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Influence of FB Conditions on Processes  
Within a Large Fuel Particle During  
Initial Phases of Conversion

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## INFLUENCE OF FB CONDITIONS ON PROCESSES WITHIN A LARGE FUEL PARTICLE DURING INITIAL PHASES OF CONVERSION

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### ABSTRACT

A theoretical study has been performed in order to investigate the interaction between fluidized bed (FB) temperature and original size of coal, and the pressure rise within a large coal particle during the initial phases of the combustion process. A mathematical model, describing the devolatilization process, has included the internal and external heat transfer, primary decomposition reactions and mass transfer. The model has shown how the FB temperature and original size of coal reflect on the pressure profile of the coal particle during the devolatilization. One of the major consequences of coal devolatilization in the fluidized bed is the primary fragmentation; hence, the special attention has been paid to this process. On the basis of the devolatilization model results, a physical model of the primary fragmentation in FB is proposed.

### INTRODUCTION

The burning of a coal particle occurs in two consecutive phases: generation and combustion of volatiles and char oxidation. Combustion of volatiles generates up to 50% of the total coal combustion heat. Thus, an understanding of the devolatilization and consequent processes is of great importance for designing models of coal conversion. The model presented here is focused on transport processes within a volatile-rich coal particle, large enough to be non-isothermal.

Coal devolatilization is caused and accompanied by a number of physical and chemical phenomena. Particle heats-up by convection and radiation from the FB to the particle surface, and by heat conduction. Intraparticle temperature gradients cannot be neglected, because Biot number ( $Bi_c = r_c \alpha / \lambda_c$ ) of the coal particle is larger than  $\frac{1}{2}$  (its diameter exceeds 3 mm). Initially, the release of volatiles is mainly a physical transformation during which the particle dries, and trapped gases ( $\text{CO}_2$ ,  $\text{CH}_4$  and  $\text{C}_2\text{H}_6$ ) leave the particle. Once the particle reaches the temperature of  $200^\circ\text{C}$ , the chemical decomposition reactions start, and in the temperature range  $200\text{--}500^\circ\text{C}$ , emerging gases produce a pressure increase in the particle core (1). Due to the pressure gradient, a convective flow towards the particle surface arises.

Inside the particle, the concentration gradient causes diffusive mass transport, which can be molar and molecular, depending on the size of the pores. Having analyzed developed devolatilization models of various coals (2, 3, 4, 5, 6), the following facts have been distinguished, which should not be omitted in modeling:

- coal has a porous structure,
- internal heat transfer is the rate controlling process,
- in the pressure rise calculation both Knudsen (prevails in the micropores) and molar (prevails in the macropores) diffusion should be taken into account,
- the generation and transport processes depend on the coal size, coal thermal properties, FB temperature, chemical reactions parameters and the porosity of the coal.

One of the major consequences of coal devolatilization in FB is primary fragmentation - coal particle breakage during devolatilization. This process exerts influence on volatile release, as well as on the combustion process, the char combustion rate and particle emission (7). An insight into the fragmentation, its causes and mechanism, enables more accurate predictions of changes in particle size distribution. The comminution causes axial and radial particle segregation, which influences the bed dynamics and heat transfer in the bed (8, 9). The change of particle size distribution should be taken into account in heat calculation (heat released in bed and freeboard), as well as the utility design (choice of circulation and separation systems).

Factors influencing fragmentation, identified and discussed before (10, 11, 12) are: the original size of coal, the bed temperature, the particle residence time, the volatile matter content, the coal hardness, the fluidizing medium, the diameter of convective pores, the volatile viscosity. Factors less effective on coal breakage during devolatilization are: the chemical kinetics, the coal thermal diffusivity and the bed heat transfer coefficient.

In order to design a mathematical model to predict the primary fragmentation, a mechanism of the phenomenon should be explained. Here, the devolatilization model has been used in attempt to establish a primary fragmentation physical model, and to test it on factors marked as the most significant ones (original size of coal and FB temperature).

