a single coal particle (Slovak brown coal [5]) using a thermogravimetric experimental apparatus [5—8] was carried out enabling a detailed investigation of the development of internal pore structure during combustion [8, 9]. Based on these results (development of the internal structure and visualization of the cross-section of partially combusted particle) several models describing the combustion of a single coal char particle were assumed [6, 10].

The aim of this paper is to compare the two mechanisms of single coal char particle combustion at different initial conditions (initial combustion temperature and oxygen concentration in the inlet gas stream). Mathematical modelling of single coal particle combustion is also discussed.

MATHEMATICAL MODEL

The coal char combustion is represented by a great number of reactions. Heterogeneous reactions (*A*—*C*) and a homogeneous one (*D*) are taken as dominant, whereby the reaction (*B*) is strongly dependent on the combustion temperature

$$\mathrm{C(s)} + \mathrm{O_2} \rightarrow \mathrm{CO_2} \qquad (A)$$

$$\mathrm{C(s)} + \mathrm{CO_2} \rightarrow \mathrm{2CO} \qquad (B)$$

$$\mathrm{C(s)} + 1/2\mathrm{O_2} \rightarrow \mathrm{CO} \qquad (C)$$

$$\mathrm{CO} + 1/2\mathrm{O_2} \rightarrow \mathrm{CO_2} \qquad (D)$$

The reaction rates for reactions (*A*—*D*) are usually given by the following equation

$$\dot{\xi}_{\mathrm{V}j} = k_{\mathrm{V}j,\infty} \exp\left(-\frac{E_j}{RT}\right) C_i^{m_{j,i}} C_{ii}^{n_{j,ii}} \quad j = 1, \dots, 4 \qquad (1)$$

where the reaction rate $\dot{\xi}_{\mathrm{V}j}$ is based on the volume unit of the particle, $k_{\mathrm{V}j,\infty}$ is the frequency factor for the *j*-th reaction, *C* is concentration of the *i*-th gas reactant and the *ii*-th solid reactant, *m*, *n* are stoichiometric coefficients of the reactants in reactions (*A*—*D*) [10]. Gaseous components, namely $\mathrm{O_2}$, $\mathrm{CO_2}$, and CO, were assumed, $i = 1$, 2, and 3, respectively. The only solid component was C, $ii = 4$.

The combustion temperature and the oxygen concentration are the key factors influencing the combustion mechanism, which is the base for the development of an appropriate mathematical model. Thus, also the model solution depends on the conditions, for which the model was derived [7]. At low temperatures, the combustion proceeds according to the reaction-diffusion mechanism. At higher temperatures the shell-progressive mechanism was noticed [6]. Previously, detailed information about the shell-progressive mechanism of combustion was published [5, 7, 10].

Dimensionless forms of the model equations consisted of mass balances for gaseous components inside the coal particle

$$\frac{\partial\left(\varepsilon_{\mathrm{P}} Y_i^{\mathrm{S}}\right)}{\partial\tau} = \left(\frac{\varepsilon_{\mathrm{P}}}{\varepsilon_{\mathrm{P}}^0}\right)^{\alpha} \omega_1 \nabla^2 Y_i^S + Th^2 \sum_{j=1}^{3} \nu_{ij} P_j R_j + \\ + \varepsilon_{\mathrm{P}} Th^2 P_4 R_4 \qquad (2)$$

The solid carbon mass balance in the dimensionless form is given by

$$\frac{\partial Y_4^{\mathrm{S}}}{\partial\tau} = -\Omega Th^2 \sum_{j=1}^{3} \nu_{j4} P_j R_j \qquad (3)$$

where *Y* is dimensionless concentration of gaseous or solid components, ε_{P} is porosity of the solid phase, ν is stoichiometric coefficient of the gaseous or solid components, *Th*, *P*, and *R* are dimensionless parameters.

