

Modelling of Nonlinear Behaviour during Combustion of Single Coal Char Particle*

Ľ. JELEMENSKÝ**, J. MARKOŠ, R. ŽAJDLÍK, and B. REMIAROVÁ

*Department of Chemical and Biochemical Engineering, Faculty of Chemical Technology,
Slovak University of Technology, SK-812 37 Bratislava
e-mail: jelemen@cvt.stuba.sk*

Received 19 May 2000

Experimental and theoretical investigation of combustion of a single coal char particle is presented. As a model of coal char particle combustion the shell progressive mechanism was considered. The porous structure of an original, devolatilized and partially combusted particle was analyzed. Due to the bimodal character of the porous structure, the pore size distribution was determined by a sorption method and mercury porosimetry. Combustion experiments were carried out in an equipment where the TGA method was applied for process monitoring. This equipment allowed to study the behaviour of the coal char particle during the process of drying, degassing, and combustion. During the combustion process, the particle consisted of two regions – the noncombusted core and the ash layer. The time dependences of the particle mass, temperature in the particle and gas phase, and composition of the combustion products were measured. The obtained experimental results confirmed that the shell progressive mechanism can be applied for the mathematical description of combustion of single coal char particle.

The mechanism of coal combustion is not simple. It consists of various processes, which proceed at various rates and mutually interplay. This process can be elucidated on the basis of the history of a single particle. Immediately after the entry of a coal particle into the combustion device, a rapid release of humidity and volatile substances into the surroundings occurs as a result of the influence of high temperature. The basic process, however, is the combustion itself, which can be characterized as a noncatalytic G-S reaction.

In looking for an appropriate mathematical model, the majority of authors started from several models for noncatalytic reactions, the final forms of which differed in their complexity. The choice of the model solution depended on the conditions for which the model was derived. This choice was mainly influenced by the structure of the solid phase and by the transport and reaction rates. The complexity of the model depended mainly on the type of the heterogeneous reaction and simplifying assumptions. According to the assumptions on which these models were built, the homogeneous reaction took place only in a thin layer around the particle.

A relatively great number of papers were reported that dealt with the modelling of the carbon combustion process at steady-state conditions with the goal of

separating the influence of other factors on the final solution. These factors are: the flow-rate of gas [1], changes of the concentration of oxygen [2] and coal properties [3–5], form of the reaction scheme [6, 7], rates of the heterogeneous reaction [8], or the influence of transport processes [9].

In terms of the structure of the solid phase, the published papers dealt with the modelling of combustion of porous and nonporous single coal particles, which, in the majority of cases, did not contain further components. The dynamic models of these systems can be divided in dependence on the character of the solid phase into:

- models, in which the particle does not contain solid components forming ash [10–14];
- models taking into account also the presence of other solid components forming ash [15–18].

It is clear that the temperature is crucial for the model describing the process. At low temperatures, the process can proceed according to the homogeneous model, at high temperatures in accordance with the shell progressive model and in the intermediate temperature region the zone model of the heterogeneous reaction is applied [15]. Some works indicate that the process of coal combustion proceeds in the majority of cases at high temperatures. Therefore, it is convenient

*Presented at the 27th International Conference of the Slovak Society of Chemical Engineering, Tatranské Matliare, 22–26 May 2000.

**The author to whom the correspondence should be addressed.

to describe the coal combustion process by the shell progressive model. The ash layer formed around the particle is little heat conductive, a high overheating of the particle therefore occurred [16, 17].

Some information about the combustion mechanism can be obtained from the investigation of the porous structure of coal particle and its changes during the reaction. The pore structure depends on the origin and pretreatment of coal. It has been shown in several experimental studies [19, 20] that the original porous structure is characterized by a bimodal pore distribution. Nearly all internal surface area belongs to the region of micropores (pore radius $R_P < 1$ nm) and mesopores ($1 \text{ nm} < R_P < 25$ nm), while the large pores ($R_P > 25$ nm) account for a significant part of the total porosity.

The overall chemical reactivity depends on the accessibility of the internal surface area to the gaseous reactants, which is determined by the porous structure of the coal particle. The micropores may not be accessible to the gaseous reactants unless the feeder pores are large enough.

The aim of this paper is to present the experimental results obtained by the application of the TGA method to the combustion of a coal char particle at a

low oxygen concentration in the inlet gas. The work is also focused on the estimation of the porous structure characteristics and the mathematical model of coal char particle combustion and the estimation of combustion kinetic parameters.

EXPERIMENTAL

Coal char from the coal (coal mine Čígeľ, Slovakia) was used. The following composition of the coal char was determined by the elemental analysis: 72.3 mass % carbon, 0.5 mass % hydrogen, 1.3 mass % nitrogen, and 2.7 mass % sulfur.

