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Modelling and experimental studies on oxy-fuel combustion of coarse size coal char

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ABSTRACT

Oxy-fuel combustion of single coarse sub-bituminous coal char particle is investigated in an isothermal mass loss apparatus. Experimental studies are performed at the reactor temperature of 1100 K and in varying O_2 concentrations of 42–60% in both O_2-CO_2 and O_2-N_2 environments. A fully transient model is developed for the combustion and gasification reactions including the transport of heat and mass in the porous char particle and the gas film. The model is validated with experimental findings of the present authors as well as that reported in literature over a wide range of O_2 concentrations. Simulation study is carried out to assess the effect of the particle size, the reactor temperature and the gas composition. The simulation shows that low diffusivity of O_2 within the reactor in CO_2 environment and the endothermic gasification reaction are mainly responsible for lowering the peak temperature and the rate of combustion of char than that in O_2-N_2 environment. It is also observed that though the effect of CO_2 on the combustion rate at low temperatures is insignificant, it is considerable at the reactor temperature of 1273 K and above in O_2-CO_2 environment. The model is expected to provide vital information for reactor design under oxy-fuel combustion and its integration with CFD analysis for identifying the optimum particle size, reactor temperature and oxygen concentration.

1. Introduction

Due to its low price and abundance, coal will continue to remain the primary source of energy in foreseeable future for the developing countries including India. Even in a developed country like Australia, around 85% of the electricity is derived from coal [1]. The usage of coal is increasing every day due to the high energy need of the developing civilization. This has eventually increased the CO_2 emanation to approximately 75% of the total greenhouse gas emission globally. Nearly 40% of the CO_2 released into atmosphere is contributed by the thermal power plants using coal. The use of coal in power generation and the release of CO_2 are likely to go up further in future [2,3]. Hence the recent research focus has shifted towards the development of technologies for CO_2 capture and storage (CCS) for possible continued utilization of coal in thermal power plants. The CCS technologies include pre-combustion capture [4], post combustion capture [5], oxy-fuel combustion [6] and chemical looping combustion [7]. Techno-economic feasibility studies have shown that oxy-fuel technology is the most promising option among the CCS technologies approaching commercialization. Not only is it capable of producing a highly concentrated CO_2 stream, it has also great flexibility, as it can be adapted in new installations as well as used in retrofitting both the existing pulverized and fluidized-bed coal fired power plants. Oxy-fuel combustion is one of the clean coal technologies which have attracted research interest in the present day. It has numerous advantages over the traditional air combustion technique; it reduces greenhouse gas (GHG) emission as well as enables easy sequestration of CO_2 due to less volume of the flue gas [7]. Moron et al. [8] proposed the additional advantage in oxy-fuel combustion, where the effluent flue gas contains mostly CO_2 and a little amount of H_2O causing easy sequestration of CO_2 due to its higher concentration than in case of combustion with air.

Presently some of the pilot plants on oxy-fuel combustion are in operation all over the globe including Germany, Japan, Australia Spain and USA. The pilot plant facility in Aioi, Japan is used to test different coals in air and oxy-fuel conditions. These studies are expected to be beneficial for the assessment of flame stability analysis, combustion behaviour, gaseous emissions, fly ash characteristics, plant operation, and development of comprehensive mathematical model of the plant. The study showed that under oxy-fuel combustion (21% O_2 and 79% CO_2), the flame temperature is 100-150 °C lower than that in air (21% O_2 and 79% N_2) combustion, due to the higher heat capacity of CO_2 and lower rate of combustion [7]. The lower flame temperature leads to lower particle temperature consequently the burn out time becomes longer. In contrast, the combustion reaction rate in O_2/N_2 atmosphere is comparatively faster and the burn-out time is less.

Recovery of CO_2 in conventional coal power plants is highly energy intensive due to its low concentration, typically 14–16% in the flue gas

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Nomenclature

Notations

k_{s1}^0, k_{s2}^0	Pre-exponential factors of heterogeneous reactions (1 & 2), mol K m^{-2} atm^{-1} s^{-1}
k_{v3}^0	Pre-exponential factor of CO combustion reaction, mol m^3 s^{-1}
T	Temperature, K
R_{s1}	Reaction rate of O_2 combustion, mol m^{-2} s^{-1}
R_{s2}	Reaction rate of CO_2 gasification, mol m^{-2} s^{-1}
$R_{v3}^{'}$	Reaction rate of homogeneous CO combustion, mol m^{-3} s^{-1}
E	Activation energy, J mol^{-1}
R	Universal gas constant, 8.314 J mol^{-1} K^{-1}
p_{O2}, p_{CO2}	Partial pressure of O_2 & CO_2.
c_k	Concentration of gaseous component k, mol m^{-3}
r	Distance from the particle's centre, m
D_p	Particle size, mm
M	Molecular weight, kg mol^{-1}
W_c	Instantaneous mass concentration of carbon in solid char, kg m^{-3}
C_p	Heat capacity, J kg^{-1} K^{-1}
R_v	Reaction rate, mol m^{-3} s^{-1}
t	Time, s
D	Molecular diffusivity, m^2 s^{-1}
S	Specific pore surface area, m^2 m^{-3}
r_o	Particle radius, mm
N_t	Total molar flux of gas mixture, mol m^{-2} s^{-1}
c_t	Total concentration of gaseous mixture, mol m^{-3}
Y	Mass fraction