Enthalpy balance for the combusted particle can be expressed as

$$\left[(1-\varepsilon_{\mathrm{P}})\,\Xi_1 + \varepsilon_{\mathrm{P}}\Xi_2\right]\frac{\partial\Theta}{\partial\tau} + \Theta\left[\Xi_2 - \Xi_1\right]\frac{\partial\varepsilon_{\mathrm{P}}}{\partial\tau} = \\ = \Lambda\nabla^2\Theta + Th^2\sum_{j=1}^{3}\beta_j P_j R_j + \varepsilon_{\mathrm{P}} Th^2 \beta_4 P_4 R_4 \qquad (4)$$

Expressions for porosity were based on the assumption that the porosity value is changing due to the decrease of the carbon content inside the particle

$$\varepsilon_{\mathrm{P}} = \varepsilon_{\mathrm{P}}^0 + \psi_{\varepsilon}\left(1 - Y_4^{\mathrm{S}}\right) \qquad (5)$$

$$\frac{\mathrm{d}\varepsilon_{\mathrm{P}}}{\mathrm{d}\tau} = -\psi_{\varepsilon}\frac{\mathrm{d}Y_4^{\mathrm{S}}}{\mathrm{d}\tau} \qquad (6)$$

Both, thermal conductivity and effective diffusion coefficient varied with the porosity

$$\Lambda = \frac{\lambda_{\mathrm{U}}}{\lambda_{\mathrm{U}}^0} = \left[1 - \left(1 - \frac{\lambda_{\mathrm{A}}}{\lambda_{\mathrm{U}}^0}\right)\left(1 - Y_4^{\mathrm{S}}\right)\right] \qquad (7)$$

$$D_{\mathrm{e}i} = D_{\mathrm{e}i}^0\left(\frac{\varepsilon_{\mathrm{P}}}{\varepsilon_{\mathrm{P}}^0}\right)^{\alpha} \qquad (8)$$

where α is equal to 2 for random pore distribution [11].

The initial conditions for the single coal char particle combustion were as follows

$$\begin{aligned} &\varphi \in \langle 0, 1\rangle \\ &\qquad Y_i^{\mathrm{S}} = 0 \quad i = 1, 2, 3 \\ &\qquad Y_4^{\mathrm{S}} = 1 \\ &\qquad \varepsilon_{\mathrm{P}} = \varepsilon_{\mathrm{P}}^0 \\ &\qquad \Theta = 1 \\ &\qquad D_{\mathrm{e}i} = D_{\mathrm{e}i}^0 \\ &\qquad \Lambda = 1 \end{aligned} \qquad (9)$$

Boundary conditions applied for $t > 0$ and $\varphi = 0$

$$\frac{\mathrm{d}Y_i^{\mathrm{S}}}{\mathrm{d}\tau} = \frac{\mathrm{d}\Theta}{\mathrm{d}\tau} = 0 \qquad (10)$$

and for $t > 0$ and $\varphi = 1$

$$\begin{aligned} \frac{\mathrm{d}Y_i^{\mathrm{S}}}{\mathrm{d}\tau} &= \frac{Bi_{\mathrm{m}}}{\omega_i}\left(\frac{\varepsilon_{\mathrm{P}}^0}{\varepsilon_{\mathrm{P}}}\right)\left(Y_i^{\mathrm{g}} - Y_i^{\mathrm{S}}\right) \\ \Lambda\frac{\mathrm{d}\Theta}{\mathrm{d}\tau} &= Bi_{\mathrm{h}}\left(1 - \Theta\right) + \theta(1 - \Theta^4) \end{aligned} \qquad (11)$$

During the model development several assumptions and simplifications were considered, *i.e.* non-isothermal conditions; constant pressure; complete devolatilization of the coal particle at a time equal to zero; constant pellet size during the combustion (deviation ± 5 % of initial particle diameter); increasing porosity of the particle with time and with the carbon conversion (and consequently also the change of diffusion coefficients of gaseous reactants and the thermal conductivity with time and location within the coal particle); no solid products originate in reactions (A—D), removal of the reaction heat from the particle by convection and radiation; no catalytic effect of ash on the combustion process; perfect mixing of the gas phase surrounding the particle.