The combustion experiments were carried out using a single coal char particle and applying the thermogravimetric method. The set-up (Fig. 1) allowed to perform measurements at different experimental conditions, *i.e.* temperature, mass of the particle, composition of the gas feed (Table 1). To avoid the volatilization process, pretreated coal particles were used. The pretreatment procedure was as follows:

1. Coal particle preparation – a spherical particle (diameter 5–10 mm) was obtained by cutting coal.
2. Drying in flowing air and/or nitrogen at 100°C during 4 h. To avoid a particle rupture, the heating

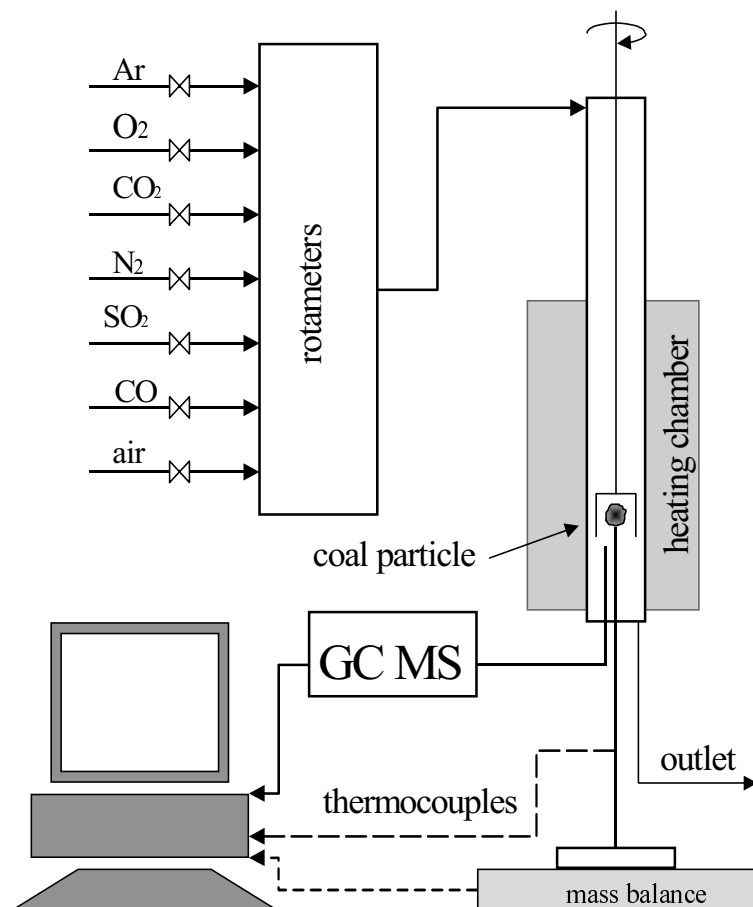


Fig. 1. Experimental set-up.

Table 1. Experimental Conditions of Single Coal Particle Combustion

Temperature/°C	530
Pressure/Pa	1.01×10^5
Mole fraction of inlet oxygen	0.05–0.15
Mass of the coal particle/kg	0.4×10^{-3} – 0.6×10^{-3}
Mass of the char particle/kg	0.2×10^{-3} – 0.3×10^{-3}
Coal particle diameter/m	8.0×10^{-3} – 1.0×10^{-2}
Volumetric flow-rate/m ³ s ⁻¹	1.4×10^{-5} – 5.6×10^{-5}

rate was 2 °C min⁻¹ up to temperature of 100 °C. The mass loss after drying was approximately 10 %.

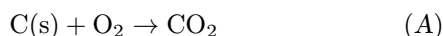
3. Devolatilization ensures the removal of volatile substances by heating to temperature of 800 °C in flowing nitrogen. The heating rate was 2 °C min⁻¹ and 5 °C min⁻¹ up to temperature of 500 °C and 800 °C, respectively. Volatile compounds represent 40 % of the original mass of the coal particle.

In order to obtain the information about the content of nonvolatile substances in the coal char particle, several thermogravimetric analyses were carried out. The mass changes of the particle within the temperature range of 100–800 °C were studied. The content of volatile substances in coal at 800 °C was about 4 %. It means that the effect of these substances on the combustion process of the degassed particle was negligible.

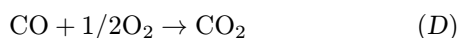
The coal char particle was kept in flowing nitrogen and/or argon stream and the inlet gas temperature was set at 530 °C. After switching the feed stream to the air stream, the particle started burning process itself. The experiment was completed when the mass of the particle remained constant.

THEORETICAL

Mathematical model of the coal char particle combustion is presented. The combustion process of a coal char particle can be described by the following heterogeneous reactions



and one homogeneous reaction



The model equations are derived under the following assumptions: shell progressive mechanism, non-isothermal conditions, constant pressure, constant pellet size during combustion, complete devolatilization of the coal particle at time equal to zero, and pseudo-

steady state for gas components [21].

The reaction rates for the reactions (A–C) are given by

$$\xi_{\text{S},j} = k_{j,\infty} \exp\left(-\frac{E_j}{RT}\right) C_{\text{s},i}^{a_j} C_{\text{s},k}^{b_j} \quad (1)$$

where ξ_{S} is the rate of reaction per unit area, k_{∞} is a frequency factor for j -th reaction, C is a concentration for i -th gas component and k -th solid component, a and b are the orders of j -th reaction. For the sake of simplicity, three components are supposed: oxygen ($i = 1$), CO₂ ($i = 2$), and CO ($i = 3$). The only solid component is carbon.

The reaction rate for gas-phase reaction (D) can be expressed as

$$\xi_{\text{g},D} = k_{D,\infty} \exp\left(-\frac{E_D}{RT}\right) C_{\text{g},1}^{a_D} C_{\text{g},3}^{b_D} \quad (2)$$

where the rate of reaction is expressed per unit area of the external surface of particle. The reaction orders (a , b) in eqns (1) and (2) are supposed to be equal to the stoichiometric coefficients of reactions (A–D).

