

# Chemical, thermal and dilution effects of carbon dioxide in oxy-fuel combustion of wood in a fixed bed<sup>†</sup>

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## Abstract

Experimental and numerical modeling was performed on eucalyptus wood combustion under oxy-fuel conditions using a fixed bed reactor in order to isolate the role of various carbon dioxide effects on the burning rate. Wood combustion was investigated under four different mixtures of O<sub>2</sub> and Ar/CO<sub>2</sub>/N<sub>2</sub>: 21 % O<sub>2</sub>/79 % N<sub>2</sub>; 21 % O<sub>2</sub>/22.5 % CO<sub>2</sub>/56.5 % Ar; 40 % O<sub>2</sub>/60 % CO<sub>2</sub>; and 40 % O<sub>2</sub>/47 % CO<sub>2</sub>/13 % Ar. The first three mixtures were designed to have the same peak temperatures in order to isolate chemical and dilution effects of CO<sub>2</sub>. This was achieved by substituting some percentage of CO<sub>2</sub> with Ar in O<sub>2</sub>/CO<sub>2</sub> mixture while maintaining a constant concentration of O<sub>2</sub>. The fourth mixture was meant to isolate the thermal effect of CO<sub>2</sub>. The results were obtained from both the experimental rig and numerical simulation for a fixed bed configuration. Wood combustion in the fixed bed was modeled using Lagrange-Euler method, where gas-phase was calculated using computational fluid dynamics (CFD), that is Euler phase, while solid-phase was tracked in Lagrange phase using discrete element method (DEM). The results show that ignition time in CO<sub>2</sub> environment decreases gradually as O<sub>2</sub> concentration is increased. On the other hand, burning rate and flame front speed increase as O<sub>2</sub> concentration is increased. It was established that dilution effect is the most influential parameter on the burning rate of wood combustion in an oxy-fuel system.

**Keywords:** Burning rate; CO<sub>2</sub> effect; Fixed bed; Oxy-fuel combustion; Wood combustion

## 1. Introduction

The demand for biomass fuel has increased due to ever increasing energy need that cannot be fully satisfied by other energy sources, such as coal. Biomass is an attractive energy source as compared to coal as it is renewable. Most of the energy scenarios indicate that biomass will be increasingly used to meet increasing energy demand in future [1].

For a long time, biomass has been converted to energy using burners which operate under air-fuel conditions. However, in the last two decades, there has been increasing use of combustion of biomass in power generation [2, 3]. Oxy-fuel combustion is a technique of capturing CO<sub>2</sub> by recirculating exhaust gas. It is applicable to solid fuels [4], liquid fuels [5] and gaseous fuels [6]. The technique was introduced in power plants the first time in 1982 [7]. Since then, a lot of research, for instance [8-10], have been done to understand the combustion phenomenon.

The studies on fundamental combustion phenomena - transport, chemical and thermodynamics processes - occurring in

oxy-fuel combustion are based on models and experiments on laboratory-scale devices. These include studies on ignition delay time in coal [11], ignition temperature, burnout and NO<sub>x</sub> emission in biomass and coal blends [12], and gaseous emissions from biomass/coal co-firing [13]. Such studies provide insights into combustion phenomena in practical oxy-fuel environment [12, 13]. The presence of CO<sub>2</sub> in oxidizer alters physical and thermal properties of the gas mixture, which has impact on fuel reactivity, flame temperature and emissions. Unlike inert species such as argon and nitrogen which have only thermal and dilution effects on combustion processes, addition of reactive species such as CO<sub>2</sub> introduces a chemical effect [14, 15]. Dilution effect is the reduction of concentration of oxidizer caused by addition of CO<sub>2</sub>, thermal effect is the decrease in temperature caused by addition of CO<sub>2</sub> and chemical effect is the direct active participation in the chemical reactions.

The three roles played by CO<sub>2</sub> addition can be separated by adjusting the flame temperature to a value corresponding to a reference condition without change in oxidizer and fuel relative concentrations [15, 16]. This technique has been applied to study the effects of CO<sub>2</sub> on soot formation, but it can also be applied to study the effects on other combustion properties [17].