Table 1. Experimental Conditions of a Single Coal Particle Combustion

Parameter	Value
Initial temperature/ °C	450—800
Pressure/Pa	atmospheric
Inlet concentration of oxygen/vol. %	3—21
Mass of particle/kg	0.5×10^{-3}—1.0×10^{-3}
Mass of degassed particle/kg	0.3×10^{-3}—0.7×10^{-3}
Flow rate of gas mixture/(m^3 s^{-1})	2.8×10^{-5}
Particle diameter/m	7.0×10^{-3}—10.0×10^{-3}

EXPERIMENTAL

Coal particles prepared from brown coal (coalmine Nováky, Slovakia; C$^{\mathrm{d}}$ 47.35 mass %, H$^{\mathrm{d}}$ 4.6 mass %, N$^{\mathrm{d}}$ 1.0 mass %, S$^{\mathrm{d}}$ 3.0 mass %) were used. The single spherical coal char particles were combusted in an experimental equipment, which is described in detail elsewhere [5, 8]. Experimental conditions are summarized in Table 1.

Prior to combustion the particles were dried, devolatilized and preheated to the initial combustion temperature in a nitrogen atmosphere. The particle was combusted in a flowing mixture of nitrogen and oxygen to different burnout degrees. Then the feed stream was switched to nitrogen again and the combustion experiment was stopped. The internal core structure was investigated after discharging ash. It was found that the internal pore structure of a particle core strongly depended on the origin and pretreatment of the coal particle. Development of micro- and mesoporous structures was determined by the measurement of adsorption and desorption isotherms of nitrogen at its boiling point on a SORPTOMATIC 1900 instrument (Fisons Instruments, Milano, Italy). To detect the changes in the macroporous structure of the partially combusted coal particles, the mercury porosimetry method (POROSIMETER 2000, Fisons Instruments, Milano, Italy) was used.

RESULTS AND DISCUSSION

In Table 2 the influence of the initial conditions on the combustion process is summarized. It offers a concise conclusion of experimental study of the coal combustion using the TGA equipment, which could be considered general for different types of coal combustors. Mathematical simulation of combustion was carried out successfully for the conditions corresponding to the shell-progressive mechanism, published in previous paper [5].

Concentration of Oxygen above 5 vol. %, Initial Temperature above 530 °C

Particles were combusted starting at the initial

Tabl n Mechanisms for Wider

Initi		ntent in inlet gas	
		5	above 5 vol. %
b		on	Shell-progressive mechanism
al		ve	Shell-progressive mechanism

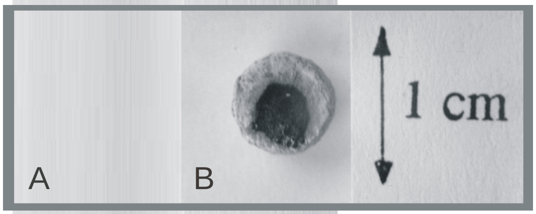

Fig. 2. Cross-sections of the particles combusted to a 50 % burnout degree, at the initial temperatures 450 °C (A) and 650 °C (B), 5 vol. % content of oxygen in the feed stream.

