Acta Geodyn. Geomater.Vol.1, No.2 (134), 261-274, 2004

MODELLING OF EFFECTS OF OPERATING CONDITIONS AND COAL REACTIVITY ON TEMPERATURE OF BURNING PARTICLES IN FLUIDIZED BED COMBUSTION

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(*Received* December 2003, *accepted* February 2004)

ABSTRACT
Two simplified models for estimation of temperatures of smaller, low ash char particles and bigger high ash char particles burning in fluidized bed (FB) have been formulated and solved in our study. For smaller, low ash char particles constant temperature across char particles was assumed. In the case of bigger, high ash char particles with reaction zone moving from surface to the inner part of the char radial profile of temperature within the particles was considered. Results of the model solutions have shown, that the temperature of burning char particles increases significantly with increasing oxygen concentration in flue gas, with increasing operating pressure, decreasing char particle size and increasing reactivity/porosity of the char. The temperature difference between burning char temperature and FB temperature can attain values between 40 and 150 ^{o}C for atmospheric conditions and values between 200 and 500 ^{o}C for pressurized FB combustion. Solution of the model for temperature of bigger, high ash char particles revealed, that under specific conditions (e.g. lower operating pressure, low thermal conductivity of porous, surface ash layer, low resistance in ash layer for oxygen diffusion) the temperature within the burning char particle, on the reaction sphere, can be even higher than the temperature in the stage of surface char burning.
Theoretical estimates of temperatures of burning char particles are important for forecasting and avoiding ash particle agglomeration in FB combustion and in modeling of emissions.

KEYWORDS: modelling, char temperature, fluidized bed combustion

1. INTRODUCTION

Temperature of burning solid fuel particles (e.g. coal and biomass) in fluidized bed (FB) is higher than the measured average „bulk“ temperature of FB. This fact is necessary to respect in modelling of FB combustion processes (Hannes J., 1996, Saastomoinen et al., 1996, Svoboda et al., 1999) agglomeration phenomena in FB (Kobylecki R. et al., 2003, Kouki et al., 2003) formation and reduction of gaseous emissions (Lin W. 1994, Braun A., 1998) mainly NO_x N_2O CO etc.

Temperature difference between temperature of a burning solid fuel particle and average measured temperature of a fluidized bed (consisting of inert ash particles and burning fuel particles) depends on major number of factors (Joutsenoja et al. 1999). The most important factors influencing this temperature difference are: concentration of oxygen in flue gas, temperature of fluidized bed, operating (overall) pressure, fuel reactivity, particle size of solid fuel and fluidized bed particles, ash content and composition of solid fuels and others. Difference of temperatures between burning particles and "bulk" temperature of fluidized bed can reach under atmospheric combustion conditions (0.1 MPa) even several hundreds ^{o}C at higher concentrations of oxygen in gas phase. As a result of intensive mixing of particles in fluidized bed, the heat transfer within a fluidized bed (i.e. output of heat energy from burning particles) is relatively high. In a case of entrainment of small burning particles from dense fluidized bed to the region above the fluidized bed (so called "freeboard"), the temperature of the char particles elevates as consequence of lower heat transfer from the particles to the surroundings. This means, that in the region above the dense fluidized bed the temperature difference elevates and particularly for small burning coal particles with small difference between gas and coal/char particle velocity the difference can reach under pressurized conditions (0.3 – 0.8 MPa) even values over 600 ^{o}C (Saastomoinen et al., 1996).

Exact modeling of temperatures of burning particles is very difficult, because direct, precise measurement of surface temperature and determination of parameters of burning solid fuel particles in FB are practically infeasible and because of non-existence of exact correlations for such important parameters as e.g. surface molar CO/CO_2 ratio in burning of different coal and biomass particles in fluidized bed in a broad range of conditions. As well correlations for heat transfer by convection and radiation in FB for a broader range of particle size are only approximate or intended for a limited range of conditions (e.g. only for small particles or only for bigger particles above 1 mm). Reaction order of oxidation/combustion related to oxygen is considered (for simplicity) to be equal one. Parameters of heat and mass transfer in fluidized bed depend on particle properties, regime of fluidization existence appearance size and frequency of gas bubbles in FB etc.

In this study we prefer simplified approach and relatively simple correlations (Hannes J., 1996, Lin W., 1994) based on a simple thermal balance and steady state conditions.

Two basic theoretical models are considered for char combustion in FB: one for smaller, low ash particles with supposed uniform temperature across the particle and another one for relatively bigger, high ash char particles with different temperature at the surface and inside particles.

Three basic kinds of coals (chars) are considered: smaller particles (below 1.0 mm) of more and less reactive low ash coals and bigger, high ash coal particles (above 1.1 mm) corresponding to model situation of burning char particles with different temperatures on the surface and inside char particle. For solution of the simplified models table sheet calculator in the frame of Excel was used.

2. THEORETICAL MODEL FOR SMALLER BURNING CHAR PARTICLES WITH SUPPOSED UNIFORM TEMPERATURE ACROSS THE CHAR PARTICLE

The model for estimation of temperature of burning coal/char particle is based on heat balance. For simplicity we consider only burning of char without volatiles under steady state conditions. This assumption is near the realistic situation in burning of reactive coals (Svoboda et al., 1999).

Under steady state conditions the heat generated by char burning is equal to the heat transferred to surroundings:

$$Q_{gen} = Q_{tr} \quad (2.1)$$

where Q_{gen} is the heat generated by burning of a char particle and Q_{tr} is the heat transferred to surroundings (to the fluidized bed).

Heat generation rate $\boldsymbol{Q}_{\mathrm{gen}}$ in char combustion can be expressed as:

$$\boldsymbol{Q}_{\mathrm{gen}} = r_{\mathrm{char}}\ \Delta H_C \quad (2.2)$$

(in W, kW or kW/m^3 of solid fuel).

where r_{char} is reaction rate of carbon burning (e.g. mol/s or mol/(s*m^3 fuel)) and ΔH_C is reaction enthalpy related with burning of char particle, generally resulting in formation of CO and CO_2 mixture (in J/mol or kJ/mol).

Burning of carbon generally leads to formation of CO and CO_2 according to the equation:

$$C + (1/\Phi)\, O_2 \rightarrow (2 - 2/\Phi)\, CO + (2/\Phi - 1)\, CO_2 \quad (2.3)$$

where parameter $\Phi = n_C/n_{O2}$ (ratio of reacting moles of carbon and oxygen). For combustion process leading to pure CO_2 $\Phi = 1$ and for formation of pure CO $\Phi = 2$.

Parameter Φ is related to parameter $\Phi_C = n_{CO2}/n_{CO}$ (ratio of CO_2 moles and CO moles):

$$\Phi = n_C/n_{O2} = n_C/(0.5n_{CO} + n_{CO2}) = (2 + 2\Phi_C)/(1+ 2\Phi_C) \quad (2.4)$$

Parameter Φ_C is function of combustion temperature, oxygen concentration, char size, char reactivity and catalysis by ash components (Tognotti et al., 1990, Hannes J.1996). According to Tognotti et al., 1990, the dependence of Φ_C on temperature and oxygen concentration can be expressed by the following equation for common coal char at atmospheric pressure:

$$\Phi_C = 0.02027\, (P_{O2})^{0.21} \exp(3000/T) \quad (2.5)$$

where P_{O2} is partial pressure of oxygen (in bar) and T is absolute temperature in K.

Dependence of parameter Φ on char particle size is supposed for particle diameters d_p in a range: d_p = 0.1 – 1.1 mm (Hannes J., 1996). For bigger char particles Φ is supposed to be 1.

The correction on char particle size has a form:

$$\Phi_p = (2 + 2\Phi_C - (d_p - 0.05)/(1 + \Phi_C))/(1+ 2\Phi_C) \quad (2.6)$$

where Φ_p is the corrected parameter Φ and d_p is diameter of burning char particles in mm for the supposed size range 0.1 – 1.1 mm.

