



# Devolatilization of a single fuel particle in a fluidized bed under oxy-combustion conditions. Part B: Modeling and comparison with measurements



Changsheng Bu<sup>a,b</sup>, Bo Leckner<sup>b</sup>, Xiaoping Chen<sup>a,\*</sup>, Alberto Gómez-Barea<sup>c</sup>, Daoyin Liu<sup>a</sup>, David Pallarès<sup>b</sup>

<sup>a</sup> Key Laboratory of Energy Thermal Conversion and Control of Ministry of Education, School of Energy and Environment, Southeast University, Nanjing 210096, China

<sup>b</sup> Department of Energy and Environment, Chalmers University of Technology, Göteborg 41296, Sweden

<sup>c</sup> Chemical and Environmental Engineering Department, University of Seville, Seville 41092, Spain

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## ABSTRACT

A detailed one-dimensional transient model is developed to describe the conversion of a single fuel particle in  $O_2/N_2$  and  $O_2/CO_2$  atmospheres in a fluidized bed (FB). The model takes into account the main relevant phenomena occurring from the addition of a particle to the FB up to the instant when most of the volatiles have been released. The model accounts for the rates of drying, fuel devolatilization, homogeneous combustion of volatiles in a thin flame, heterogeneous combustion of char, and mass and heat transfer, the latter involving the heat transfer from the FB reactor and flame to the particle. The model is used to simulate and explain the experiments given in Part A of the present work, which includes tests with four ranks of coal (from anthracite to lignite) and one type of wood in  $O_2/N_2$  and  $O_2/CO_2$  atmospheres with the  $O_2$  volume concentration varying in the range of 0–40% at a fixed bed temperature of 1088 K. The predicted history of the temperature of the fuel particle and of the volatiles flame agrees well with the measurements. The simulated results indicate that the heat transfer processes at the particle scale are similar in pure  $N_2$  and  $CO_2$ . The model reveals that only a small amount of heat from the flame is transferred to the fuel particle, explaining why the rate of particle heating is hardly affected by the flame. The decrease in the devolatilization time measured at higher  $O_2$  concentration is explained by heterogeneous (char) combustion, which is seen to be significant during the last stages of devolatilization. The model shows that the char combustion is limited by the rate of diffusion of  $O_2$  to the particle and justifies the lower heating rate observed in  $O_2/CO_2$  compared to in  $O_2/N_2$ . A sensitivity analysis shows that the thermal capacity and conductivity of the fuel, as well as the convective heat transfer coefficient, are the most influencing parameters affecting the time of devolatilization.

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## 1. Introduction

Devolatilization of solid fuel involves complex mechanisms of chemical reactions (devolatilization reactions, homogeneous and heterogeneous reactions) coupled with internal and external heat and mass transfer. Numerous simulation studies [1,2] have been performed on the pyrolysis of coarse solid-fuel particles taking into account both heat transfer (internal and external) and chemical kinetics of pyrolysis (i.e., the single step model, the two-parallel reaction model, three competitive reaction model and the distributed activation energy model), indicating that the process of pyrolysis can be approximately described by a progressing temperature

front in the particle [3]. In an oxidizing environment, Higuera [4] simulated the devolatilization behavior of an isolated coal particle moving relative to the surrounding gas, using a competing reaction model of pyrolysis, assuming a uniform particle temperature and that the released volatiles burned in a thin diffusion flame in the vicinity of the coal. The author indicated that many characteristics of the devolatilization process are not qualitatively altered by the motion of the particle, and that the size of the flame increases with the size of the particle and decreases with the concentration of oxygen in the bulk gas. The evolution and combustion of volatiles released from a single isolated coal particle in stagnant and convective environments was also numerically studied by Agarwal [5].

When  $O_2/N_2$  is replaced by  $O_2/CO_2$ , the chemical reactions and heat and mass transfer could be changed by the greater heat sink (the product of heat capacity and density), and lower  $O_2$  diffusion

\* Corresponding author. Fax: +86 25 83793453.

E-mail address: [xpchen@seu.edu.cn](mailto:xpchen@seu.edu.cn) (X. Chen).