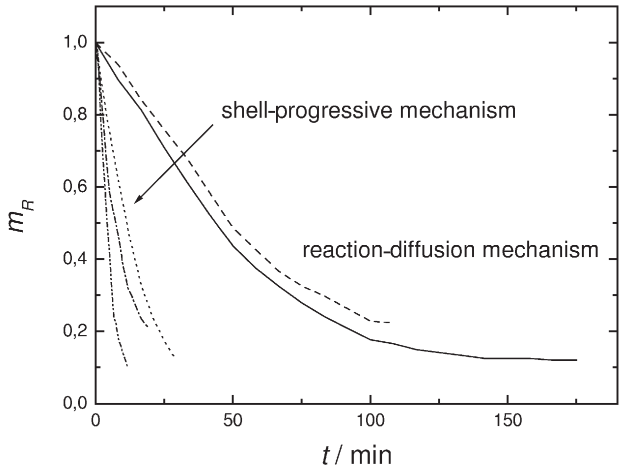

Fig. 3. Time dependences of the particles relative mass at initial temperature of 530 °C and at different oxygen contents in gas phase: 3 % (solid line), 5 % (dashed line), 10 % (dotted line), 15 % (dotted-dashed line), and 21 % (dashed-dotted-dotted line).

temperatures of 530 °C, 650 °C, and 800 °C in the atmosphere containing 10 vol. %, 15 vol. %, and 21 vol. % of oxygen in the inlet gas. For given conditions, intense preheating of the particle, and hence acceleration of combustion was observed. The time of burnout of the whole coal particle was apparently shorter than the combustion time measured for low oxygen content in the inlet gas (Figs. 3 and 4).

In the cross-section of partially combusted particle two different regions could be recognized (Fig. 2B). The reactions were assumed to occur only at a sharp interface between the exhausted outer shell (ash) and the unreacted core of the solid (coal char). Oxygen was immediately consumed by the reaction at the shell—core interface. The ash shell, with a macroporous structure and a high porosity, did not represent any diffusional resistance for the gas components [8]. Radius of the unreacted core was shrinking as the reaction proceeded, but the properties of the core surface area were not changing considerably (Table 3). Due to this fact, the shell-progressive mechanism was proposed and the corresponding mathematical model was derived to describe the coal particle combustion [5].

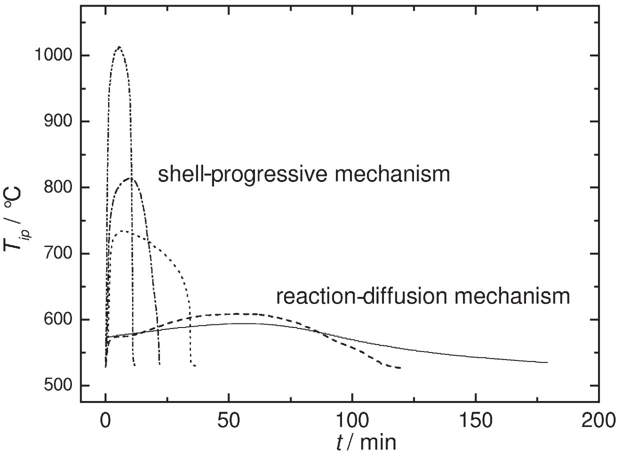

Fig. 4. Time dependences of the temperature inside the particles at the initial temperature of 530 °C and at different oxygen contents in gas phase: 3 % (solid line), 5 % (dashed line), 10 % (dotted line), 15 % (dotted-dashed line), and 21 % (dashed-dotted-dotted line).

At the oxygen concentration higher than 15 vol. % and the initial temperature above 530 °C, a considerable overheating of the particle core (above 900 °C) was detected during its combustion (Fig. 4). At these conditions also endothermic reaction (B) between solid carbon and diffused carbon dioxide is feasible. As a result of the solid carbon consumption in reaction (B), an increase of the specific surface area in the microporous and mesoporous regions of the unreacted core was observed (Table 3). This observation was supported by repeated combustion experiments followed by the analysis of the core internal surface.