The enthalpy ΔH_C related with combustion of char carbon to a mixture of CO and CO_2 is given by equation:

$$\Delta H_C = (2 - 2/\Phi_p) \cdot 112 + (2/\Phi_p - 1)\cdot 395 \text{ (kJ/mol)} \quad (2.7)$$

where the reaction enthalpy for combustion of carbon to CO is 112 kJ/mol and for CO_2 formation 395 kJ/mol. The ΔH values for CO and CO_2 formation (112 and 395 kJ/mol) are assumed to be independent on reaction temperature.

MODEL FOR BURNING OF SMALLER CHAR PARTICLES

The model is based on assumption of shrinking spherical carbon particle with surface heterogeneous reaction and gaseous film in surroundings of the carbon (char) particles (Hannes J., 1996, Svoboda et al., 1999). The model situation is near the real situation of burning of smaller char particles of low ash coals at not too high temperatures and pressures. For combustion rate r_{char} of char/carbon particle the following equation is assumed:

$$r_{char} = (6/d_p)\, k_{rea}\ (P/\boldsymbol{R}\, T_g)\, (X_{O2}sur)^n \quad (2.8)$$

where $\boldsymbol{R}$ is universal ideal gas constant (8.314 Jmol^{-1} K^{-1}), P is overall pressure (Pa), T_g is the characteristic temperature in gas phase (K), k_{rea} is kinetic reaction rate constant (m/s), $X_{O2}sur$ is molar concentration of oxygen ($X_{O2}sur = n_{O2}/\Sigma n_{gases}$) at the surface of burning particles, n is reaction order (assumed to be equal one) and r_{char} is combustion rate of carbon/char related to volume unit of char (mol m^{-3} s^{-1}).

Diffusion of oxygen from the fluidized bed to the surface of burning char particles is described by equation:

$$r_{char} / \Phi_p = (6/d_p)\, k_{diff}\, (P/\boldsymbol{R}\, T_g)\, (X_{O2}b - X_{O2}sur) \quad (2.9)$$

where k_{diff} is diffusion coefficient of oxygen in gaseous film (m/s), $X_{O2}b$ is molar concentration of oxygen in "bulk" of fluidized bed (equal to molar concentration of oxygen in flue gas).

If both, the chemical reaction of heterogeneous char burning and diffusion of oxygen through the gaseous film are important, the following equation can be derived:

$$r_{char} = (6/d_p)\, k_{char}\, (P/\boldsymbol{R}\, T_g)\, (X_{O2}b)^{1} \quad (2.10)$$

where

$$k_{char} = 1/(1/k_{rea} + 1/(k_{diff}\, \boldsymbol{\Phi_p})) \quad (2.11)$$

For temperature T_g in gaseous film the following simple equation was (as usually) adopted:

$$T_g = (T_p + T_{fl})/2 \quad (2.12)$$

Where T_g is the mean temperature in gaseous film around burning char particles, T_p is temperature of reacting-burning char particle and T_{fl} is the measured "bulk" temperature of fluidized bed.

$$k_{rea}\ (m/s) = \mathbf{A}\, \exp(-E_a/(\boldsymbol{R} T_p)) \quad (2.13)$$

A is the pre-exponential factor (for common coals **A** is assumed to be approximately 600 - 900 m/s) and E_a is activation energy ($E_a/\boldsymbol{R}$ for common more reactive coals is assumed usually between 8000 and 10000 K). In our modeling we have arbitrarily chosen the following values for A and $E_a/\boldsymbol{R}$: For "less" reactive (usual) sub-bituminous coals the values **A** = 800 m/s $E_a/\boldsymbol{R}$ = 10 000 K have been chosen. For very reactive lignite coals the values **A** = 800 m/s and $E_a/\boldsymbol{R}$ = 8000 K have been considered.

The following equations are supposed for estimation of k_{diff} :

$$k_{diff} = Sh\ D/d_p \quad (2.14)$$

$$Sh = 2\, \varepsilon_g + 0.69\, Sc^{0.33}\, Re^{0.5} \quad (2.15)$$

where Sh, Sc, Re are respectively Sherwood, Schmidt and Reynolds number, ε_g is volume fraction of gas in fluidized bed (according to regime of fluidization the ε_g values can be supposed between 0.55 – 0.65). The Sh, Sc and Re numbers are defined:

$$Sc = \mu_g / (Ro_g\ D_g) \quad Re = v_g\ d_p\, Ro_g / \mu_g$$
$$Sh = k_{diff}\ d_p / D_g \quad (2.16)$$

where D_g is diffusivity of gaseous reagent - oxygen (m^2/s), Ro_g is flue gas density, μ_g is flue gas viscosity and v_g is linear gas velocity in fluidized bed.

For estimation of D_g the correlation derived by Verweyen N. 1993 is employed:

$$D_g = D_{g0} * (T/T_0)^{1.64}\ P_0/P \quad (2.17)$$

where the values with index 0 are: T_0 = 298 K, P_0=1.013 bar, D_{g0} = 2.21*10^{-5} m^2/s.

The equations used for computation (estimation) of flue gas viscosity μ_g flue gas density Ro_g, thermal conductivity of flue gas λ_g and specific heat C_p of flue gas are summarized in **Table I**.

In all applications of the relations given in **Table I,** assumption of independence of viscosity, thermal conductivity and thermal capacity of flue gas on operating pressure was used. The dependence of flue gas density on operating pressure and temperature was considered the same as for ideal gas. For estimation of gas temperature T_g in computations of flue gas properties arithmetic average values according to eq. (2.12) have been accepted. Overall heat generation rate $\boldsymbol{Q}_{gen}$ by char burning is then computed:

$\boldsymbol{Q_{gen}}$ = ΔH_C (from eg. 2.7) r_{char} (from eq. 2.10) (kW/m^3 char) (2.18)

HEAT TRANSFER (COOLING) RATE OF BURNING CHAR PARTICLES

For bigger char particles (above approx. 1 mm) a correlation for Nu – number is supposed (Hannes J., 1996):

$$Nu_1 = 3539*(d_p/d_{av})^{0.257} \cdot Ar^{0.105\ ET} \cdot$$
$$\cdot\, (0.844 + 0.0756\ T_{fl} / 298) \quad (2.19)$$

where Ar is Archimedes number, ET = $(d_p/d_{av})^{0.082}$,d_p is diameter of burning char particles and d_{av} is average (mean) diameter of particles in fluidized bed (so called Sauter diameter).

$$Ar = g \cdot (d_{av})^3\, Ro_s\, Ro_g / (\mu_g)^2 \quad (2.20)$$

g is acceleration due to gravity, Ro_s is density of solid particles in fluidized bed.

For smaller particles (usually below 0.5 mm) Nusselt number is composed of two members for heat transfer by convection and radiation (Hannes J. 1996):

$$Nu_2 = Nu_{conv} + Nu_{rad} \quad (2.21)$$

$$Nu_{conv} = 2 + 0.69\, Re^{0.5}\, Pr^{0.33} \quad (2.22)$$

$$Pr = \mu_g\, C_p/\lambda_g \quad (2.23)$$

(Prandtl number)

where μ_g is viscosity of flue gas (Ns/m^2) C_p is specific heat of flue gas (J$kg^{-1}deg^{-1}$) and λ_g is thermal conductivity of flue gas (W$m^{-1}deg^{-1}$).

$$Nu_{rad} = \boldsymbol{\sigma}\, \boldsymbol{\epsilon}\, [(T_p)^4 - (T_{fl})^4]\, d_p/T_p - T_{fl)}\, \lambda_g) \quad (2.24)$$

where $\boldsymbol{\sigma}$ is Stefan Boltzman constant =5.67 10^{-8} Wm^{-2} K^{-1}, $\boldsymbol{\epsilon}$ is emissivity of burning char particles

Table 1 Equation used for estimation of properties (viscosity, density, thermal capacity and thermal conductivity) of flue gas.

