Numerical research on the homogeneous/heterogeneous ignition process of pulverized coal in oxy-fuel combustion

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Chun Zou *, Lei Cai, Chuguang Zheng

State Key Laboratory of Coal Combustion, Huazhong University of Science and Technology, Wuhan 430074, PR China

ABSTRACT

Oxy-fuel combustion technology has been deemed a promising technology to reduce CO_2 emissions from coal-fired power stations. The ignition processes of pulverized coal in oxy-fuel combustion were detailedly simulated using a CFD model with a new devolatilization sub-model. The profiles of the rates of devolatilization, volatile content, char and coal combustion during the homogeneous and heterogeneous ignition process were obtained by the numerical simulation. The present CFD model was validated by the comparison of the predicted ignition positions of a coal particle with a diameter of 85 μm and Jovanovic's experimental results for four different temperatures of the secondary oxidant: 1073 K,1273 K, 1473 K and 1623 K, and oxygen mole fractions of 0.21 and 0.35 in nitrogen or carbon-dioxide. The ignition mechanisms were determined at the position of particle ignition based on three criteria conditions of the homogenous, heterogeneous, and heterogeneous–homogeneous ignition. The three conditions were implemented in the FLUENT code by user-defined function (UDF). The mechanisms of the coal ignition in O_2/CO_2 atmospheres are that for an O_2 mole fraction of 0.21 in CO_2, a coal particle with a diameter of 85 μm ignites homogeneously when the secondary air temperature ranges from 1073 K to 1473 K. The particle ignites heterogeneously when the secondary air temperature exceeds 1473 K. When the mole fraction of O_2 in CO_2 increases to 0.35, homogeneous ignition occurs at secondary air temperatures of 1073 K and 1273 K, while heterogeneous ignition occurs at temperature higher than 1273 K. The rates of devolatilization, char and coal combustion at the ignition position changed slightly when the secondary air temperature increased. However, the rate of volatile combustion at the ignition position drastically decreased as the secondary air temperature was increased. The drastic variance of the rate of volatile combustion at the ignition position caused the change in the ignition mechanism of coal in oxy-fuel combustion. During homogeneous ignition in O_2/CO_2 atmospheres, the char generally ignites at the maximum mole fraction of volatiles near the surface of the coal particle. The devolatilization and volatile combustion processes are not affected by the char combustion process. During heterogeneous ignition in O_2/CO_2 atmospheres, volatiles generally ignite at the maximum mole fraction of volatiles near the surface of coal particle. The interaction between the combustion of volatiles and char is significant. The curve of the rate of char combustion features a v-notch due to the combustion process of volatiles, and the curves of the rate of volatiles combustion and mole fraction of volatiles are skewed due to the char combustion process.

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1. Introduction

O_2/CO_2 recycled combustion, a typical oxy-fuel combustion technology, has been deemed a promising technology to reduce CO_2 emissions from coal-fired power stations [1–5]. During O_2/CO_2 recycled combustion, the combustion of fuel occurs in an atmosphere of oxygen and recycled flue gas (RFG), i.e., O_2/CO_2.

The combustion characteristics of coal in oxy-fuel are evidently different from those observed in conventional air combustion because of the significant differences between the physical and chemical property of CO_2 and N_2 [6–13]. Many studies have examined the combustion characteristics of coal in oxy-fuel combustion using a thermogravimetric analyzer (TGA) [6–8], drop tube furnace (DTF) [6,9,10] and entrained flow reactor (EFR) [11–13].

Coal ignition is closely associated with coal devolatilization, the homogeneous combustion of volatiles and the heterogeneous combustion of char and coal. Coal can be homogeneously, heteroge-

* Corresponding author. Tel.: +86 2787542417x8314; fax: +86 2787545526.
E-mail address: zouchun@hust.edu.cn (C. Zou).

Nomenclature

A	pre-exponential factor, s^{-1}	hom	homogeneous reaction
Ea	activation energy, J/kmol	het	heterogeneous reaction
R_{gas}	gas constant, J/mol/K	vol	volatiles
T_p	particle temperature, K	A_{het}	pre-exponential factor, $kg/m^2/s/P$
K	devolatilization rate, $kmol/s/m^3$	E_{het}	activation energy, J/kmol
W	mass of volatiles, kg	M_{vol}	molecular weight of volatiles
A_P	surface area of the particle, m^2	C_{vol}	concentration of volatiles, $kmol/m^3$
ρ	gas density, kg/m^3	CO_2	concentration of O_2, $kmol/m^3$
T_{ox}	local temperature of oxidant in the gas, K	$A_{hom,vol}$	pre-exponential factor, $kg/m^2/s/P$
f_{ox}	local mass fraction of oxidant in the gas	$E_{hom,vol}$	activation energy, J/kmol
M_{ox}	local molecular weight of oxidant in the gas, kg/kmol	$\Re_{dvol}$	devolatilization rate, $kmol/s/m^3$
R	chemical rate, $kmol/s/m^3$	$\Re_{hom,vol}$	reaction rate of volatiles combustion, $kmol/s/m^3$
D_0	bulk molecular diffusion rate, m^2/s	$\Re_{het}$	reaction rate, $kmol/s/m^3$
d_P	particle diameter, m	$\Re_{het,coal}$	reaction rate of non-devolatilization coal combustion, $kmol/s/m^3$
C_1	mass diffusion coefficient, m^2/s		
T_∞	ambient gas temperature, K	$\Re_{het,char}$	reaction rate of devolatilization char combustion, $kmol/s/m^3$
T_0	reference temperature, K		
V_{cell}	volume, m^3		
Sh	Sherwood number correlation		