The zone surrounding the particle is assumed to be perfectly mixed. The mass balance for gas components in the gas phase around the particle is given by the following dimensionless equation

$$Y_{\text{g},i}^{\circ} - St_{\text{g},i} \frac{(Y_{\text{g},i} - Y_{\text{s},i})}{\left[1 + Bi_{\text{m},i} \frac{1-\varphi}{\varphi}\right]} + \nu_{D,i} \Xi R_{\text{g},D} = Y_{\text{g},i} \Theta_{\text{g}} \quad (3)$$

where $Y_{\text{g},i}^{\circ}$ stands for the dimensionless inlet concentration of the gas component at reference temperature T_{g}° , Bi_{m} and St_{g} are the dimensionless parameters, $Y_{\text{g},i}$, $Y_{\text{s},i}$ are the dimensionless concentrations of the component in the gas and solid phase, Θ_{g} is a dimensionless temperature in the gas phase, and $\nu_{D,i}$ is a stoichiometric coefficient of i -th component for the (D) reaction.

The mass balance of gas components in the particle in the dimensionless form is given by

$$Y_{\text{g},i} - Y_{\text{s},i} = Da_i \left[1 + Bi_{\text{m},i} \frac{1-\varphi}{\varphi}\right] \varphi^2 \sum_{j=1}^J \nu_{j,i} p_j R_{\text{S},j} \quad (4)$$

where Da_i is a dimensionless parameter, φ is a dimensionless radius of the particle, and p_j is a dimensionless parameter.

The mass balance of the solid component in the dimensionless form can be expressed as

$$\frac{d\varphi}{d\tau} = \sigma Da_1 \sum_{j=1}^J \nu_{j,k} p_j R_{\text{S},j} \quad (5)$$

The initial condition for $\tau = 0$ is $\varphi = 1$.

The enthalpy balance for the single particle is given by

$$\Psi_s \varphi^2 \sum_{j=1}^J \beta_j p_j R_{S,j} = \frac{h_\lambda (1 + \varphi) (\Theta_\varphi - \Theta_p)}{\ln(1/\varphi^2)} \quad (6)$$

and

$$\frac{h_\lambda (1 + \varphi) (\Theta_\varphi - \Theta_p)}{\ln(1/\varphi^2)} = h_g (\Theta_p - \Theta_g) + h_e (\Theta_p^4 - \Theta_g^4) \quad (7)$$

where Ψ_s , h_g , h_e , h_λ , β are the dimensionless parameters.

The enthalpy balance for the gas around the particle is given by the following dimensionless equation

$$\begin{aligned} 1 + h_g (\Theta_p - \Theta_g) + h_e (\Theta_p^4 - \Theta_g^4) + \Psi_h R_{g,D} = \\ = \Omega \Theta_g^2 + h_w (\Theta_g - \Theta_w) \end{aligned} \quad (8)$$

where Ψ_h , h_w , Ω are the dimensionless parameters.

The effective diffusivity of gas in the solid, which is included in the parameter B_{i_m} in eqns (3) and (4), is approximated by the Fuller method for binary gas systems [22]. The mass-transfer coefficient for gas components, which is involved in the parameters Da , B_{i_m} , and St_g is estimated from the experimental results reported in [23].

The surface consumption rate of carbon from the experimental data is obtained by

$$(r_C)_S = - \frac{1}{S_P} \frac{dm}{dt} \quad (9)$$

where m is a mass of the coal particle and S_P is the reaction surface at time t expressed by the equation

$$S_P = 4\pi \left(R_p (1 - X(t))^{1/3} \right)^2 \quad (10)$$

where R_p is a radius of the particle and X is a carbon conversion at time t .

RESULTS AND DISCUSSION

The identification of the porous structure was performed using the principles of gas adsorption and mercury penetration. The porous structure of the original degassed particle and the partially combusted particle was estimated.

In order to obtain a partially combusted particle the feed stream was switched to nitrogen after desired combustion time and the experiment was stopped.

The results of our experiments showed that the specific surface area of the original coal particle was negligible. The devolatilization of the coal particle had an important influence on its porous structure. The removal of volatile organic compounds had an influence on the accessibility of the micropore region. The total porosity increased from 5 % to 10 %. During the combustion of a coal char particle, changes occurred, which were closely linked with the conditions of the process. Due to a slow progress of the reaction proceeding at a low initial combustion temperature (380–500 °C) and lack of oxygen, the inner surface of the particle was successively being opened. The porous

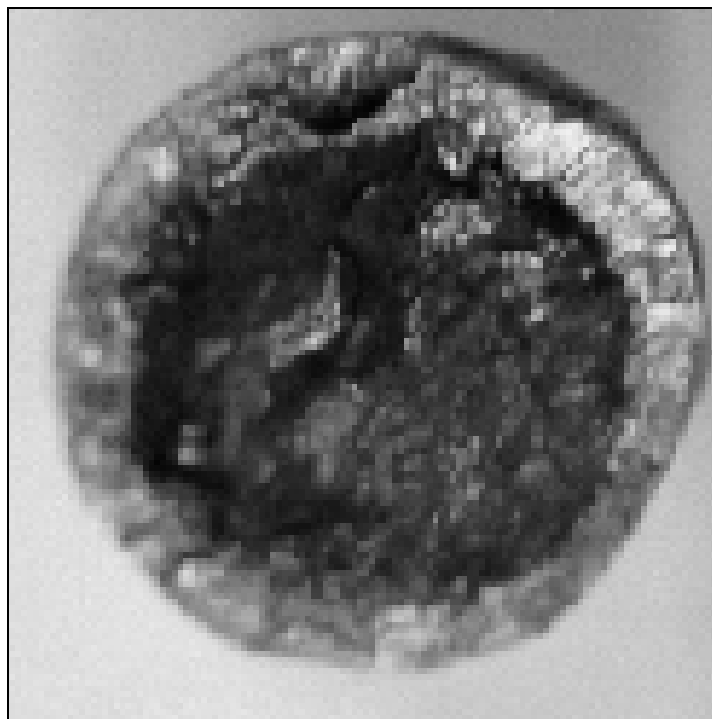


Fig. 2. The cross-section of a partially combusted particle.