Concentration of Oxygen above 5 vol. %, Initial Temperature below 530 °C

Particles were combusted starting at the initial temperature of 460 °C and 530 °C in the presence of 10 vol. % and 15 vol. % of oxygen in the nitrogen stream. Increase of the internal surface area in the microporous region was detected, when the temperature inside the particle during combustion was higher than 850 °C. Due to a lower initial temperature, the

Table 3. Development of the Internal Specific Surface Area of the Particles Combusted to a 50 % Burnout Degree at Different Initial Conditions

Initial temperature/ °C	Oxygen content in inlet gas/vol. %	Specific surface/(m^2 g^{-1}) below 50 nm	Specific surface/(m^2 g^{-1}) above 50 nm
		3.6[a]	6.41[a]
		115.2[b]	9.31[b]
450	5	263.7	16.3
	10	137.7	18.8
	15	156.0	18.6
550	5	113.6	16.1
	10	143.3	21.3
	15	138.5	17.1
650	5	130.5	21.7
	15	143.2	13.3
800	5	172.1	6.2
	15	165.5	12.1

a) Original coal; *b*) degassed coal.

combustion lasted obviously longer compared to the previous experiments. On the other hand, the combustion time was apparently shorter than in the case of experiments carried out at lean oxygen conditions (Fig. 3), when a sharper mass loss was observed [6]. The shell-progressive mechanism was confirmed also by visual observations of the partially combusted particles and the development of internal structure of unreacted cores (Table 3).

Concentration of Oxygen below 5 vol. %, Initial Temperature above 530 °C

Particles were combusted starting from the initial temperature of 550 °C, 650 °C, and 800 °C at a lean oxygen conditions. The development of the internal structure was different for each initial temperature used. At initial temperature of 550 °C, specific surface area of the particle core was similar to that of uncombusted particle. At a temperature of 800 °C, the development of the core microporous structure was influenced by the endothermic reaction (*B*).

The combustion rate at 550 °C and low oxygen (5 vol. %) content in the gas phase was very slow (Figs. 3 and 5) and the overheating of the particle was negligible (Fig. 4). The development of the internal structure followed the shell-progressive mechanism when the combustion was carried out at higher initial temperatures. Due to depletion of oxygen at the shell—core interface, changes in the internal structure were negligible. Combustion took place just at the sharp boundary.

The initial temperature range of 530—550 °C could be assumed as a turning point of the reaction mechanism between the shell-progressive and the reaction-diffusion one. The limiting factor was the concentration of oxygen in the inlet gas stream.

The shell-progressive mechanism was ascribed also to the combustion of commercial char in an atmosphere with a low oxygen content at the initial temperature of 800 °C [8, 9]. At the same time, an increase of the specific surface area was detected due to the reaction (*B*).

Detailed kinetic study of combustion under the conditions described above was published recently [5]. In the case of the shell-progressive mechanism, the reactions were assumed to proceed in a thin layer between the ash shell and the noncombusted core interface. The combustion rate was related to the reaction surface area, *i.e.* geometric surface of the unreacted particle core. It was assumed that the reactions were not catalyzed by inorganic compounds in the ash and depended solely on the reacting component's concentrations and the temperature. The transport properties like porosities and thermal conductivities of the core and ash were constant throughout the process. It was verified that the reaction orders (m, n) in eqn (*1*) were equal to the stoichiometric coefficients in reactions (*A*—*D*).

For the estimation of kinetic parameters of eqn (*1*) used with the shell-progressive mathematical model for single coal char particle, sets of experimental data (temperature inside the particle, around the particle, and in the main flow of gas) were used [5]. Kinetic parameters of reactions were in a good agreement with relevant data available in the literature [11].

Optimized kinetic parameters were used to simulate the single coal char particle combustion at the conditions suitable for shrinking core mechanism. Very good agreement of experimental and simulated data verified correctness of the assumed simple kinetic equation (eqn (*1*)) [5].

In general, behaviour of particles combusted at high temperature was the same at similar initial conditions. Prediction of changes in the values of the unreacted core properties during combustion is not necessary due to the principles of shell-progressive mechanism [8, 9].

