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A char combustion sub-model for CFD-predictions of fluidized bed combustion - experiments and mathematical modeling

Jakub Bibrzycki [a,b], Marco Mancini [b], Andrzej Szlęk [a], Roman Weber [b,*]

[a] Institute of Thermal Technology, Silesian University of Technology, Konarskiego 22, Gliwice 44-100, Poland
[b] Institute for Energy Process Engineering and Fuel Technology, Clausthal University of Technology, Agricolastrasse 4, Clausthal-Zellerfeld 38678, Germany

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ABSTRACT

The Grain-Thermo-Balance (GTB) rig was built for generation of the char, at high heating rates, and for experimental determination of its oxidation rates. A zero-dimensional mathematical model for calculating oxidation rates of millimeter-size char particles was developed to serve as a char particle sub-model in a CFD-based software for predicting performance of fluidized bed boilers. When morphology of the char was determined using mercury porosimetry and the char oxidation rates in the kinetic regime were measured using TGA, the zero-dimensional Shrinking Particle Model was able to reproduce the GTB measurements well - with exception of the last 2% burnout where due to a model singularity the calculated temperatures exceeded the measured values. When the char was generated in TGA, at low heating rates, its intrinsic reactivity was four times lower and the reactivity decrease was attributed to alterations to the char morphology (40% slow-down) and annealing (60%).

1. Introduction and objectives

In industrial coal-fired fluidized beds, the dense bed is formed using inert (sand) particles typically not larger than 1 mm whereas fuel particles can be as large as 3–8 mm. Bed temperatures are typically in the 1150–1230 K range. Current research efforts, aiming at development of CFD-based mathematical models for performance predictions of fluidized bed combustors [1], concentrate on handling the complex fluid dynamics of two-phase flows. As reviewed by Singh et al. [2], there are three numerical methods available and these are (a) Eulerian–Lagrangian methods which use single particle, particle parcel or a group of particles description of the solid-phase, (b) Eulerian–Eulerian Two Fluid Model methods and (c) Discrete-Element Method which also uses the Eulerian–Lagrangian framework. The three zones of fluidized bed combustion namely, dense bed, splash zone and free board, require different CFD-methods and fluid dynamics of the first two zones is the most difficult to simulate. CFD-simulations of such a complex fluid dynamic structure require a constant intervention of the modeler to force and secure convergence and computational times are very long. Adamczyk et al. [3] have recently modeled an industrial circulating fluidized bed boiler using a hybrid Euler–Lagrange approach and, since it was not possible to achieve a steady-state convergence, the model was run as time-dependent until oscillations around a mean value were observed. One may question such an approach but this is the state of CFD-modeling in fluidized bed technology today. It is then perhaps not too surprising that at this stage of the CFD-modeling, BCURA-type models [4] are used [2,3,5] to compute oxidation rates of char particles. In such models, the oxidation rates are computed by taking into account both oxygen diffusion through the particle boundary layer and an Arrhenius expression accounting for kinetics.

The objective of our work is to develop a zero-dimensional mathematical model for calculating oxidation rates of millimeter-size char particles which is to serve as a sub-model in CFD-based software for predicting performance of fluidized beds. The goal is to develop and validate a char oxidation model which goes beyond BCURA-formulation [4] by taking into account both reactants transport and reactions inside the porous structure. There exist many models that just do that, as exemplified by works of Simons [6] and Haugen et al. [7]; however, they are too complex to be incorporated into a CFD software handling fluidized bed combustion. In other words, zero-dimensionality is the constraint we must adhere to. In reviews by Laurendeau [8] and Smith [9] (see also Weber and Mancini [10]) the framework of the mathematical modeling has been summarized and since then a proliferation of models have been developed which can

List of acronyms: BCURA, British Coal Utilisation Research Association; FB, Fluidized Bed; GTB, Grain Thermo-Balance; IR, InfraRed; RPM, Random Pore Model; SCM, Shrinking Core Model; SPM, Shrinking Particle Model; TGA, ThermoGravimetric Analysis/Analyzer.

* Corresponding author.
E-mail addresses: jakub.bibrzycki@wp.pl (J. Bibrzycki), mancini@ievb.tu-clausthal.de (M. Mancini), andrzej.szlek@polsl.pl (A. Szlęk), roman.weber@ievb.tu-clausthal.de, weber.rom@gmail.com (R. Weber).