## Nomenclature

$a$	heating rate of the sample in a thermogravimetric analyzer (K/s)	$T$	temperature (K)
$A$	area (m <sup>2</sup> )	$u$	velocity (m/s)
$A_{hete,k}$	frequency factor of heterogeneous combustion (kg/(m <sup>2</sup> s kPa))	$v$	volume (m <sup>3</sup> )
$A_{pyro}$	frequency factor of pyrolysis (1/s)	$V$	mass yield of volatile matter released up to a certain instant of time (kg/kg)
$C_p$	thermal heat capacity (J/(kg K))	$V^*$	total volatile content of the fuel (kg/kg)
$C$	amount of carbon in the coal (kg/kg <sub>daf</sub> )	$Y_{O_2,\infty}$	mass concentration of oxygen (kg/kg)
$D$	diffusion coefficient (m <sup>2</sup> /s)		
$E_{hete,k}$	activation energy of heterogeneous combustion (J/mol)	<i>Greek letter</i>	
$E_{pyro,0}$	mean activation energy of pyrolysis (J/mol)	$\alpha$	thermal diffusivity (m <sup>2</sup> /s)
$F_{cbp}$	fraction of total heat transferred to the particle surface due to convection between FB reactor and particle (-)	$\gamma$	stoichiometric oxygen to fuel mass weight ratio (-)
$F_{ccp}$	fraction of total heat transferred to the particle surface due to char combustion (-)	$\delta$	boundary layer thickness (m)
$F_{rbp}$	fraction of total heat transferred to the particle surface due to radiation between FB reactor and particle (-)	$\varepsilon$	emissivity, or bed voidage (-)
$F_{rfp}$	fraction of total heat transferred to the particle surface due to radiation between flame and particle (-)	$\lambda$	thermal conductivity (W/(m K))
$h_{conv}$	convective heat transfer coefficient (W/(m <sup>2</sup> K))	$\rho$	mass density (kg/m <sup>3</sup> )
$h_m$	mass transfer coefficient (kg/(m <sup>2</sup> s kPa))	$\sigma$	Stefan-Boltzmann constant (W/(m <sup>2</sup> K <sup>4</sup> ))
$H$	amount of hydrogen in the coal (kg/kg <sub>daf</sub> )	$\sigma_E$	standard deviation of the activation energy (J/mol)
$\Delta H_{vap}$	heat of vaporization (J/kg)	$\phi_A$	volume fraction of ash (v/v)
$\Delta H_{hete}$	heat released from heterogeneous combustion (J/kg)	$\phi_C$	volume fraction of carbon (v/v)
$\Delta H_{vol,c}$	heat released from volatiles combustion (J/kg)	$\phi_M$	volume fraction of moisture (v/v)
$\Delta H_{pyro}$	global heat of devolatilization (J/kg)	$\phi_V$	volume fraction of volatiles (v/v)
$k_{vap}$	rate of vaporization (kg/s)		
$k_{hete}$	specific rate of heterogeneous combustion (kg/(m <sup>2</sup> s))	<i>Subscripts</i>	
$k_{pyro}$	rate of devolatilization (kg/s)	$b$	fluidized bed
$m$	mass (kg)	$daf$	dry and ash-free
$N$	amount of nitrogen in the coal (kg/kg <sub>daf</sub> )	$c$	combustion
$Nu$	Nusselt number (-)	$eff$	effective
$O$	amount of oxygen in the coal (kg/kg <sub>daf</sub> )	$ef$	evaporation front
$P$	pressure (kPa)	$f$	volatiles' flame
$Q_t$	total amount of heat transferred to the particle surface (J)	$fi$	final
$Q_{cfb}$	rate of heat transferred by conduction between flame and bed (W)	$g$	gas
$Q_{cfp}$	rate of heat transferred by conduction between flame and particle (W)	$h$	heat
$Q_{rfb}$	rate of heat transferred by radiation between flame and bed (W)	$hete$	heterogeneous
$Q_{rfp}$	rate of heat transferred by radiation between flame and particle (W)	$in$	internal
$r$	spherical coordinate (m)	$k$	kinetic
$r_{hete,k}$	kinetic coefficient of the effective combustion rate (kg/(m <sup>2</sup> s kPa))	$low$	lower part of the particle
$r_{eff,hete}$	effective coefficient of the heterogeneous combustion rate (kg/(m <sup>2</sup> s kPa))	$m$	mass
$R$	particle radius (m)	$mf$	at minimum fluidization conditions
$R_g$	universal gas constant, (kPa m <sup>3</sup> /(mol K) or J/(mol K))	$p$	particle
$S$	amount of sulfur in the coal (kg/kg <sub>daf</sub> )	$o$	oxygen
$Sh$	Sherwood number (-)	$t$	time
$S_r$	source term in Eqs. (1) and (2) (kg/(m <sup>3</sup> s) or W/m <sup>3</sup> )	$up$	upper part of the particle
$t$	time (s)	$vol$	volatiles
		$0$	initial value
		<i>Abbreviations</i>	
		AC	anthracite coal
		BC	bituminous coal
		DAEM	distributed activation energy model
		FB	fluidized bed
		LC	lignite coal
		SBC	sub-bituminous coal
		SW	Schima wood
		TGA	thermogravimetric analyzer

rate in CO<sub>2</sub> compared to N<sub>2</sub>, and even CO<sub>2</sub> gasification with carbon could occur at high temperature [6]. A longer ignition delay time of volatiles from pulverized coal in O<sub>2</sub>/CO<sub>2</sub> than in O<sub>2</sub>/N<sub>2</sub> was experimentally observed by Molina and Shaddix [7], who demonstrated by modeling that the higher heat sink of CO<sub>2</sub> contributes to this behavior. Maffei et al. [8] developed a comprehensive model of coal combustion in O<sub>2</sub>/CO<sub>2</sub> and O<sub>2</sub>/N<sub>2</sub>, and found that the lower diffusion rate of O<sub>2</sub> in CO<sub>2</sub> and CO<sub>2</sub> gasification of carbon reduced

the temperature of the burning pulverized coal compared to that in N<sub>2</sub>. However, less work has been done on modeling of devolatilization of coarse fuel particles in an O<sub>2</sub>/CO<sub>2</sub> atmosphere, which are typically used in fluidized bed (FB). Guedea et al. [9] studied devolatilization and combustion of large fuel particles ( $d_p = 3\text{--}4$  mm) in O<sub>2</sub>/N<sub>2</sub> and O<sub>2</sub>/CO<sub>2</sub> at 1123 K in a thermo-gravimetric analyzer (TGA), proposing a model which predicted slightly longer devolatilization time in O<sub>2</sub>/CO<sub>2</sub> than in O<sub>2</sub>/N<sub>2</sub>, in agreement with the

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