## MODEL

The model structure is linear, and it consists of submodels for heat transfer, chemical reactions and mass transfer. The general assumptions are: the coal particle is a homogenous porous sphere with constant diameter (there is no swelling or primary fragmentation), the environment pressure is atmospheric, and the coal particle is at the ambient temperature before being introduced into the FB. Processes of devolatilization and char combustion are completely separate, which is justifiable for large coal particles on FB temperatures lower than 1150°C (13). For numerical purposes (to keep the constant density), the spherical coal particle has been divided into the numerous concentric layers of the same volume.

It has been assumed that the devolatilization is a thermally neutral process, and that there is no thermal influence of the volatiles combusting in the particle surroundings. Although the thermal diffusivity of coal actually increases during the process (14, 15), in the case of models which neglect the reaction heat, better agreement with

experimental results has been accomplished assuming the thermal properties of coal are constant (15, 16).

Heat balance, which determines the temperature along the radius of the coal particle, is described by the following partial differential equation:

$$\frac{\partial}{\partial \tau} [\rho_c c_c T(r, \tau)] = \frac{1}{r^2} \frac{\partial}{\partial r} \left[ r^2 \lambda_c \frac{\partial T(r, \tau)}{\partial r} \right],$$

with constant initial temperature:

$$T(r, 0) = T_0,$$

and boundary condition:

$$\alpha A [T_b - T(r_c, \tau)] = \lambda_c \left( \frac{\partial T(r, \tau)}{\partial r} \right) \Big|_{r=r_c}.$$

Convective heat transfer coefficient between the coal particle surface and the fluidized bed is described by the correlation obtained on the basis of prior experimental investigations (17).

Chemical reactions have been described by the distributed activation energy model. Each reaction is described by a first order equation, where the reaction rate is defined by Arrhenius law:

$$\frac{dVM_i(r, \tau)}{d\tau} = k [VM_i^* - VM_i(r, \tau)].$$

Chemical reactions submodel gives the amount of released volatiles and the rate of devolatilization:

$$VM(r, \tau) = VM^* \left\{ 1 - \int_0^\tau \exp \left[ - \int_0^\tau k(E) d\tau \right] \left[ \sigma (2\pi)^{1/2} \right]^{-1} \exp \left[ - \frac{(E - E_0)^2}{2\sigma^2} \right] dE \right\},$$

$$\Gamma(r, \tau) = \frac{\partial VM(r, \tau)}{\partial \tau}.$$

Devolatilization process implies release of great volume of gaseous components, followed by pressure and concentration gradients within the particle. Depending on the process nature and pore size, three mechanisms of mass transfer are possible in a porous coal particle: convective transfer, molar and Knudsen diffusion. If the process is assumed to be pseudo-steady, the mass balance of volatiles is:

$$\frac{1}{r^2} \frac{\partial}{\partial r} (r^2 N) = \rho_o \Gamma.$$

The mass flux of the released volatiles is:

$$N = - \frac{M}{R_g T} \frac{1}{r^2} \left( D_{eff} + \frac{\beta o P}{\mu} \right) \left( \frac{\partial (r^2 P)}{\partial r} \right).$$

Integration with the boundary condition  $P(r_c, \tau) = P_0$  gives the pressure profile as a function of radial position and time.

## RESULTS AND DISCUSSION

In order to validate the model, temperature histories of coal particle centers are given

for different particle sizes (Fig. 1) and for different FB temperatures (Fig. 2). As expected, heating rates are higher for smaller particles (Fig. 1) and heating rate increases in hotter fluidized bed (Fig. 2). Also, the devolatilization time (time needed for releasing 95% of total volatile amount) increases with the diameter of the coal particle. It has been shown that variation in bed temperature has only a small effect on devolatilization times.

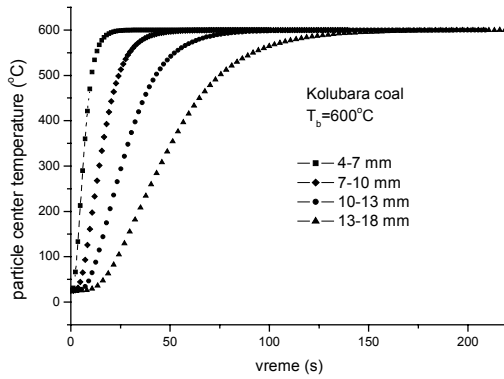


Figure 1. Temperature histories of the coal particle center for different particle size classes, the model results