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List of symbols

A	Ash content in coal, %
A_{int}	Pre-exponential factor for intrinsic kinetics, m/s
c_{ash}	Specific heat capacity of ash, kJ/(kg · K)
c_C	Specific heat capacity of carbon, kJ/(kg · K)
c_{char}	Specific heat capacity of solid material in char, kJ/(kg · K)
C_{CO_2}	Molar concentration of carbon dioxide, kmol CO_2/m_g^3
C_{O_2}	Molar concentration of oxygen, kmol O_2/m_g^3
$c_{p\,air}(T_p)$	Specific heat capacity of air at constant pressure, at T_p, kJ/(kg · K)
c_p	Specific heat capacity of char particle, kJ/(kg · K)
$c_{r\,av}$	Average char conversion rate, kg/s
D_{eff}	Effective diffusivity, m^2/s
D_g	Gas diffusivity, m^2/s
D_{gb}	Gas diffusivity at bulk temperature, m^2/s
D_k	Knudsen diffusivity, m^2/s
$d_{pore\,av}$	Average pore diameter at time, τ m
$d_{pore\,av0}$	Initial average pore diameter, m
d_p	Particle diameter, m
d_{p0}	Initial particle diameter, m
$d_p{}^*$	Equivalent particle diameter, m
$E_{a\,int}$	Activation energy, kJ/kmol
g_{ash}	Ash mass fraction in char, kg ash/kg char
g_C	Carbon mass fraction in char, kg C/kg char
$h_{CO_2}^{Tp}$	Specific enthalpy of carbon dioxide at T_p, kJ/kg
$h_{CO_2}^{298.15}$	Specific enthalpy of carbon dioxide at 298.15, K kJ/kg
h_{CO}^{Tp}	Specific enthalpy of carbon monoxide at T_p kJ/kg
$h_{CO}^{298.15}$	Specific enthalpy of carbon monoxide at 298.15, K kJ/kg
h_{O2}^{Tb}	Specific enthalpy of oxygen at T_b, kJ/kg
$h_{O_2}^{298.15}$	Specific enthalpy of oxygen at 298.15, K kJ/kg
Δh_r	Reaction enthalpy of carbon oxidation, kJ/kg C
$\Delta h_r(CO)$	Reaction enthalpy of carbon oxidation to CO, kJ/kg C
$\Delta h_r(CO_2)$	Reaction enthalpy of carbon oxidation to CO_2, kJ/kg C
k_{int}	Intrinsic kinetics constant, m/s
k_{pseudo}	Pseudo-kinetics constant, m/s
L_V	Volumetric pore length, m/m^3
m	Mass of char sample at time t, kg
M	Moisture content in coal, %
m_0	Initial mass of char sample, kg
m_{ash}	Mass of ash, kg
M_C	Molar mass of carbon, kg C/kmol C
M_{CO}	Molar mass of carbon monoxide, kg CO/ kmol CO
M_{CO_2}	Molar mass of carbon dioxide, kg CO_2/kmol CO_2
M_{O_2}	Molar mass of oxygen, kg O_2/kmol O_2
p	Absolute pressure, Pa
S_{ext}	External particle surface area, m^2
S_{m0}	Initial char specific internal surface area, m^2/g
S_V	Char volumetric internal surface area at time t, m^2/m^3
S_{V0}	Initial char volumetric internal surface area, m^2/m^3
T_A	Activation temperature, K
T_b	Gas temperature at bulk conditions, K
T_p	Particle temperature, K
T_{wall}	Pipe internal surface temperature, K
t	Time, s
V	Volatiles content in coal, %
V_p	Particle volume, m^3
V_{pore}	Total intrusion volume of mercury per gram of char, m^3/g
V_{sample}	Volume of char sample, m^3
w	Average velocity from outflow of the ceramic pipe, m/s
X	Char burnout
X^*	Char burnout in 20–95% range
z_{N_2}	Molar content of N_2 in the gas mixture
z_{O_2}	Molar content of O_2 in the gas mixture
DTG	Normalized sample mass loss rate, 1/s
HHV	Higher heating value of coal, kJ/kg
LHV	Lower heating value of coal, kJ/kg
c	carbon mass fraction in coal, %
h	hydrogen mass fraction in coal, %
s	sulfur mass fraction in coal, %
n	nitrogen mass fraction in coal, %
o	oxygen mass fraction in coal, %
Nu	Nusselt number
Re	Reynolds number
Pr	Prandtl number
Sc	Schmidt number
Sh	Sherwood number
α	Convective heat transfer coefficient, $kW/(m^2 \cdot K)$
β_{eff}	Effective mass transfer coefficient of O_2, m/s
δ_{m-mod}	Relative difference of average conversion rates, %
ϵ	Char porosity at time t, m_g^3/m^3
ϵ_0	Initial char porosity, m_g^3/m^3
ϵ_p	Emissivity of the char particle surface
ϵ_{p-pw}	Mutual emissivity of the char particle-wall arrangement
η	Effectiveness factor
μ_b	Gas dynamic viscosity at bulk temperature, Pa · s
λ_b	Gas thermal conductivity at bulk temperature, kW/(m · K)
γ	Stoichiometric coefficient in reaction (3), kmol O_2/kmol C
$\gamma_{CO2} = 1$	Stoichiometric coefficient of carbon/CO_2 reaction kmol, CO_2/ kmol C
ρ_{app}	Apparent char density at t, kg/m^3
ρ_{app0}	Initial apparent char density, kg/m^3
ϕ	Thiele modulus
ψ	Pore structural parameter
$\rho_{air}(T_p, p)$	Density of air calculated at $p = 1$bar and T_p, kg/m^3
ρ_{true}	True char density, kg/m_{solid}^3
σ	Stefan-Boltzmann constant, $kW/m^2 \cdot K^4$
τ_{pore}	Pore tortuosity

Subscripts

0	Initial
app	Apparent
b	Bulk
g	Gas
p	Particle

Superscripts

ad	Air dried conditions
daf	Dry ash-free basis
exp	Experimental
mod	Modeling

be classified into shrinking particle models (SPM) and shrinking core models (SCM). In the latter models, the particle diameter remains constant during oxidation, and the reactions take place at the sharp interface between the unreacted core and the ash layer. The ash layer

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