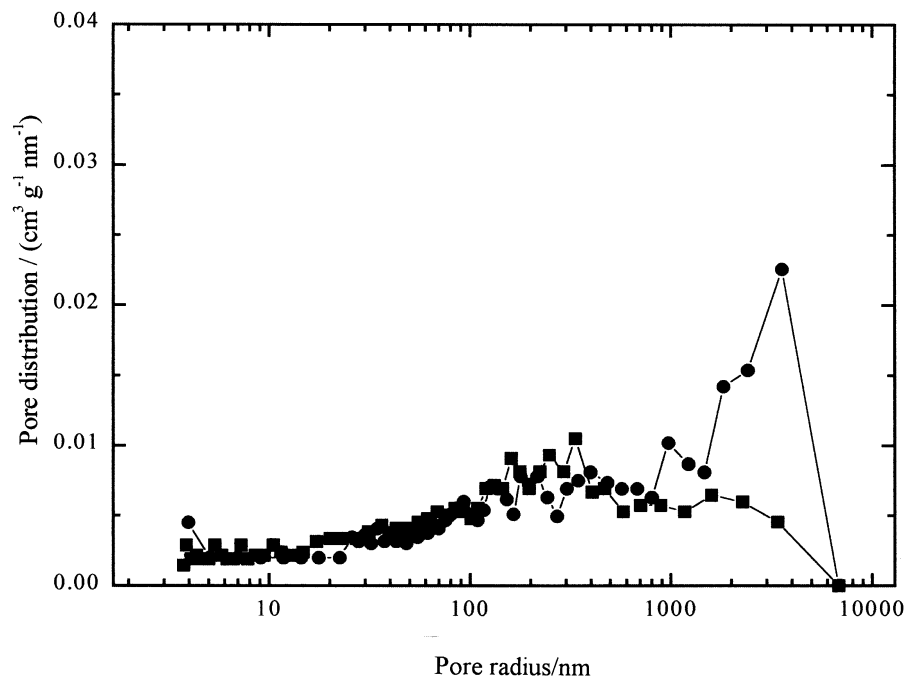


Fig. 3. Pore size distribution of partially combusted particles determined by mercury porosimetry. Inlet oxygen concentration: 10 mole %. Combustion temperature: ■ 460°C, ● 550°C.

structure of this particle was formed by pores with a diameter from 10 nm to 2000 nm. Thus, the inside of the particle became more accessible for the diffusion of both reactants and products. At a high initial combustion temperature (500–800°C) and oxygen concentration values, when the reaction proceeded faster, a significant ash shell was formed on the geometrical surface of the particle (Fig. 2). The thickness of this shell increased with time. Since the porosity of the ash was high (72 %), the access of reactants to the non-combusted core was not hindered. On the other hand, this layer was not sufficiently thermally conductive. This caused an overheating of the particle, which contributed to a faster course of the reaction proceeding by the shell mechanism. The structure of the core was predominantly formed by micropores. The dimension of these pores was a limiting factor of the diffusion inside the particle when the pores were inaccessible to the molecules of oxygen. This also supports the assumption of the shell mechanism of combustion. The pore size distributions of partially combusted particles at different temperatures are shown in Fig. 3.

Eqns (3), (4), and (6–8) represent a system of nonlinear equations which were solved for each integration step of the ordinary differential equation (5). Because this system of equations is a stiff one, Gears' method was used for its solution [24]. The model equations were solved for the mass of the coal char particle, temperature inside particle, temperature of the external particle surface, temperature of the gas and the combustion products, and the composition of gas com-

Table 2. Values of Optimized Parameters

Reaction	$E/(\text{kJ mol}^{-1})$	k_{∞}
(A)	140.5	$3.4 \times 10^2 \text{ m}^4 \text{ mol}^{-1} \text{ s}^{-1}$
(B)	143.0	$6.5 \times 10^5 \text{ m}^4 \text{ mol}^{-1} \text{ s}^{-1}$
(C)	100.0	$3.6 \times 10^7 \text{ m}^{2.5} \text{ mol}^{-0.5} \text{ s}^{-1}$
(D)	130.0	$5.0 \times 10^6 \text{ m}^{2.5} \text{ mol}^{-0.5} \text{ s}^{-1}$

E – activation energy, k_{∞} – frequency factor.

ponents at the sharp interface between the ash layer and the reaction surface.

The model kinetic parameters (activation energy E and frequency factor k_{∞}) have been obtained by an optimization procedure using experimental data sets for measurement conditions given in Table 1. The optimization procedure used a modified Levenberg–Marquardt method and an active set strategy to solve nonlinear least-squares problems subject to simple bounds on the variables [24]. For nonlinear least-squares problem the experimentally obtained mass of the coal particle and gas composition were used. The optimized kinetic parameters for reactions (A–D) are given in Table 2.