Property	Validity for temperatures T_g = 700 - 1150 °C
Density of flue gas Ro_g (kg/m^3)	$Ro_g = P M_{fg} /(\boldsymbol{R}\, T)$ where $M_{fg} \approx 29$
Viscosity of flue gas μ_g (Pas)	$(4.4610^{-5}/1.04) \cdot (T/1073.15)^{0.66}$
Thermal conductivity of flue gas λ_g (Wm^{-1}K^{-1})	$1.04 \cdot 0.062 + 0.0143 \cdot (T - 900)/300$
Specific heat of flue gas C_p (Jkg^{-1}deg^{-1})	$1180 + 0.2 \cdot (T – 973.15)$

(considered ϵ = 0.85) and d_p (m) is diameter of burning char particle.

Coefficient of heat transfer α_p is computed from Nu_2 :

$$\alpha_p = Nu_2 \lambda_g / d_{av} \quad (2.25)$$

To avoid discontinuities in estimation of Nu – numbers for particles in a broader size range the following correlation was introduced for Nusselt numbers Nu :

$$Nu = Nu_1 d_p/(d_p + d_{av}) + Nu_2 d_{av}/(d_p + d_{av}) \quad (2.26)$$

The mean Nu-number for usual particle size range (0.5 – 1 mm) can be roughly approximated by equation:

$$Nu = (Nu_1 + Nu_2)/2 \quad (2.27)$$

Coefficient of heat transfer α_p from burning char particles to the fluidized bed is calculated with either eq. (2.26) or eq. (2.27) :

$$\alpha_p = Nu \lambda_g /d_{av} \quad (Wm^{-2}K^{-1}) \quad (2.28)$$

Heat transfer (cooling) rate $\boldsymbol{Q_{tr}}$ is computed from equation:

$$\boldsymbol{Q_{tr}} = \alpha_p (T_p - T_{fl})(6/d_p) \quad (W\ m^{-3}\ char) \quad (2.29)$$

PROCESS OF COMPUTATION OF BURNING CHAR PARTICLE TEMPERATURE

The temperature of fluidized bed T_{fl} is chosen and first approximation of temperature of burning char particles (T_p) higher than the temperature of fluidized bed. The temperature difference is estimated according to overall conditions (e.g. 10 – 150 K).

For given temperatures T_p and T_{fl} and operating pressure the parameters of flue gas (with temperature $T_g = (T_p + T_{fl})/2$) are computed. With considered char fluidized bed particle properties and gas properties the relevant Re Sh Sc Pr Nu numbers gas diffusivities relevant parameters coefficients and char burning reaction rate the values for $\boldsymbol{Q_{gen}}$ and $\boldsymbol{Q_{tr}}$ are computed and compared.

If the cooling rate $\boldsymbol{Q_{tr}}$ is lower than $\boldsymbol{Q_{gen}}$ the temperature of burning char particles is elevated and again the values $\boldsymbol{Q_{tr}}$ and $\boldsymbol{Q_{gen}}$ are compared. This procedure is repeated until $\boldsymbol{Q_{tr}} = \boldsymbol{Q_{gen}}$ within a given (supposed) uncertainty (e.g. 1 K or 0.5 % $\boldsymbol{Q_{gen}}$).

The increase of $\boldsymbol{Q_{tr}}$ with increasing T_p is normally higher than increase of $\boldsymbol{Q_{gen}}$.

For char particles with size d_p = 0.8 mm and for average particle size d_{av} = 0.8 mm of fluidized bed inert particles the dependencies of temperature differences ΔT between burning char particles and fluidized bed particles on fluidized bed temperature, oxygen concentration in flue gas, operating pressure and char reactivity have been computed. Examples of computed dependencies of ΔT on fluidized bed "bulk" temperature and oxygen concentration (3 – 15 %vol. O_2) at two operating pressures 0.1 and 1.5 MPa are shown in Fig. 1 and Fig. 2. Dependence of ΔT on fluidized bed temperature under various operating pressures at constant oxygen volumetric concentration in flue gas for char and fluidized bed particles 0.8 mm is illustrated in Fig. 3. Effect of char reactivity on dependence of ΔT on fluidized bed temperature, oxygen concentration and operating pressure is obvious from comparison of Fig. 4 (for more reactive lignite coal with $E_a/\boldsymbol{R}$ = 8 000 K) with Figs. 1, 2 and 3 for less reactive coal char with $E_a/\boldsymbol{R}$ = 10 000 K. More reactive coal chars have relatively smaller difference in ΔT due to increase of operating pressure than less reactive coal chars.

The burning char temperature increases with increasing oxygen concentration in flue gas, with operating pressure and with increasing reactivity of coal char.

Increasing char particle size causes decrease of ΔT under practically all combustion conditions. For char particles bigger than 1.1 mm we supposed for simplicity that the same value of combustion enthalpy holds as for particles with diameter 1.1 mm, i.e. burning of char to practically only product CO_2. Dependence of ΔT on particle size of burning char particles at temperatures of fluidized bed 750, 850 and 950 °C for fluidized bed inert particle size 0.5 mm is given in Figs. 5 and 6.

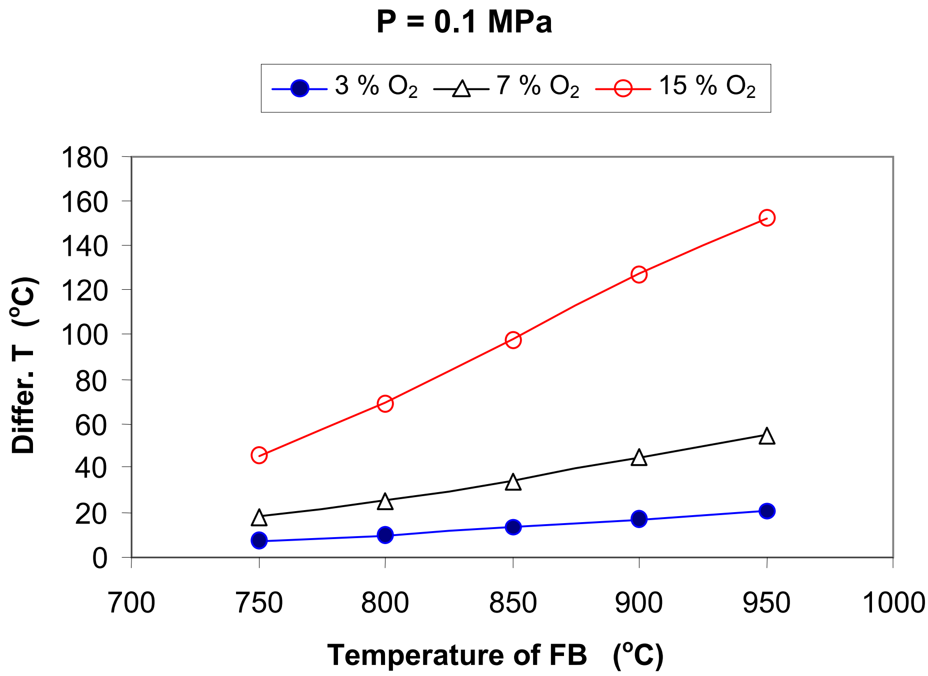

Fig. 1 Dependence of temperature difference between burning char temperature and FB temperature on “bulk”temperature of FB and effect of oxygen concentration in flue gas. Size of char particles and fluidized bed inert particles = 0.8 mm, operating pressure = 0.1 MPa, linear gas velocity in fluidized bed = 0.5 m/s, less reactive coal char ($E_a/\boldsymbol{R}$ = 10 000 K).