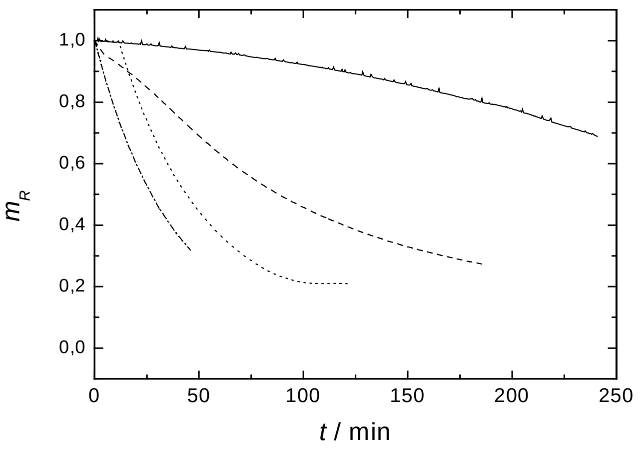

Fig. 5. Time dependences of the particles relative mass for the oxygen concentration of 5 vol. % and at different initial temperature: 460 °C (solid line), 530 °C (dashed line), 650 °C (dotted line), 800 °C (dotted-dashed line).

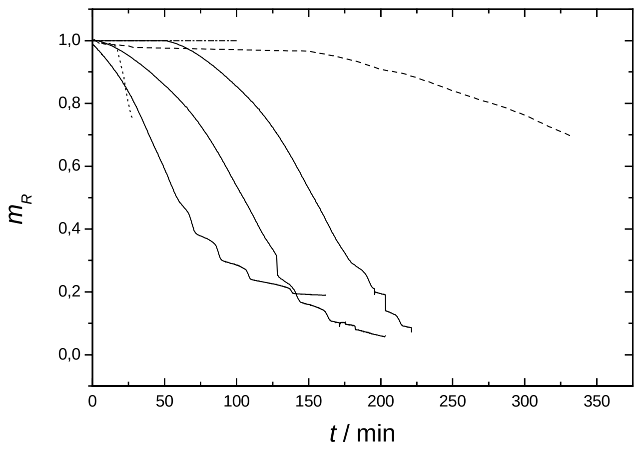

Fig. 6. Time dependences of the particles relative mass of six different particles prepared from one piece of coal, combusted at the same initial conditions (460 °C and 5 vol. % of oxygen in the inlet stream).

Concentration of Oxygen below 5 vol. %, Initial Temperature below 530 °C

Due to the low oxygen content (max. 5 vol. %) and low initial temperature (max. 530 °C) the reaction proceeded very slowly, with a small heat release. The higher temperature of the particle did not accelerate the chemical reactions (Figs. 3—5) as it was in the case of higher initial temperatures. During experiments it was found that each particle burned out in a different way. Repetition of experiments using the same initial conditions did not lead to the same results.

In such case, the amount of oxygen in the gas surrounding the particle was not sufficient to ignite the reactions (Fig. 6, dotted-dashed line). **At given conditions, temperature oscillations during the combustion of several coal char particles were observed**. On the other hand, when the accumulation of oxygen was sufficient, the reactions were ignited. Due to the fast chemical reactions, oxygen in the particle pores and on their surface was quickly consumed. As the transport of oxygen through the particle pores was fairly slow, the reactions were **decelerated** and the temperature fell down (Fig. 6, solid lines; temperature oscillations are shown in Fig. 7). New **acceleration** of combustion reactions occurred first when a sufficient amount of oxygen was accumulated in the particle pores. This sequence was periodically repeated and the measured temperatures and concentrations of the gaseous product exhibited oscillations (Fig. 7) [7].

Due to the different nature of individual coal particles different behaviour was observed, *e.g.* the reaction proceeded very slowly (Figs. 4 and 6, dashed line). However, even if the reaction started, it was extinguished after a certain time (Fig. 6, dotted line). As the combustion rate was very slow, the particle composition played a key role in this process. Therefore, it was impossible to predict the sample behaviour and the evolution of core properties during the particle combustion.