The surface rates of carbon consumption calculated from the experimental data and from the model are compared in Fig. 4. It is clear that the surface rate of carbon consumption increases with an increase in the partial pressure of oxygen. From the experimental results regression (Fig. 4) follows the fact that

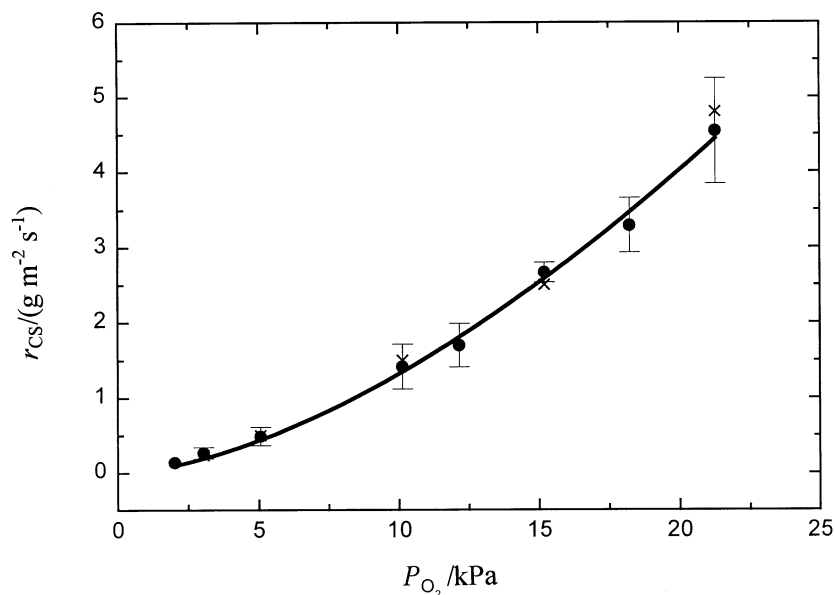


Fig. 4. Dependence of the surface consumption rate of carbon on the mole fraction of oxygen. ● Experimental data, × model and solid line – regression of experimental points.

the surface reaction rate can be expressed as $r_{CS} \approx k P_{O_2}^{1.7}$. Fig. 4 also shows a very good agreement between the surface rate calculated from experimental data and from the model. Furthermore, both the gas feed rate and the external mass transfer rate do not significantly affect the overall reaction rate.

Fig. 5 shows the experimental and computed time dependences of the temperature inside the particle and gas temperature around the particle. This figure confirms that the model is able to predict the temperature in the particle during the combustion process.

The experimental and theoretical concentrations of oxygen, CO₂, and CO during combustion are compared in Fig. 6. This figure shows that the presented model predicts oxygen and CO₂ concentrations satisfactorily. On the other hand, the theoretical concentration of CO is systematically higher than the experimental one and this prediction error varies from 30 % to 80 %.

Fig. 7 shows the experimental and computed dependences of the particle mass *vs.* combustion time. It follows from this figure that the computed particle mass, when all temperature values are calculated simultaneously, is in a good agreement with the experimental data.

For the comparison, the combustion process of the coal char particle, which was started up at a low combustion temperature, was observed. During the combustion process when the oxygen concentration was 4.8 mole % and the temperature of inlet gas was 460 °C, the oscillations of temperature inside the particle were observed (Fig. 8). From this figure it is clear that the combustion process is different from the combustion process started up at 530 °C. It was mentioned above that the combustion proceeded slowly at a low

initial combustion temperature and the inner surface of the particle was successively opened. The inside of the particle became more accessible for the diffusion of oxygen. From this it follows that the origin of this oscillation behaviour is in the transport limitation of oxygen through the particle. During the combustion, the surface rate and temperature increase very fast but, on the other hand, the transport of oxygen through the particle is very slow and it is not able to supply sufficiently the reaction surface. The rate of surface reaction and temperature decrease, then the oxygen concentration inside the particle increases and the particle is burnt again at the reaction surface.

CONCLUSION

The porous structure of the coal char particle during the combustion was closely linked with the condition of the process. The ash shell was not formed on the geometrical surface of the particle when the combustion process started up at a low combustion temperature (350–500 °C). During the combustion process started up at a high combustion temperature (500–800 °C), the particle consisted of two regions – the noncombusted core and the ash layer. The combustion did not cause changes in the pore distribution and porosity in the core of the partially combusted particle. Porosity of the ash layer indicates a low diffusional resistance for reactants. The obtained experimental results confirm that the presented shell progressive mechanism can be applied for the mathematical description of the combustion of a single coal char particle.

The model was found to describe the time functions of the decrease in the particle mass and tem-