neously and hetero-homogeneously ignited based on the interaction of these processes. Homogeneous ignition is generally thought to be a two-stage process. The primary step consists of the initial ignition of volatiles accumulated around the coal particle. Subsequently, the homogeneous combustion of volatiles ignites the char particle [14]. Heterogeneous ignition can occur via the direct attack of oxygen on the coal or char particle. In hetero-homogeneous ignition, char and volatiles ignite simultaneously. Although the definition of ignition differs according to the experimental facilities and conditions adopted in the studies [15–17], the particle diameter, heating rate, oxygen mole fraction, coal type and ambient gas temperature are widely accepted to have significant effects on the ignition mechanism [14,18–21]. Homogeneous ignition usually occurs when large particles are heated slowly and/or in low oxygen fractions, while heterogeneous ignition mostly takes place when small particles are heated quickly or the oxygen mole fraction is high. Heterogeneous ignition is more likely to occur for low-rank coals at high ambient temperatures [14].

Many researchers have examined the ignition mechanism and process of coal in oxy-fuel combustion [9, 12, 13, 22–26]. Khatami et al. [9] investigated the ignition mechanism of single particle coal and char particles in O_2/N_2 and O_2/CO_2 atmospheres with oxygen mole fractions in the range of 20–100%. They claimed that heterogeneous ignition is likely to occur in the O_2/CO_2 atmospheres, and homogeneous ignition in the O_2/N_2 atmospheres. They mainly attributed this preference to the lower devolatilization rate of the coal particles in the CO_2 atmosphere compared to N_2. In contrast with air combustion, ignition is commonly thought to be delayed in oxy-fuel combustion at O_2 concentration of 21% due to the thermal capacity (ρc_p) of CO_2, which is greater than that of N_2. Using US eastern bituminous coal and an entrained flow reactor, Molina and Shaddix [12] found that high concentrations of CO_2 had no evident effect on the time of volatile combustion from ignition to burnout under a homogeneous gas-phase ignition regime. Further studies by Shaddix et al. [13] indicated that the present of CO_2 does not affect the volatile fuel consumption rate, but slightly impacts the volatile cloud combustion rate because of a slightly lower diffusivity of volatiles in CO_2 than in N_2. Liu [22] studied the ignition delay of a pulverized coal stream using identical experimental facilities and found that the ignition time strongly depends on the furnace gas temperature and coal particle size. Zhang [23] imaged the ignition of a low-volatile bituminous coal particle in two O_2/CO_2

mixtures. They observed the homogeneous ignition sequence using a high-speed camera and claimed that the volatiles that accumulated on char surface mainly converted into CO, and coal ignition in ~30%O_2–70%CO_2 essentially matches that in air. Jovanovic et al. [24] experimentally and numerically studied the ignition of coal in DTF. The ignition point positions predicted by their modified sequential coal model agree with the experimental results. Their later studies [25] indicated that the FG model can successfully predict the ignition point position.

The aforementioned works mainly qualitatively examined the ignition phenomena in O_2/N_2 and O_2/CO_2 atmospheres. Few studies have attempted to quantify the interaction between devolatilization, the combustion of volatiles and coal or char combustion in the ignition process, which are significant to understand the ignition mechanism of coal and the effects of these processes on the ignition mechanisms in O_2/CO_2 atmospheres.

Numerical simulation is an important tool to study combustion. For instance, the rate of devolatilization and reaction rates of volatiles, coal and char in the ignition process are easily calculated by numerical simulation. Recently, several CFD models have successfully predicted the ignition point position and delay time of coal combustion in O_2/CO_2 atmospheres [24,25]. Therefore, this study had two primary objectives to further understand the ignition mechanism of coal in O_2/CO_2 atmospheres:

- The first objective was to study the homogeneous and heterogeneous processes in O_2/CO_2 atmospheres in detail by numerical simulation.
- The second objective was to examine the effects of ambient gas temperatures and particle sizes on the ignition mechanism of coal particles in O_2/CO_2 atmospheres.

2. Modeling approach

2.1. Coal combustion models

A commercial CFD code, ANSYS Fluent version 12, was adopted to simulate the ignition process of coal in this study. The coal combustion process was modeled in the Eulerian–Lagrangian frame [27]. For continuous phase modeling, the time-averaged mass, momentum, energy and species transport equations were solved in the Eulerian frame. Because the back flow in DTF was absent,