Greek letters

ΔH	Heat of reaction, J mol^{-1}
ε	Porosity
ε_r	Char emissivity
η	Mole ratio of product CO/CO_2
γ_{kl}	Reaction stoichiometry for component k, in reaction no. l.
λ	Thermal conductivity of char, J m^{-1} s^{-1} K^{-1}
λ_r	Reference thermal conductivity of gas, Wm^{-1} K^{-1}
ρ	Density, kg m^{-3}
ψ	Pore parameter
σ	Stephan–Boltzmann constant, 5.67×10^{-8} Wm^{-2} K^{-4}
τ	Tortuosity factor of char
ζ	Local carbon conversion in solid char

Subscripts

s	Particle surface or solid phase
b	Bulk value
av	Average value
c	Carbon
g	Gas phase

[9], diluted by the N_2 in air. The concentration of CO_2 can be increased by separating the nitrogen from the air before its entry to the combustor, reducing thereby the cost of recovery of CO_2. Therefore, in oxy-fuel technology, combustion of coal takes place in presence of oxygen (>21%) and flue gas rich in CO_2. Generally the flue gas is recycled to regulate the combustion temperature and moderate the effective heat transfer [10].

A number of investigations on oxy-fuel coal combustion have focused on the O_2-N_2 and O_2-CO_2 environment in order to study the effect on char burnout time, char particle temperature and char combustion rate [3,4]. Bu et al. [10,11] performed both experimental and modelling investigations for coarse size (6 mm) single coal particle, in oxy-fuel environment and reported that the low diffusivity of O_2 in presence of CO_2 is primarily responsible for variation in burn out time and particle temperature along with slower combustion rate in O_2-CO_2 than in O_2-N_2 environments. They experimentally investigated the effect of slow and endothermic CO_2 gasification reaction on the conversion and temperature profiles in O_2-CO_2 environment. Kim et al. [12] observed through simulation studies that the endothermic CO_2 gasification reaction lowers char particle temperature, thereby reducing the oxidation rate.

Juan et al. [13] incorporated the Stefan flow and oxidation of CO in gas boundary layer for the development of combustion model and predicted the experimental findings like particle temperature and burn-out time accurately. They did a thorough study and observed that combustion dynamics is highly influenced by Stefan flow and CO oxidation rate during combustion at low bulk temperature for large particle size in presence of low O_2 concentration. However, they concluded that effect of Stefan flow is insignificant for reaction during gas diffusion controlled regime. Further, Juan et al. [14] also investigated the effect of Stefan flow and CO oxidation rate on mass transfer coefficients of O_2 and CO_2 during oxy-fuel combustion of coal char. Bejarano et al. [15] investigated the combustion behaviour of bituminous, lignite coal and synthetic char at different O_2 concentrations in N_2 and CO_2 environment and reported that coal particle burns at relatively higher temperature and requires less burnout time in O_2/N_2 atmosphere than in O_2/CO_2 atmosphere. Maffei et al. [16] experimentally investigated the combustion behaviour of single coal particle in O_2/N_2 and O_2/CO_2 atmospheres in a drop tube furnace and measured the particle temperature with the help of three-color pyrometer system. In model they coupled the heat and mass transfer phenomena for devolatilization, combustion and gasification. Sadhukhan et al. [17] studied coarse particle coal combustion in a fluidized bed and presented a comprehensive model considering coal devolatilization, volatile combustion in the boundary layer, combustion of residual char, CO oxidation within the pores of the char as well as in the gas boundary layer, coupled with heat transfer model for both devolatilization and char combustion. They made a detailed investigation on burnout time, centre and surface temperature profiles. Murphy et al. [18] investigated the combustion of bituminous coal char in oxygen-enriched environment (6–36 mol%) at reactor temperatures of 1047–1527 °C in an entrained flow reactor. They estimated the char burnout time from combined equation of chemical kinetics and heat transfer. Germyachkin et al. [19] modelled the combustion process of porous carbon particle in oxygen atmosphere. They proposed that the combustion reaction proceeds through two regimes: 1. Oxygen penetrates into the porous structure of the carbon particle from ambient and reacts over the entire particle volume producing both carbon monoxide and carbon dioxide. 2. Oxygen reacts on the particle outer surface producing only carbon monoxide. The carbon monoxide gradually diffuses out into the gas boundary layer and oxidizes to carbon dioxide. Zhou et al. [20] studied the effect of CO_2 on single particle oxy-fuel combustion and reported that the particle temperature is lower by 220 °C when N_2 (21% O_2, 79% N_2) is replaced by CO_2 (21% O_2, 79% CO_2). This is due to combined effect of the higher density and heat capacity of CO_2 and the presence of endothermic CO_2-gasification reaction. Zhang et al. [21] also investigated the effect of CO_2 on oxy-fuel combustion and reported that chemical attributes, specific heat, radiation characteristics and mass diffusivity of CO_2 are the main governing parameters in ignition delay of pulverized coal combustion in O_2-CO_2 environment compared to that in O_2-N_2 environment.

Brix et al. [22] experimentally investigated the oxy-fuel combustion of millimeter-sized (2–4 mm) coal char particles in a fixed bed reactor maintained at 1073 K in presence of varying oxygen concentration (5–80%) both in O_2-CO_2 and O_2-N_2 environments. The researchers experimentally studied the evolution of peak particle temperature and burnout time with O_2 concentration. They observed that the particle peak temperature is always higher in O_2-N_2 environment than that in