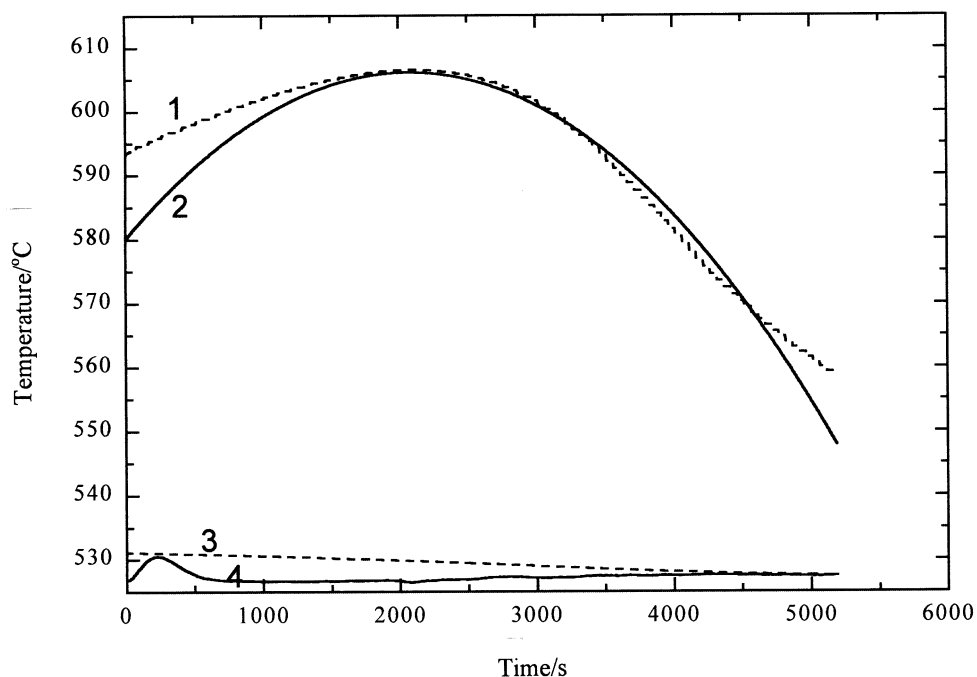


Fig. 5. Comparison of the experimentally obtained and calculated temperatures during the combustion at the inlet oxygen concentration of 4.8 mole %. Temperatures inside the particle: 1. model, 2. experimental. Temperatures around the particle: 3. model, 4. experimental.

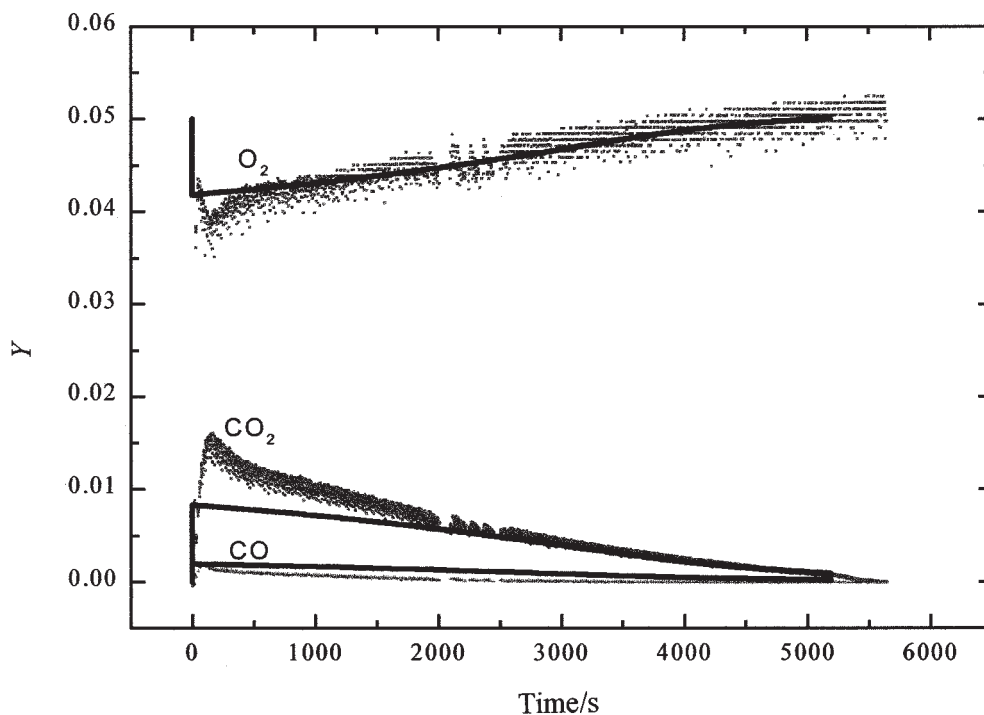


Fig. 6. Concentrations of oxygen, CO_2 , and CO in the outlet gas as a function of the combustion time at the inlet oxygen concentration of 4.8 mole %. Solid lines – model.

perature inside the particle and around the particle during the combustion very well. Furthermore, the model prediction of the combustion products is in a quantitative agreement with experimental observations.

On the other hand, during the combustion process started up at a low combustion temperature, the oscillations of temperature inside particle were observed. The origin of this oscillation behaviour is in transport limitations of oxygen through particle.