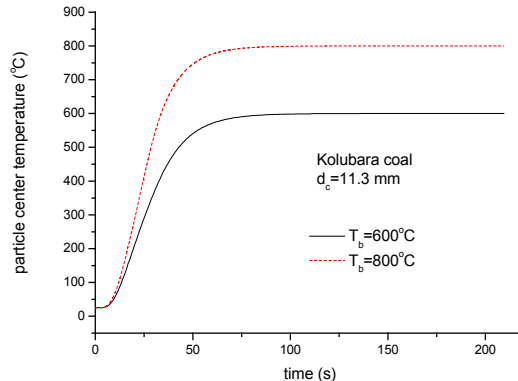


Figure 2. Temperature histories of the coal particle center on different FB temperatures, the model results

The results of the mass transfer submodel have shown how the volatile pressure changes depending on the radial position (Fig. 3) and time (Fig. 4). It can be seen that volatile pressure reaches the highest values in the center of the particle (Fig 3), and shortly after its introduction into the fluidized bed (Fig. 4). It is important to note that these pressure values are not real, because the change in porosity has not been taken into account (porosity increases during the process and pore size distribution changes). These values are used only as an indicator of the pressure rise trend.

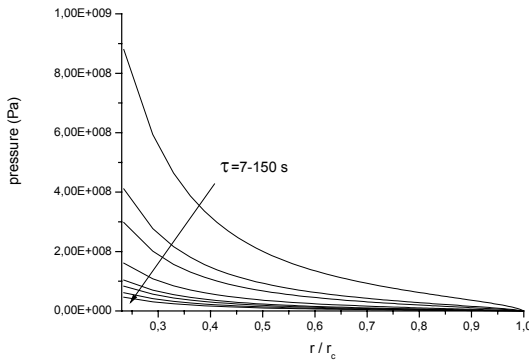


Figure 3. Pressure of released volatiles in the coal particle ( $d_c=5,7$  mm,  $T_b=700^\circ\text{C}$ ), depending on radial position, the model results

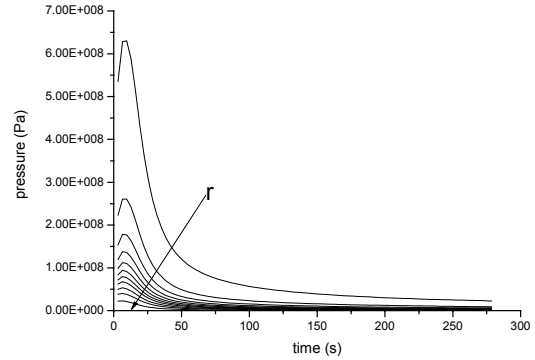


Figure 4. Pressure of released volatiles in the coal particle ( $d_c=5,7$  mm,  $T_b=700^\circ\text{C}$ ), depending on time, the model results

It might be concluded that initial crack develops in the center of the particle, which is the first point where applied forces of released volatiles become equal to the resultant of the coal resistance forces.

From previous investigations (10, 11, 15) FB temperature and original size of coal could be distinguished as factors of unambiguous influence on primary fragmentation process – it is more intense for larger particles and those at higher bed temperatures. There are a lot of dissonances about the relevance of other factors such as: total volatile amount, coal porosity, volatile viscosity, fluidization ratio, type of inert FB material, etc. This is the reason why the FB temperature and the size of coal have been selected to test the primary fragmentation physical model presented here.

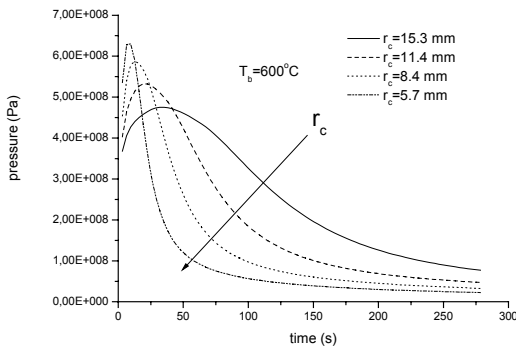


Figure 5. Pressure maximum of released volatiles for different particle size classes, the model results