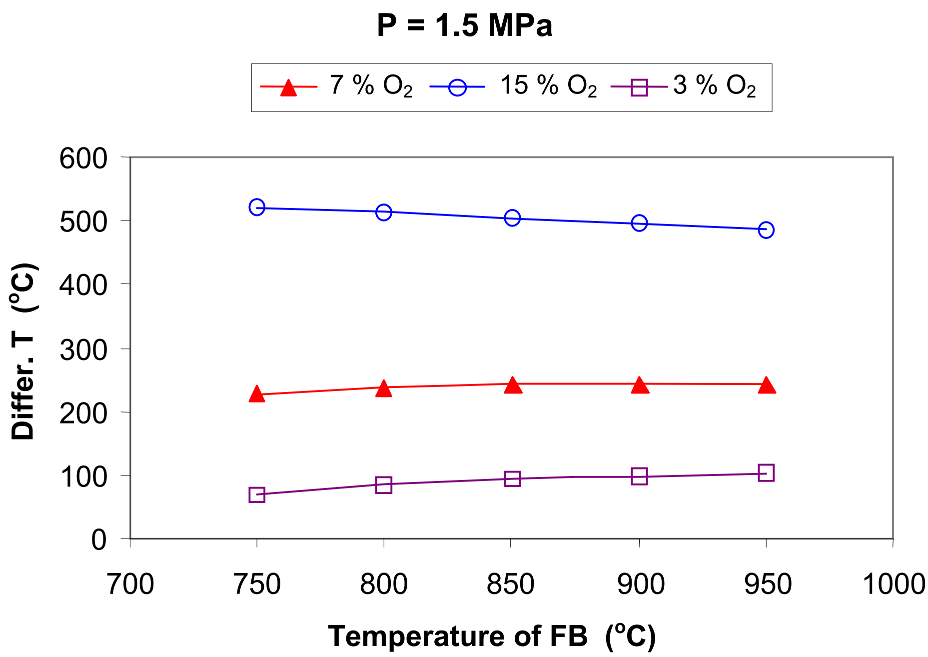

Fig. 2 Dependence of temperature difference between burning char temperature and FB temperature on “bulk” temperature of FB and effect of oxygen concentration in flue gas. Operating pressure 1.5 MPa, other conditions the same as in Fig. 1

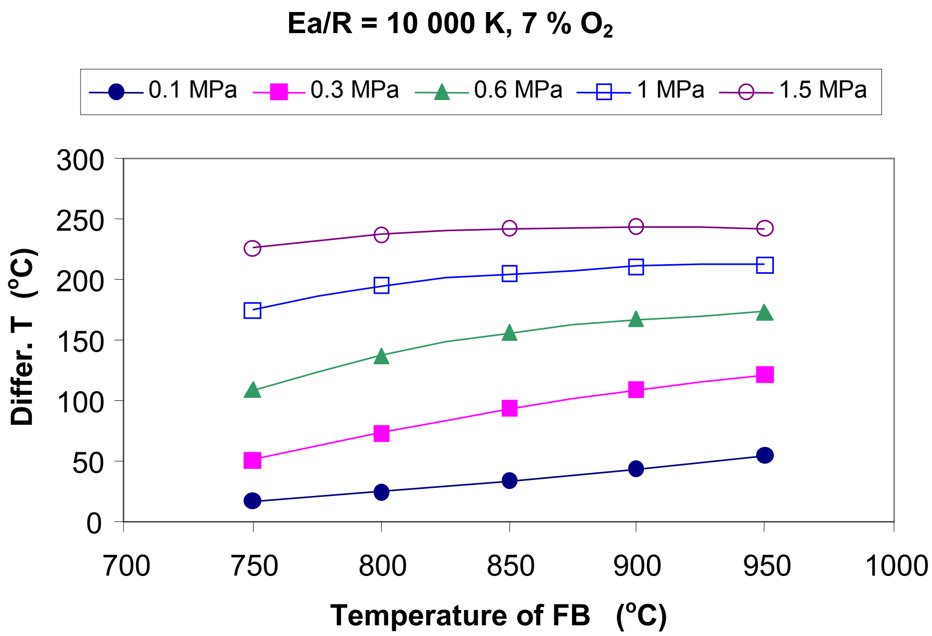

Fig. 3 Dependence of temperature difference between burning char temperature and FB temperature on "bulk" temperature of FB and effect of operating pressure at oxygen concentration in flue gas 7 vol. %. Size of char particles and fluidized bed inert particles = 0.8 mm, linear gas velocity in fluidized bed = 0.5 m/s, less reactive coal char ($E_a/\boldsymbol{R}$ = 10 000 K).

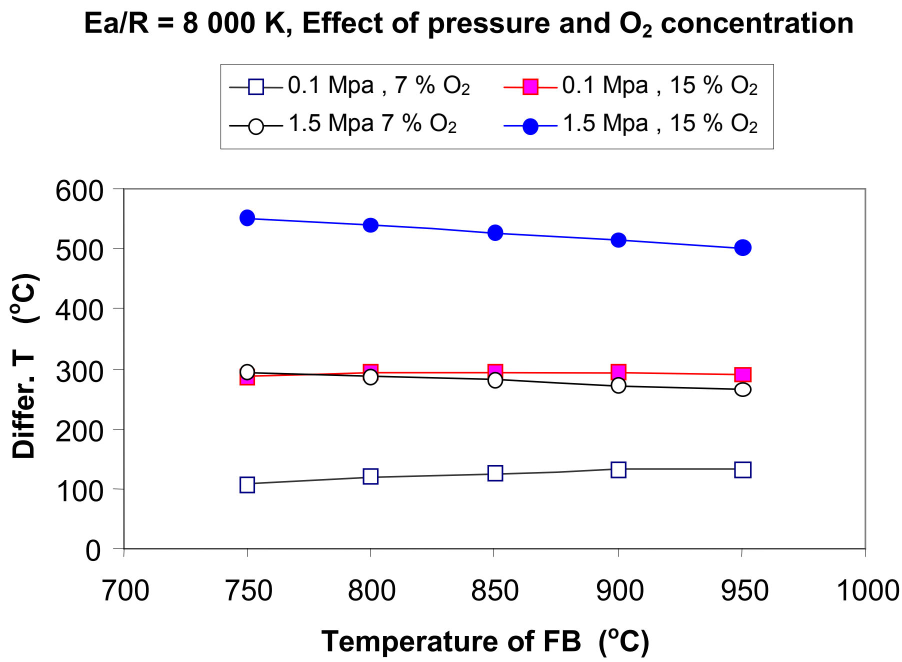

Fig. 4 Dependence of temperature difference between burning char temperature and FB temperature on "bulk" temperature of FB and effect of operating pressure at oxygen concentrations in flue gas 7 and 15 vol. % for more reactive coal char ($E_a/\boldsymbol{R}$ = 8 000 K). Size of char particles and fluidized bed inert particles 0.8 mm, linear gas velocity in fluidized bed 0.5 m/s.

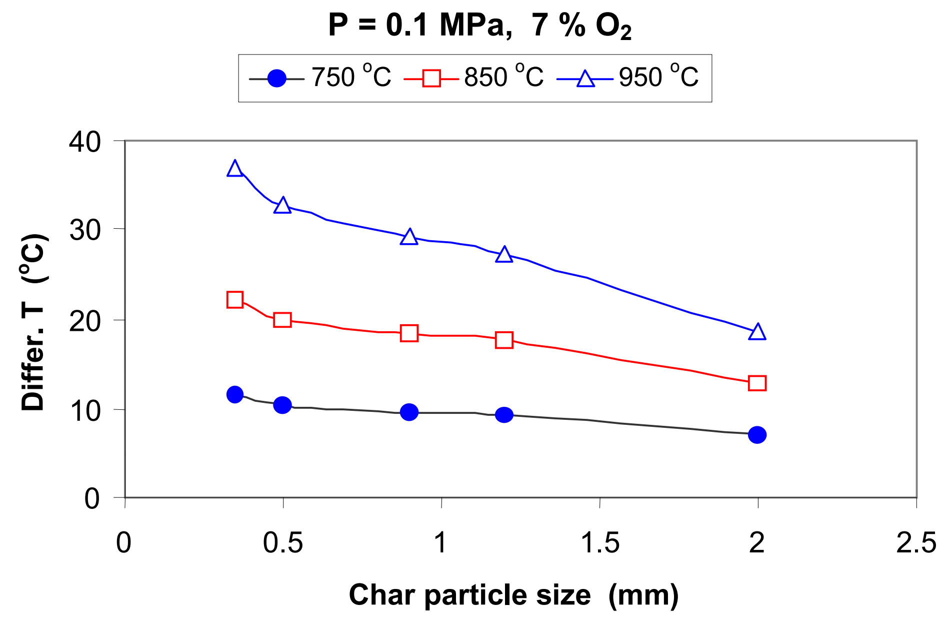

Fig. 5 Dependence of temperature difference between burning char temperature and FB temperature on char particle size and effect of "bulk" FB temperature at operating pressure 0.1 MPa and oxygen concentration in flue gas 7 vol. %. Size of fluidized bed inert particles 0.5 mm, linear gas velocity in fluidized bed 0.5 m/s, less reactive coal char ($E_a/\boldsymbol{R}$ = 10 000 K).