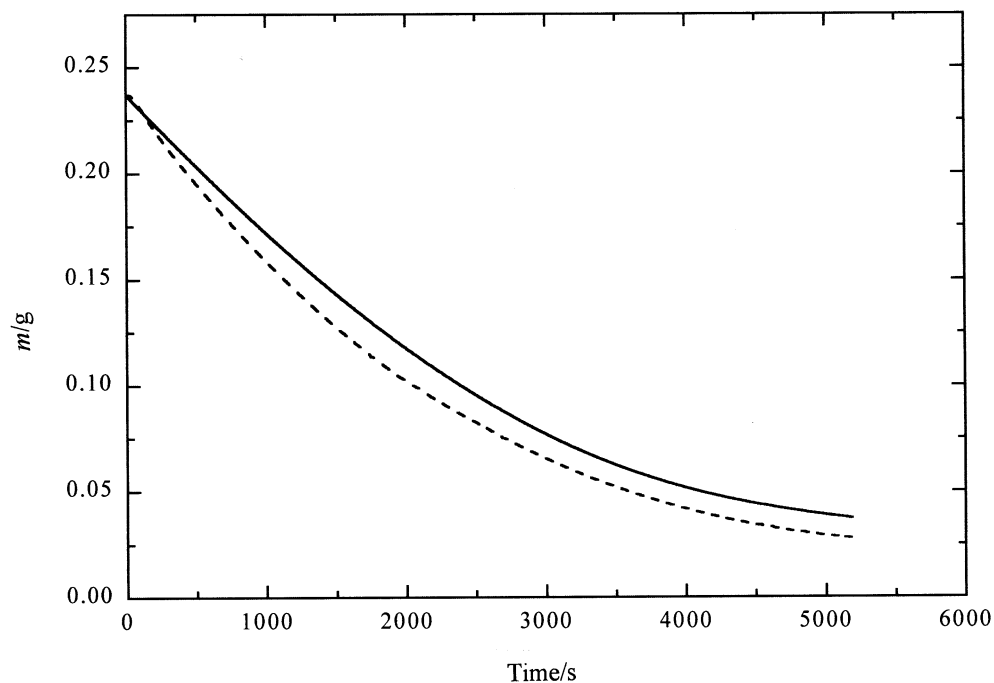


Fig. 7. Comparison of the experimentally obtained and calculated mass values of the coal particle during the combustion at the inlet oxygen concentration of 4.8 mole %. Solid line – experiment, dashed line – model.

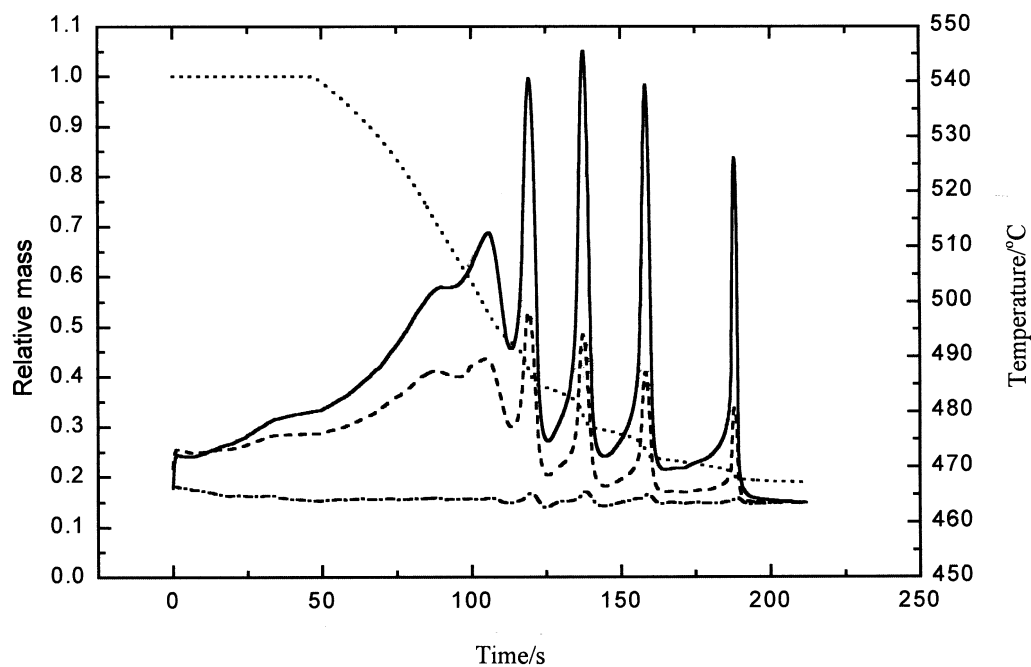


Fig. 8. Oscillation of temperature inside and outside the particle during the combustion at the inlet oxygen concentration of 4.8 mole % and at temperature of inlet gas 460°C. Solid line – temperature inside the particle, dashed line – temperature close to the particle surface, dashed dotted line – temperature outside the particle and dotted line – relative mass of the particle.

Acknowledgements. This work was supported by the Grant VEGA No. 1/7351/20 from the Slovak Scientific Grant Agency.

SYMBOLS

a, b	order of reaction		
C	concentration	mol m^{-3}	
A_r	surface area of reaction zone	m^2	
Bi_m	dimensionless parameter $k_g R_p / D_{s,i}$		
Da	dimensionless parameter $\xi_S^0 / C_g^0 k_g$		
D_s	effective diffusivity of gas in the solid	$\text{m}^2 \text{s}^{-1}$	

$c_{p,g}$	heat capacity	$\text{J kg}^{-1} \text{K}^{-1}$	i	index of the gas component
E	activation energy	J mol^{-1}	j	index of the reaction
ΔH	heat of reaction	J mol^{-1}	k	index of the solid component
k_∞	frequency factor, dimension is dependent on the type of equation		p	ash
k_g	mass-transfer coefficient	m s^{-1}	s	solid phase
m	mass of coal particle	g	S	reaction surface
h_g	dimensionless parameter $4\pi R_p^2 \alpha_g / \dot{V}^o \rho_g^o c_{p,g}^o$			
h_e	dimensionless parameter $4\pi R_p^2 \chi \varepsilon T_g^3 / \dot{V}^o \rho_g^o c_{p,g}^o$			
h_w	dimensionless parameter $A_r \alpha_w / \dot{V}^o \rho_g^o c_{p,g}^o$			
h_λ	dimensionless parameter $4\pi R_p^2 \lambda_p / \dot{V}^o \rho_g^o c_{p,g}^o$			
p_j	dimensionless parameter $\xi_{S,j}^o / \xi_{S,1}^o$			
R_p	radius of the particle	m		
R	gas constant	$\text{J mol}^{-1} \text{K}^{-1}$		
$R_{S,j}$	dimensionless reaction rate $\xi_{S,j} / \xi_{S,j}^o$			
R_g	dimensionless reaction rate $\xi_{g,4} / \xi_{g,4}^o$			
r_C	surface consumption rate	$\text{g m}^{-2} \text{s}^{-1}$		
T	temperature	K		
t	time	s		
V	volumetric flow of the gas phase	$\text{m}^3 \text{s}^{-1}$		
S_P	reaction surface	m^2		
St_g	dimensionless parameter $4\pi R_p^2 k_g / \dot{V}^o$			
w	linear velocity	m s^{-1}		
Y_i	dimensionless concentration in the gas phase C_i / C_g^o			
X	carbon conversion			