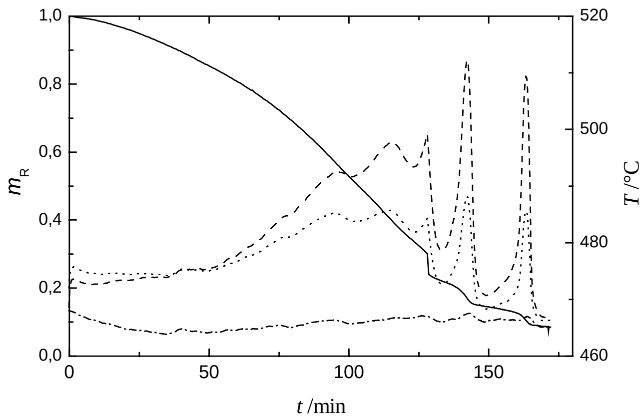

Fig. 7. Combustion of coal particle at 460 °C and for oxygen concentration of 5 vol. %. Time dependences of the particle relative mass (solid line) and the temperature in the centre of the particle (dashed line), temperature on the geometric surface (dotted line), temperature of the gas close to the particle surface (dotted-dashed line) [7].

It was assumed that the reaction rates depended principally on the initial combustion temperature and the content of oxygen in close neighbourhood of the coal particle and that they were independent of the composition of the solid particle material, *i.e.* the reactions were noncatalytic and dependent only on the gaseous reactants concentration and temperature. In general, the reaction rates were slow and varied for each experiment, even if the same conditions were used (Fig. 6). Therefore, one may speculate that the catalytic effect of the inorganic matter, ash, should be taken into account. Nowadays, it is practically impossible to appreciate the catalytic influence of the inorganic substances in the ash on the reaction order, activation energy, and the frequency factor.

Pranda et al. [3] discussed about the catalytic effect of the mineral matters on the carbon gasification. Alkali metal compounds used in this study exhibit a beneficial effect on the combustion reactions, decreasing the ignition temperature. The same authors [12] found a positive effect of alkali metal carbonates on the decrease of CO generation in favour of CO_2. The effect of coal-burning additives (CBA) on the coal combustion was also studied [13]. As a coal-burning additive, a powder composed mainly of metal and semi-metal oxides, such as Mg, Fe, Mn, Al, Si, and B, was used. CBA dopping had no significant effect on the energetic value of the coal types used. However, it was shown that the carbon ignition temperature decreased as the CBA was applied. Furthermore, the kinetic study showed that CBA was able to change the course of carbon oxidation by catalytic action, reducing the apparent activation energy and accelerating the burning/oxidation of graphite. In the presence of CBA, catalytically active centres were formed, at which the reactions took place.

The presented reaction-diffusion mathematical model of combustion includes many parameters. All these parameters are dependent on the original properties of the coal, its pretreatment before combustion, and finally on the combustion conditions. The analytical methods employed for the determination of the coal properties are mostly destructive for the particle. One particle could not be used for analyses and also for the combustion experiment. Coal is a natural material and its properties are changing from piece to piece. A small sample (particle with a diameter less than 1 cm) is not representative for the parameters estimation. On the other hand, by using a higher amount of coal for the parameters determination, one can obtain their average values, which sometimes are far from the actual values in the simulation of a certain particle used in the combustion experiment.