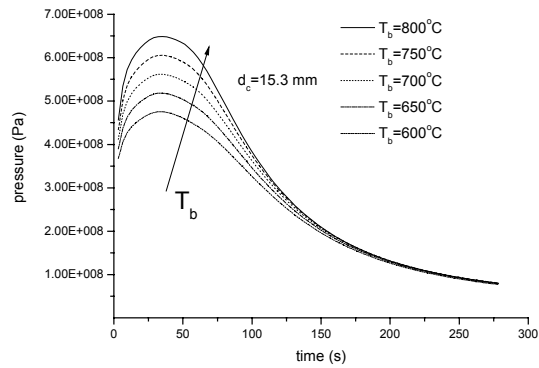


Figure 6. Pressure maximum of released volatiles for different FB temperatures, the model results

In Figure 5, the calculated change of the pressure of released volatiles in the center of particles, for different original coal particle size classes, is presented. Pressure in the center of smaller particles reaches higher values within a shorter period. The initial crack, appearing in the center of the smaller particle expands to the particle surface, which leads to pressure decrease, and, consequently, the particle does not break. This is in accordance with the hypothesis of critical diameter - the size of the particle is sufficiently small not to fragment (10). In the case of a larger particle, maximum pressure, in the center, does not have such a high value, but it decreases more slowly. The initial crack from the center meets with other cracks, developed in the particle periphery, and the particle fragments.

Figure 6 shows the computed change of released volatiles' pressure in the center of particles, for different FB temperatures. It has been shown before, that the primary fragmentation process is more intensive for higher FB temperatures. From the figure it is evident that particles at higher FB temperatures have higher pressures in the center.

**CONCLUSION**

A mathematical model of the devolatilization process has been developed. The model structure is linear, and it consists of submodels for heat transfer (internal and external), chemical reactions (multiple independent parallel first order model) and mass transfer (volatile convective flow, molar and Knudsen diffusion). It has been designed for low-rank volatile-rich coals.

A physical model of the primary devolatilization process has been proposed. It is assumed that the main cause of coal particle breakage is the pressure increase of

releasing volatiles. The initial crack appears in the center of the particle and expands towards the surface. If the particle diameter is larger than critical, the initial crack joins other cracks, developed in the meantime, and particle fragmentation occurs. In the case of particles with diameter smaller or equal to the critical, the crack grows out to the surface and the pressure decreases. One more experimentally proved effect has been explained: particles at higher FB temperatures fragmentate more intensively because of higher pressure in their center.

## NOTATION

$Bi_c$	Biot number $Bi_c = r_c \alpha / \lambda_c$	[-]
$c_c$	specific heat of coal	[J/kgK]
$d_c$	original diameter of coal particle	[m]
$D_{eff}$	effective diffusivity	[m <sup>2</sup> /s]
$E$	activation energy	[J/mol]
$E_o$	mean value of activation energy	[J/mol]
$k$	reaction rate	[s <sup>-1</sup> ]
$N$	mass flux	[kg/m <sup>2</sup> s]
$M$	molar mass of volatiles	[kg/mol]
$P$	pressure	[Pa]
$r$	radius, radial position	[m]
$r_c$	original radius of coal particle	[m]
$R_g$	gas constant	[J/molK]
$T$	temperature	[K]
$VM$	released volatiles in a particle segment as a function of time $\tau$	[kg/kg coal or %]
$VM^*$	released volatiles in a particle segment when $\tau \rightarrow \infty$	[kg/kg coal or %]
$u$	flow velocity	[m/s]

## Greek letters

$\alpha$	heat transfer coefficient	[W/m <sup>2</sup> K]
$\beta_o$	viscous permeability	[m <sup>2</sup> ]
$\varepsilon$	porosity	[%]
$\Gamma$	rate of volatile release	[1/s]
$\lambda_c$	thermal conductivity of coal	[W/mK]
$\mu$	viscosity of volatiles	[Pas]
$\rho$	density	[kg/m <sup>3</sup> ]
$\tau$	time	[s]

## Subscripts

$b$	fluidized bed
$c$	coal
$i$	volatile species
$o$	ambient

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