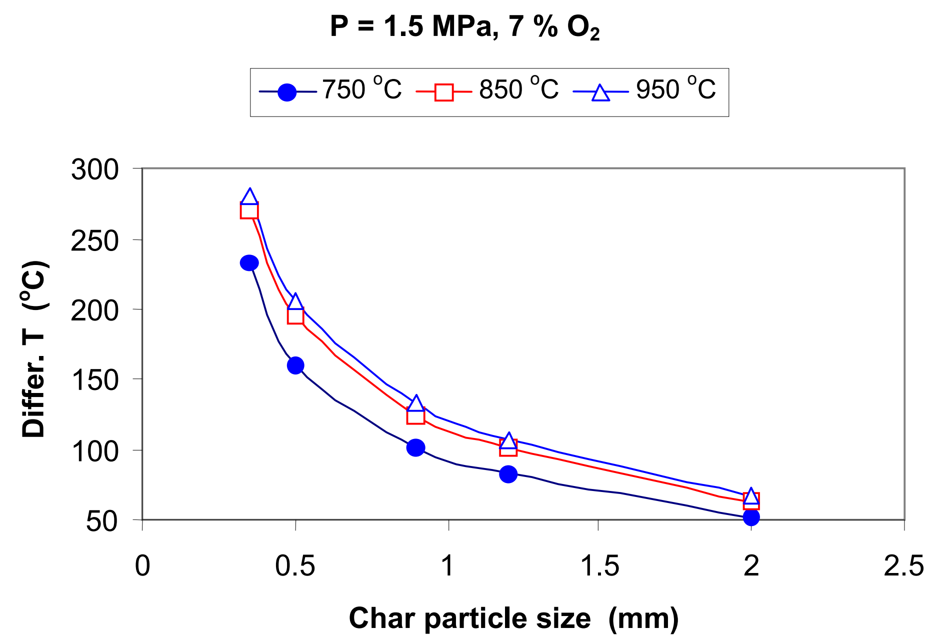

Fig. 6 Dependence of temperature difference between burning char temperature and FB temperature on char particle size and effect of "bulk" FB temperature at operating pressure 1.5 MPa and oxygen concentration in flue gas 7 vol. %. Size of fluidized bed inert particles 0.5 mm, linear gas velocity in fluidized bed 0.5 m/s, less reactive coal char ($E_a/\boldsymbol{R}$ = 10 000 K).

3. THEORETICAL MODEL FOR BURNING OF BIGGER HIGH ASH COAL-CHAR PARTICLES WITH TEMPERATURE DISTRIBUTION ACROSS THE PARTICLE DIAMETER

The model for burning of bigger char particles in fluidized bed is based on the shrinking core model for high ash coal particles (Lin W. 1994). The simplified scheme of the model situation for char particles is depicted in Fig. 7. The char particles are supposed to have constant diameter during char burning (no shrinking of ash layer).

The dimensionless concentration profile c* of oxygen in char particle (Lin W. 1994) is given by equation:

$$(dc^*/d\lambda) = (\Phi_{core})^2/(3\lambda^2) / [1/\lambda^2 + (1/\lambda_c - 1)\cdot(\Phi_{core})^2/3 + (\Phi_{core})^2/(3Sh')] \quad (3.1)$$

where $c^* = c_{O2}/c_{O2b}$, $\lambda = r/R_o$, R_o being radius of reacting char particle, r is ranging from R_c to R_o, $\lambda_c = R_c/R_o$, where R_c is radius of the reaction-burning sphere within char particle:

$$(\Phi_{core})^2 = 3R_o k_{rea}/D_{eff} \quad (3.2)$$

D_{eff} is effective diffusivity of oxygen between char radius levels R_c and R_o and $Sh' = R_o * k_{diff}/D_{eff} = Sh*D_g/(2*D_{eff})$ is a modified Sherwood number

$$D_{eff} = (\varepsilon / \psi)\cdot 1/(1/D_g + 1/D_{Knud}) \quad (3.3)$$

where ε is char porosity in the relevant region, ψ is char pore tortuozity D_g is gas phase diffusivity of oxygen and D_{Knud} is Knudsen diffusivity of oxygen in pores of char particles

$$D_{Knud} = (2/3)\, \boldsymbol{r}\ (\text{radius of pores}) \sqrt{8\mathbf{R}T/\pi M_{ox}} \quad (3.4)$$

where M_{ox} is molar mass of oxygen molecules (g/mol).

For our conditions estimation of D_{eff} by approximate relation was considered:

$$D_{eff} \approx 0.3\, D_g \quad (3.5)$$

thus

$$(dc^*/d\lambda)_{\lambda=\lambda c} = (\Phi_{core})^2/3 / [1 + (\lambda_c - \lambda_c\lambda_c)\cdot(\Phi_{core})^2/3 + \lambda_c\lambda_c(\Phi_{core})^2/(3Sh')] \quad (3.6)$$

$$(dc_{O2}/dr) = k_{rea}\, c_{O2b}/[D_{eff}(1 + \lambda_c\lambda_c k_{rea}/k_{diff}) + R_o k_{rea}(\lambda_c - \lambda_c\lambda_c)] \quad (3.7)$$

Reaction rate of char burning (mol $m^{-2}s^{-1}$) in reaction sphere with utilization of $\boldsymbol{\Phi_p}$ is expressed:

$$(dc_{O2}/dr)_{Rc} D_{eff} = k_{rea}\, c_{O2b}/[(1 + \lambda_c\lambda_c k_{rea}/(\boldsymbol{\Phi_p} k_{diff})) + R_o k_{rea}(\lambda_c - \lambda_c\lambda_c)/D_{eff}] \quad (3.8)$$

where

$c_{O2b} = (P/\boldsymbol{R}\,T)\cdot(X_{O2}b)$ as in the eq. (2. 10).

For $R_c = R_o$, i.e. for $\lambda = 1$ the eq. (3.8) is transformed directly into form of eq. (2. 10).

METHOD OF COMPUTATION OF BURNING CHAR PARTICLE TEMPERATURE

Computation of rate of heat generation Q_{gen} for individual char particle:

$\boldsymbol{Q_{gen}}$ is computed by means of eq. (3.8) and eq. (2.7) for ΔH_C:

$$\boldsymbol{Q_{gen}} = (dc_{O2}/dr)_{Rc} D_{eff}\ \Delta H_C\ 4\pi(R_c)^2 \quad (3.9)$$

(in W or kW)

The heat generated by char burning at radius R_c is transferred by conduction in the region between spheres with radius R_c and R_o and further from the surface of char particles to the fluidized bed – as schematically shown in Fig. 7.

HEAT TRANSFER IN CHAR PARTICLES (ASH LAYER) IN REGION BETWEEN R_C AND R_O

Equation for heat transfer rate by conduction in solid phase:

$$q_r = -\lambda_s\ dT/dr \qquad (W\ m^{-2}) \quad (3.10)$$

where λ_s is thermal conductivity of ash layer between R_c and R_o, λ_s is assumed to be no function of temperature and radial position.