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SYMBOLS

Bi_{h}	dimensionless parameter $(= R_{\mathrm{P}} k_{\mathrm{H}} / \lambda_{\mathrm{U}}^0)$	
Bi_{m}	dimensionless parameter $(= R_{\mathrm{P}} k_{\mathrm{g}i} / D_{\mathrm{e}i}^0)$	
C	molar concentration	mol m^{-3}
c_{P}	heat capacity	J mol^{-1} K^{-1}
D_{e}	effective diffusion coefficient	m^2 s^{-1}
$\Delta_{\mathrm{r}}H$	reaction enthalpy	J mol^{-1}
E	activation energy	J mol^{-1}
k_{g}	mass transfer coefficient	m s^{-1}
k_{H}	heat transfer coefficient	W m^{-2} K^{-1}
$k_{\mathrm{V}\infty}$	frequency factor	m^3 mol^{-1} s^{-1}
m	mass of particle	g
P_j	dimensionless parameter $(= \dot{\xi}_{\mathrm{V}j}^0 / \dot{\xi}_{\mathrm{V1}}^0)$	
R	gas constant	J mol^{-1} K^{-1}
R_j	dimensionless reaction rate $(= \dot{\xi}_{\mathrm{V}i} / \dot{\xi}_{\mathrm{V}i}^0)$	
R_{P}	particle radius	m
r	particle radial coordinate	m
T	temperature	K
Th	dimensionless parameter $(= \sqrt{R_{\mathrm{P}}^2 \dot{\xi}_{\mathrm{V1}}^0 / D_{\mathrm{e1}}^0 C^{\mathrm{g}}})$	
t	time	s
t^0	parameter $(= R_{\mathrm{P}} / D_{\mathrm{e1}}^0)$	s
Y_4^{S}	dimensionless concentration of the solid $(= C_4^{\mathrm{S}} / C_4^{\mathrm{S0}})$	
Y_i^{g}	dimensionless concentration in the gas phase $(= C_i^{\mathrm{g}} / C_1^{\mathrm{g}})$	

Greek Letters

$\mathit{\Theta}$	dimensionless temperature $(= T^{\mathrm{S}} / T^{\mathrm{g}})$	
$\mathit{\Lambda}$	dimensionless parameter $(= \lambda_{\mathrm{U}} / \lambda_{\mathrm{U}}^0)$	
$\mathit{\Xi}_1$	dimensionless parameter $(= \rho^S c_{\mathrm{P}}^{\mathrm{S}} D_{\mathrm{e1}}^0 / \lambda_{\mathrm{U}}^0)$	
$\mathit{\Xi}_2$	dimensionless parameter $(= \rho^g c_{\mathrm{P}}^g D_{e1}^0 / \lambda_{\mathrm{U}}^0)$	
$\mathit{\Omega}$	dimensionless parameter $(= C^{\mathrm{g}} / C^{\mathrm{S}})$	
α	empirical coefficient, $\alpha = 2$ [11]	
β_j	dimensionless parameter $(= (-\Delta_{\mathrm{r}} H_j)\, D_{\mathrm{e1}}^0 C^{\mathrm{g}} / T^{\mathrm{g}} \lambda_{\mathrm{U}}^0)$	
γ_j	dimensionless parameter $(= E_j / RT^{\mathrm{g}})$	
ε	emissivity	
ε_{P}	porosity of the solid phase	
θ	dimensionless parameter $(= \sigma \varepsilon T^{\mathrm{g}3} R_{\mathrm{P}} / \lambda_{\mathrm{U}}^0)$	
λ	thermal conductivity	W m^{-1} K^{-1}
ν	stoichiometric coefficient	
$\dot{\xi}_{\mathrm{V}}$	reaction rate	mol m^{-3} s^{-1}
ρ	density	m^3 kg^{-1}
σ	Stefan—Boltzmann constant	W m^{-2} K^{-4}
τ	dimensionless time $(= t / t^0)$	
ω_i	dimensionless diffusion coefficient $(= D_{\mathrm{e}i}^0 / D_{\mathrm{e1}}^0)$	
ϑ	molar volume	
φ	dimensionless radius $(= r / R_{\mathrm{P}})$	
ψ_{ε}	parameter $(= C^{\mathrm{S}} \vartheta_4)$	m^3 mol^{-1}

Superscripts

0	initial conditions
d	based on dry material
g	gaseous phase
s	solid phase
t	time

Subscripts

1	oxygen
2	carbon dioxide
3	carbon monoxide
4	carbon
A	ash
g	gas phase
i, ii	number of component – gas or solid

ip	inside the particle
j	number of reaction
P	particle
R	relative
U	coal char
V	based on the volume unit of particle

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