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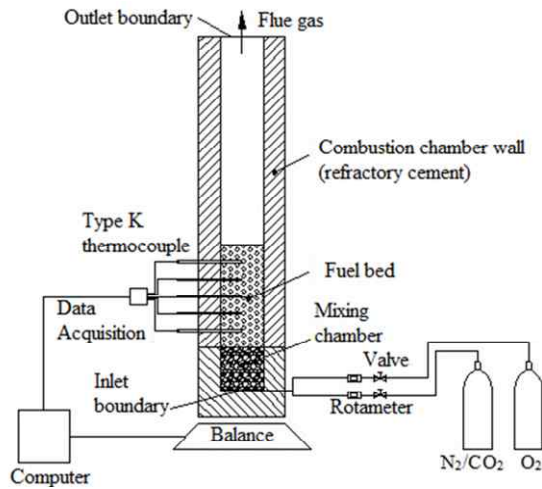


Fig. 1. Schematic diagram of experimental set-up.

Most previous studies focused on the overall effects of CO<sub>2</sub> burning environment on ignition time [18], ignition and combustion temperature [19], burnout [20], combustion intensity [19] and thermal reactivity [21]. The individual effects in terms of chemical, thermal and dilution on the combustion properties are still not clear. An understanding of these basic mechanisms through which CO<sub>2</sub> affects combustion processes is important because it helps in the design of optimized oxy-fuel burners.

The main objective of this work was to isolate the role of chemical, thermal and dilution effects of CO<sub>2</sub> on wood burning rate through numerical modeling. Four different mixtures of O<sub>2</sub> and Ar/CO<sub>2</sub>/N<sub>2</sub> were designed to separate CO<sub>2</sub> effects on wood combustion. Temperature in O<sub>2</sub>/CO<sub>2</sub> combustion environment was adjusted to be equal to that of O<sub>2</sub>/N<sub>2</sub> environment by adding an appropriate amount of Ar while O<sub>2</sub> amount remained the same. The model was validated by comparing temperature profiles with experimental values. Experiments were done on a laboratory-scale fixed bed.

## 2. Methodology

### 2.1 Experimental set-up

A schematic diagram of the experimental set-up used in this work is shown in the Fig. 1. It is a cylindrical burner made of stainless steel which is insulated with refractory cement. A detailed description of the set-up has been given in our previous paper [22].

For all the tests, the burner was filled with wood up to a height of 6 cm. Five type K thermocouples are located at an equidistant of 10 mm from one another. They are connected to a data acquisition system that records temperature every second. Temperature measurement and data acquisition using type K thermocouples were done in accordance to ASTM MNL12 [23]. Combined measurement uncertainty for thermocouple and data acquisition system depends on measured temperature and for the entire range was determined to be

between  $\pm 2.2$  °C and  $\pm 6.6$  °C. The burner was operated in a batch mode; fuel was fed once while oxidizer was supplied continuously.

### 2.2 Numerical modeling

Numerical simulations of combustion of wood in the fixed bed were carried out using a commercial software CD-Adapco (STAR CCM+ version 11.04) [24]. Wood burning in a fixed bed was simulated using Lagrange-Euler method, where gas-phase was calculated using computational fluid dynamics, that is, the Euler phase, while solid-phase was tracked in Lagrange phase, using discrete element method. The governing equations of the model are given by Eqs. (1)-(9) and fully described in Ref. [22, 24]:

- Mass conservation equation for gas-phase, Eq. (1) and solid-phase, Eq. (2):

$$\frac{\partial}{\partial t}(\chi \rho_g) + \nabla \cdot (\rho_g \mathbf{v}_g) = \sum_{i,g} w_{i,g}^{gs} \quad (1)$$

$$\frac{\partial}{\partial t}((1-\chi)\rho_s) = \sum_{i,s} w_{i,s}^{gs} \quad (2)$$

- Momentum conservation equation for gas-phase, Eq. (3):

$$\frac{\partial}{\partial t}(\chi \rho_g \mathbf{v}_g) + \nabla \cdot (\rho_g \mathbf{v}_g \mathbf{v}_g) = -\nabla p + \nabla \cdot \boldsymbol{\tau} + \rho_g \mathbf{g} + S_m \quad (3)$$

where  $S_m$  is momentum source term given as;

$$S_m = -\left( \frac{\mu}{c_1} \mathbf{v}_g + C_2 \rho_g |\mathbf{v}_g| \mathbf{v}_g \right) \quad (4)$$