In situation without heat source:

$$d/dr\,(r^2 q_r) = 0 \quad (3.11)$$

by integration of eq. (3. 11):

$$r^2 q_r = C_1 \quad (3.12)$$

after re-arrangement and substitution into eq. (3.10):

$$dT/dr = -C_1/(\lambda_s\ r^2) \quad (3.13)$$

by integration:

$$T = C_1/(\lambda_s r) + C_2 \quad (3.14)$$

where C_1 and C_2 are integration constants.

With boundary conditions:

$r = R_c$, $T = T_r$, where $T_r \geq T_p$

$r = R_o$ $T = T_p$ (3.15)

and by rearrangements (from eq. 3.14):

$$(T_r - T_p) = (C_1/\lambda_s)\cdot(1/R_c - 1/R_o) \quad (3.16)$$

C_1 can be expressed from eq. (3.16) and eq. (3.12)

$$r^2 q_r = C_1 = (T_r - T_p)\lambda_s / (1/R_c - 1/R_o) \quad (3.17)$$

and

$$q_r = (T_r - T_p)\lambda_s / [r^2(1/R_c - 1/R_o)] = d\,(\boldsymbol{Q_{con}})/d\boldsymbol{A} \quad (3.18)$$

where $\boldsymbol{Q_{con}}$ is the heat transfer rate by conduction in ash layer, which is independent on radial position in

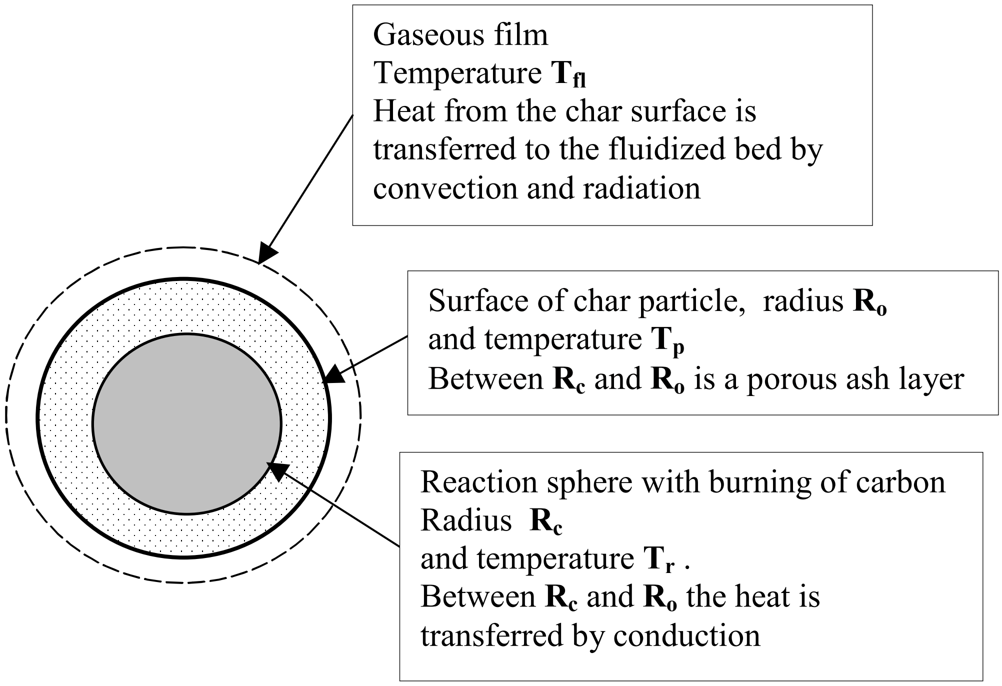

Fig. 7 Scheme of model situation and characteristic temperatures for burning of bigger char particles

the region between R_c and R_o . $\boldsymbol{A} = 4\pi\ r^2$ is surface area of a sphere with a radius r ($R_c \le r \le R_o$).

Thus for $\boldsymbol{Q_{con}}$ the following equation can be written:

$$\boldsymbol{Q_{con}} = (T_r - T_p)\lambda_s\, 4\, \pi\ R_c R_o /(R_o - R_c) \qquad (3.19)$$

Thermal conductivity of ash layer λ_s depends in reality on porosity, composition of ash and temperature. The λ_s values are probably ranging between approx. 0.1 and 10 $Wm^{-1}K^{-1}$.

In our model solutions we have used for λ_s a values 0.2 W m^{-1} K^{-1}.

This low value in model solutions gives imagination about maximum possible temperature difference between reaction zone at R_c and surface of char particles at R_o.

Heat transfer rate Q_{tr} from char particle surface to the fluidized bed

The computation of $\boldsymbol{Q_{tr}}$ is the same as in the foregoing model for smaller particles – thus computation of Nu number for bigger particles, estimate of α_p and computation of heat transfer rate to the fluidized bed for individual char particle:

$$\boldsymbol{Q_{tr}} = \alpha_p\,(T_p - T_{fl})\, 4\pi\, (R_o)^2 \quad (W) \qquad (3.20)$$

Overall method of model solution

Under steady state conditions the heat balance for burning and cooling of char particles is expressed:

$$\boldsymbol{Q_{gen}}(T_r) = \boldsymbol{Q_{con}}(T_r\ \ T_p) = \boldsymbol{Q_{tr}}(T_p\ T_{fl}) \qquad (3.21)$$

where T_r and T_p are temperatures at the reaction zone inside char particle and at the char surface respectively.

For a given temperature of fluidized bed T_{fl} the temperatures T_r and T_p are computed.

At the beginning of the computation procedure the temperature T_{fl} (1073 K - 1273 K), R_o (from initial char particle size), R_c (position of reaction zone radius in char particle), R_c = 0.35 – 0.99 R_o and the first approximation of temperature of reaction zone T_r within char particle, higher than T_{fl} are supplied.

With such values the $\boldsymbol{Q_{gen}}(T_r)$ is computed. Gas parameters and relevant dimensionless numbers are computed with temperature T_g = $(T_r + T_{fl})/2$ with given char particle size ($R_o = d_p/2$) and average size of fluidized bed particles (d_{av}).

Based on equality $\boldsymbol{Q_{con}}$=$\boldsymbol{Q_{gen}}$ and eq. (3.19) the approximation of surface temperature T_p is computed. Temperature T_p should be at least 0.2 K lower than T_r and maximum possible decrease of T_p is limited by temperature of fluidized bed T_{fl}.

With the approximated temperature T_p the heat transfer rate $\boldsymbol{Q_{tr}}$ from char surface to the fluidized bed is computed. If the $\boldsymbol{Q_{tr}}$ value is lower than $\boldsymbol{Q_{gen}}$ the next approximation of temperature T_r is higher and again the new T_p, $\boldsymbol{Q_{con}}$ and $\boldsymbol{Q_{tr}}$ values are computed. The temperatures T_r and T_p are searched repeatedly as long as the heat balance eq. (3.21) holds with acceptable precision (e.g. 0.1 - 1 %) and the difference