Greek Letters

ξ_S	reaction rate per unit area of the reaction surface	$\text{mol m}^{-2} \text{s}^{-1}$
$\xi_{g,D}$	reaction rate per unit area of the external surface of particle	$\text{mol m}^{-2} \text{s}^{-1}$
τ	dimensionless time $tk_{g,1}/R_p$	
α	heat transfer coefficient	$\text{W m}^{-2} \text{K}^{-1}$
λ_p	thermal conductivity of ash	$\text{W m}^{-1} \text{K}^{-1}$
ρ_g	gas density	kg m^{-3}
φ	dimensionless radius of the particle r/R_p	
ν	stoichiometric coefficient	
Θ	dimensionless temperature T/T_g^o	
Ξ	dimensionless parameter $4\pi R_p^2 \xi_g^o / C_g^o \dot{V}^o$	
σ	dimensionless parameter $C_g^o / C_{s,k}$	
ε	emissivity	
χ	Stefan—Boltzmann constant	$\text{J m}^{-2} \text{s}^{-1} \text{K}^{-4}$
Ω	dimensionless parameter $\rho_g c_{p,g} / \rho_g^o c_{p,g}^o$	
Ψ_s	dimensionless parameter $4\pi R_p^2 (-\Delta H_1) \xi_{S,1}^o / \dot{V}^o \rho_g^o c_{p,g}^o T_g^o$	
Ψ_h	dimensionless parameter $4\pi R_p^2 (-\Delta H_4) \xi_{g,4}^o / \dot{V}^o \rho_g^o c_{p,g}^o T_g^o$	

Superscripts

o state at reference temperature

Subscripts

g gas phase

REFERENCES

- Xu, C. R. and Fu, W. B., *Combust. Sci. Technol.* 124, 167 (1997).
- Fu, W. B. and Zheng, S. M., *Combust. Sci. Technol.* 118, 397 (1996).
- Sundaresan, S. and Amundson, N. R., *Ind. Eng. Chem. Fundam.* 19, 344 (1980).
- Sotirchos, S. V. and Amundson, N. R., *Ind. Eng. Chem. Fundam.* 23, 191 (1984).
- Fu, W. B., Zhang, B. L., and Zheng, S. M., *Combust. Flame* 109, 587 (1997).
- Caram, H. S. and Amundson, N. R., *Ind. Eng. Chem. Fundam.* 16, 171 (1977).
- Sundaresan, S. and Amundson, N. R., *Ind. Eng. Chem. Fundam.* 19, 351 (1980).
- Sotirchos, S. V. and Amundson, N. R., *Ind. Eng. Chem. Fundam.* 23, 180 (1984).
- Mon, E. and Amundson, N. R., *Ind. Eng. Chem. Fundam.* 17, 313 (1978).
- Libby, P. A. and Blake, T. R., *Combust. Flame* 36, 139 (1979).
- Mon, E. and Amundson, N. R., *Ind. Eng. Chem. Fundam.* 18, 162 (1979).
- Mon, E. and Amundson, N. R., *Ind. Eng. Chem. Fundam.* 19, 243 (1980).
- Sundaresan, S. and Amundson, N. R., *AIChE J.* 27, 679 (1981).
- Lee, J. C., Yetter, R. A., and Dryer, F. L., *Combust. Flame* 101, 387 (1995).
- Mantri, V. B., Gokarn, A. N., and Doraiswamy, L. K., *Chem. Eng. Sci.* 31, 779 (1976).
- Sotirchos, S. V. and Amundson, N. R., *AIChE J.* 30, 537 (1984).
- Sotirchos, S. V. and Amundson, N. R., *AIChE J.* 30, 549 (1984).
- Jelemenský, L., Remiarová, B., Žajdlík, R., and Markoš, J., *Petroleum and Coal* 41, 85 (1999).
- Beveridge, G. S. G. and Goldie, P. J., *Chem. Eng. Sci.* 23, 913 (1968).
- Bhatia, S. K. and Perlmutter, D. D., *AIChE J.* 26, 379 (1980).
- Froment, G. F. and Bischoff, K. B., *Chemical Reactor Analysis and Design*. Wiley & Sons, New York, 1989.
- Reid, R. C., Prausnitz, J. M., and Poling, B. E., *The Properties of Gases and Liquids*. Singapore McGraw-Hill, Singapore, 1989.
- Prince, W., *Ph.D. Thesis*. Universiteit Twente, Twente, The Netherlands, 1987.
- IMSL Math Library, Microsoft Developer Studio, Microsoft Corporation, 1995.