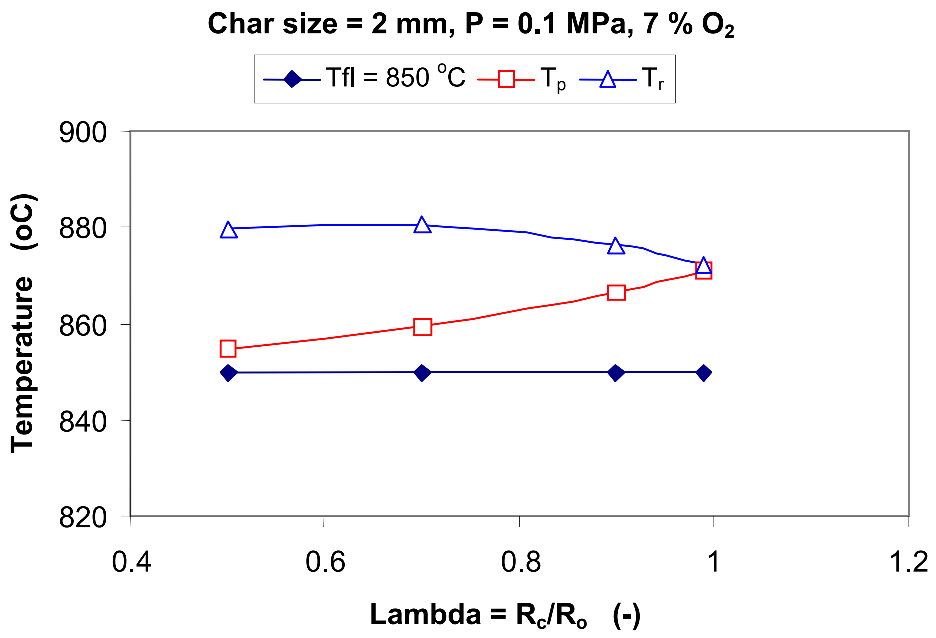

Fig. 8 Model for bigger char particles with temperature difference between reaction zone and surface of char. Dependence of char surface temperature T_p and reaction zone temperature T_r (within the particle) on the relative position of reaction zone ($\lambda = R_c/R_o$). FB temperature = 850 °C, operating pressure = 0.1 MPa, oxygen concentration = 7 vol. %, char particle $d_p = 2R_o$ = 2 mm, fluidized bed particles = 0.8 mm, linear gas velocity = 0.5 m/s, less reactive char particles ($E_a/\boldsymbol{R}$ = 10 000 K).

between the successive approximations of T_r and T_p is lower than 0.3 - 1 K. The cooling rate $\boldsymbol{Q_{tr}}$ should increase more quickly with increasing T_p, T_r than $\boldsymbol{Q_{gen}}$.

The results of model computations of dependence of temperatures T_r and T_p on ratio $\lambda = R_c/R_o$ for high ash char particles with diameter d_p = 2 mm temperature of fluidized bed T_{fl}=850 °C, effective diffusivity of oxygen in ash layer D_{eff}=0.3 D_g, supposed thermal conductivity of ash layer 0.2 W* m^{-1} K^{-1} linear gas velocity in fluidized bed 0.5 m/s and d_{av}=0.8 mm are shown in Figs. 8 and 9 for operating pressures 0.1 and 1.5 MPa at oxygen concentration in flue gas 7 vol. %. Dependence of temperatures T_p and Tr (at $\lambda = R_c/R_o$ = 0.6) on char particle size d_p for temperature of fluidized bed 850 °C oxygen concentration 7 vol % and d_{av} = 0.8 mm is illustrated in Figs. 10 and 11 for operating pressures 0.1 and 1.5 MPa.

4. RESULTS AND DISCUSSIONS

Modeling of particle temperature is limited mainly by lack of precise relevant and reliable data needed for model solution, e.g. CO/CO_2 ratio at char surface, correlations for Nu number, esp. for bigger particles, and by critical lack of experimental kinetic data, heat transfer data and various parameters for higher operating pressures and higher temperatures. Due to missing data for CO/CO_2 ratio, diffusivity and heat transfer at higher pressures the model solutions for higher operating pressures are based in fact, on extrapolations and supposed validity of the atmospheric pressure correlations for higher operating pressures.

Majority of relations for heat transfer in fluidized bed is valid for particles below 1.2 or 1.5 mm.

For bigger particles higher uncertainty resulting from extrapolations have to be taken into considerat-ion. It means, that esp. model computations of tempe-rature of burning char particles in fluidized bed for pressurized conditions and bigger char or fluidized bed particles should be taken as a “first approxima-tion”.

Due to discontinuities in correlations for partic-les in broader particle size (e.g. 0.1 – 3 mm) the dependencies of temperature differences T_r and T_p on particle size are in fact somewhat uneven, rough and having character of an approximation. We wanted to compare as well temperature of burning wood particles with coal char particles. But, even higher degree of uncertainty in parameters and missing data needed for model computation have been found for wood. From very high porosity and reactivity of wood char particles in fluidized bed combustion higher wood-char particle temperature in comparison with coal chars can be assumed.

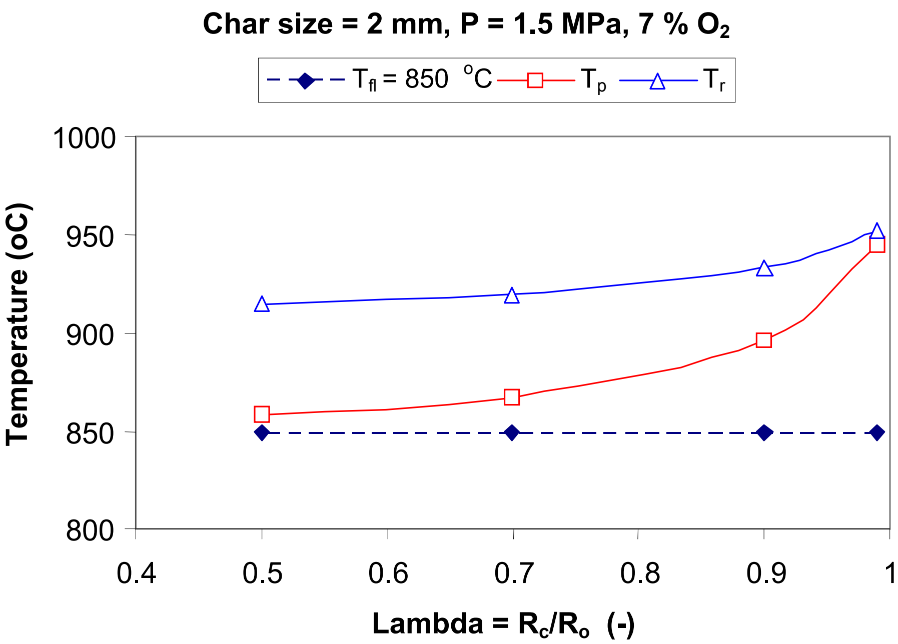

Fig. 9 Model for bigger char particles with temperature difference between reaction zone and surface of char. Dependence of char surface temperature T_p and reaction zone temperature T_r (within the particle) on the relative position of reaction zone ($\lambda = R_c/R_o$). Operating pressure = 1.5 MPa, FB temperature = 850 ^{o}C. The other conditions are the same as in **Fig. 8** .

Another difficulty in comparison of model results with experimental reality is in entrainment of smaller particles from fluidized bed. The entrained particles have in the region of "freeboard" (above the dense fluidized bed) higher temperature than within the fluidized bed. The entrainment of particles depends mainly on gas velocity, particle size, density and shape of char particles and on regime of fluidization (appearance of fluidized bed).

From the model solution for various conditions (fluidized bed temperature, oxygen concentration in flue gas operating pressure, particle size) the following knowledge has been gained:

The temperature difference between burning coal char particles and fluidized bed can attain commonly 40 – 150 ^{o}C for atmospheric pressure and several hundreds ^{o}C for pressurized conditions 1.5 MPa (Figs 1–4). Influence of fluidized bed temperature on temperature of burning char particles is generally lower at higher operating pressures. Effect of flue gas oxygen concentration on the temperature difference is higher than effect of operating pressure (see e.g. Fig. 4). The more reactive coal chars and as well wood-chars attain very quickly diffusion limitation of the burning rate and influence of oxygen concentration and operating pressure is weaker than for the less reactive coal chars (comparison of Figs. 3 and 4). Decreasing surface temperature of burning char particles with increasing char particle diameter (Figs. 5, 6) is in a qualitative agreement with experimental observations (Joutsenoja T. et al., 1999, Kobylecki et al., 2003). The dependence of burning char temperature on particle size is more significant at higher operating pressures (e.g. comparison of Fig. 5 with Fig. 6) and higher temperatures of FB at lower pressures (Fig. 5). Very small burning particles (below 0.2 – 0.3 mm) are, however, hardly accessible to reasonably precise measurement of their temperatures within fluidized bed due to significant tendency of entrainment of such particles from the fluidized bed and due to increasing probability of "sticking" of such smaller hot particles on surface of bigger, cooler particles. The theoretical finding of higher temperatures of smaller particles is in qualitative agreement with practical experience from e.g. particle agglomeration studies under conditions of atmospheric and pressurized FB combustion (Kobylecki et al., 2003). Higher temperature of burning smaller char particles has effect on emissions of nitrogen oxides and CO in FB combustion of "dusty" fuels (Svoboda et al., 2003). It seems, on basis of results of theoretical modeling, that bigger char particles of coals with higher ash content can exert higher temperature within the burning particle than the initial surface temperature in a definite stage of combustion (as shown in Fig. 8). This phenomenon is

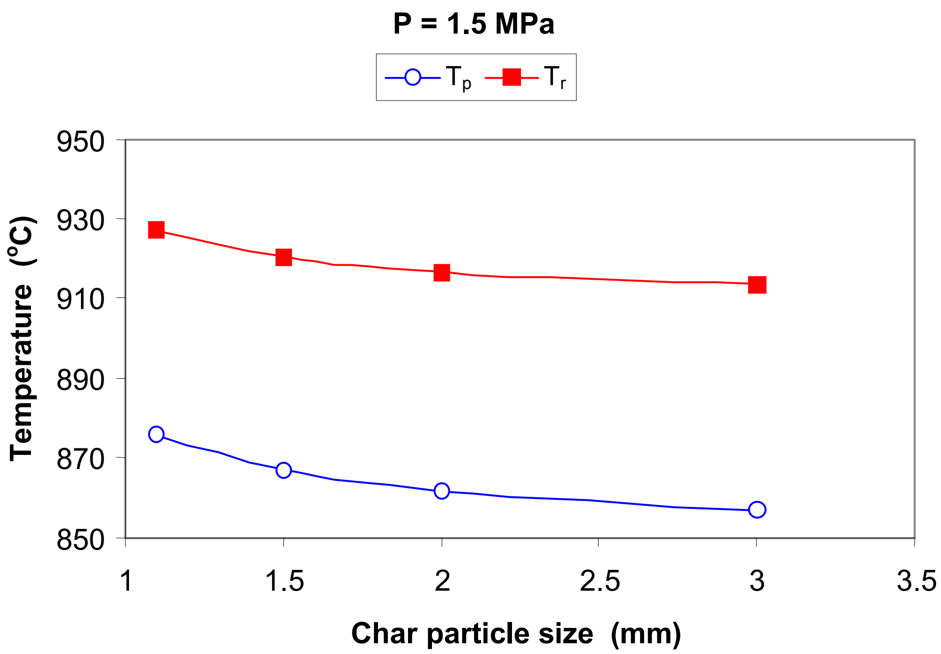

Fig. 10 Model for bigger char particles with temperature difference between reaction zone and surface of char. Dependence of char surface temperature T_p and reaction zone temperature T_r (within the particle at $\lambda = R_c/R_o = 0.6$) on char particle size. FB temperature = 850 °C, operating pressure = 1.5 MPa, oxygen concentration = 7 vol. %, fluidized bed particle size = 0.8 mm, linear gas velocity = 0.5 m/s, less reactive char particles ($E_a/\boldsymbol{R}$ = 10 000 K).

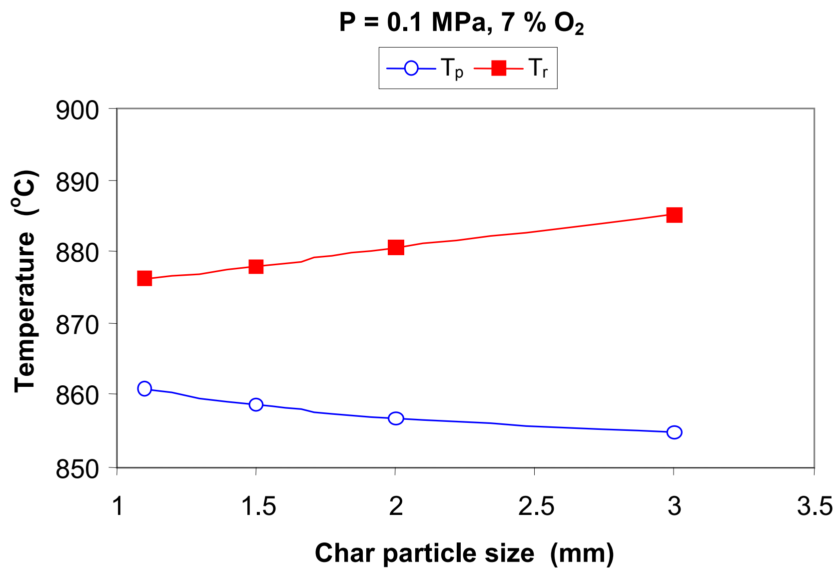

Fig. 11 Model for bigger char particles with temperature difference between reaction zone and surface of char. Dependence of char surface temperature T_p and reaction zone temperature T_r (within the particle at $\lambda = R_c/R_o = 0.6$) on char particle size. FB temperature = 850 °C, operating pressure = 0.1 MPa. The other conditions are the same as in Fig. 10.

probable only under very specific conditions of very low thermal conductivity of porous ash layer under atmospheric pressure. Under higher operating pressures (Fig. 9) the highest temperature ever attained during burning of bigger char particle is the temperature in the moment of surface oxidation.

The difference between surface and inner level burning temperature is higher for bigger particles and for higher operating pressures – as shown in Figs. 10 and 11.

Solutions of the both simplified models for temperature of burning char particles are very sensitive to values of coal char activation energies for burning (oxidation) reaction to, CO/CO_2 ratio at the surface of burning particles, to gas diffusivities thermal conductivity of ash layer in char particles etc. On the other hand, the linear gas velocity in the fluidized bed and emissivity of char particles have been found to have relatively smaller effect on the char temperature. Higher temperature of reacting char particles in FB combustion should be taken into account in modeling of nitrogen oxides and CO emissions, particularly under conditions of pressurized FB combustion (Svoboda et al., 2003).

Practical application of such model studies can be e.g. in selection of convenient conditions of FB combustion in processes with solid fuels containing ash with relatively low characteristic temperatures (ash softening, sticking, melting). To avoid undesirable particle agglomeration in FB either special conditions in FB combustion should be considered (low FB temperature, lower oxygen inlet concentration, lower operating pressure, bigger particles) or gasification processes with lower temperature of reacting fuel particles should be preferred (Čermák et al., 2001, Svoboda et al., 1999).

5. CONCLUSIONS

On basis of results from our modelling study the temperature difference between FB temperature and temperatures of burning char particles in FB combustion depends mainly on:

- char/fuel reactivity and porosity
- flue gas oxygen concentration
- operating pressure
- particle size

Dependence of the temperature difference on fluidized bed temperature is relatively weaker.

Temperature of burning char particles increases steeply with increasing oxygen concentration, operating pressure and decreasing char particles size for a given solid fuel. The temperature difference between burning char temperature and “bulk” FB temperature can attain value between 40 and 150 ^{o}C for atmospheric conditions and values between 200 and 500 ^{o}C for pressurized FB combustion.

Solution of the model for temperature of bigger high ash char particles revealed, that under specific conditions (e.g. lower operating pressure, low thermal conductivity of porous surface ash layer, low resistance in ash layer for oxygen diffusion) the temperature within the burning char particle (on the reaction sphere) can be even higher than the temperature at surface burning of char.

In practical cases particularly pressurized FB combustion of smaller coal/biomass particles with relatively low melting temperature of ash is critical from the point of view of FB particle agglomeration (Kobylecki et al., 2003). For such cases either two stage combustion with sub-stoichiometric FB combustion in the first stage (Čermák et al., 2001) or gasification processes with temperatures of reacting char particles lower than “bulk” fluidized bed temperature should be preferred. In modeling of formation and destruction of emissions (esp. NO_x, N_2O, CO etc.) in pressurized FB combustion the real temperature of burning char particles substantially higher than the FB temperature should be considered.

ACKNOWLEDGEMENTS

The financial support of this work from the Grant Agency of AS CR Grant project A 407 2201 and Grant project A407 2001) is gratefully acknowledged.

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