- Energy conservation equation for gas-phase, Eqs. (5) and (6) and solid-phase, Eq. (7):

$$\begin{aligned} & \frac{\partial}{\partial t}(\chi \rho_g h_g) + \nabla \cdot (\rho_g \mathbf{v}_g h_g) \\ &= \frac{\partial}{\partial t}(\chi p) + \nabla \cdot (\lambda_{g,e} \nabla T_g - \sum_{i=1}^{N_g} h_{i,g} J_{i,g}) + \nabla \cdot (\mathbf{v}_g p) - \nabla \cdot (\boldsymbol{\tau} \cdot \mathbf{v}_g) + S_E \end{aligned} \quad (5)$$

where  $S_E$  energy source term given as;

$$S_E = A_s h_c (T_s - T_g) - \sum_{i,g} w_{i,g}^{gs} H_{i,g} + q_R \quad (6)$$

$$\begin{aligned} \rho_s c_{ps} (1-\chi) \frac{\partial T_s}{\partial t} &= \nabla \cdot (\lambda_{s,e} \nabla T_s) + A_s h_c (T_g - T_s) + \\ & \frac{A_s}{4} Q_{a,p} (G - 4\sigma T_s^4) + \sum_{i,s} w_{i,s}^{gs} H_{i,s} \end{aligned} \quad (7)$$

- Species conservation equation for gas-phase species  $i,g$ , Eq. (8) and solid-phase species  $i,s$ , Eq. (9)

$$\frac{\partial}{\partial t}(\chi \rho_g Y_{i,g}) + \nabla \cdot (\rho_g \mathbf{v}_g Y_{i,g}) = \nabla \cdot (\rho_g D \nabla Y_{i,g}) + w_{i,g}^{gs} \quad (8)$$

Table 1. Proximate and ultimate analyses of fuel sample.

| Proximate analysis (wt%)          |       |
|-----------------------------------|-------|
| Moisture                          | 10.3  |
| Volatile matter (wt% dry basis)   | 84.9  |
| Fixed carbon (wt% dry basis)      | 14.9  |
| Ash (wt% dry basis)               | 0.2   |
| Ultimate analysis (wt% dry basis) |       |
| C                                 | 50.87 |
| H                                 | 5.73  |
| N                                 | 0.3   |
| O (by difference)                 | 43.1  |
| Gross calorific value (MJ/kg)     | 19.3  |

Table 2. Physical properties of wood.

| Particle size, $d_p$ (m)             | 0.005                                      |
|--------------------------------------|--|
| Eucalyptus wood                      |  |
| Density, $\rho$ (kg/m <sup>3</sup> ) | 1220                                       |
| Porosity, $\theta$                   | 0.64                                       |
| Specific heat, $c_p$ (J/kgK)         | $1500 + T_s$                               |
| Conductivity, $\lambda_s$ (W/mK)     | 0.2  |
| Char                                 |  |
| Density, $\rho$ (kg/m <sup>3</sup> ) | 250  |
| Porosity, $\theta$                   | 0.85                                       |
| Specific heat, $c_p$ (J/kgK)         | $420 + 2.09T_s - 6.85 \times 10^{-4}T_s^2$ |
| Conductivity, $\lambda_s$ (W/mK)     | 0.1  |

$$\frac{\partial}{\partial t} \left( (1 - \chi) \rho_s Y_{i,s} \right) = w_{i,s}^{gs} \quad (9)$$

The symbols are defined in Nomenclature. Exchange of species, mass and energy between the two phases was enabled by a two-way coupling model [22, 24].

Turbulence in both freeboard and bed region was accounted for using standard  $\kappa$ - $\epsilon$  model. Interaction between turbulence and chemistry was solved using eddy dissipation concept. Weighted-sum-of-gray-gas-model (WSGGM) [25], was used as a property model for the radiating gases.

Proximate and ultimate analyses for the samples investigated in this study are presented in Table 1 and physical properties in Table 2. The latter are based on the Mehrabian et al. [26] work.

Chemical kinetics of wood conversion in the bed was simulated using different sub-models, which consisted of drying model, pyrolysis model, homogeneous reaction model and heterogeneous reaction model. Kinetics data of these sub-models are given in Table 3. The rate expressions for these reactions are presented in Table 4. These models were adopted from previous research on wood combustion [27-32]. However, in this work oxy-fuel combustion was accounted for by incorporating a reaction involving CO<sub>2</sub> (R(10)) and its associated chain-branching reactions (R(11) and R(12)) in the ho-

mogeneous reaction sub-model. Char combustion rate was evaluated based on partial pressure of O<sub>2</sub>, CO<sub>2</sub> and H<sub>2</sub>O available at its surface [33]. The stoichiometric ratio of CO<sub>2</sub> to CO from char combustion is dependent on particle surface temperature [27]:

$$\Omega = \frac{2(1 + 4.3 \exp[-3390 / T_{particle}])}{2 + 4.3 \exp[-3390 / T_{particle}]} \quad (10)$$

Grid independent solutions were achieved by meshing computational domain into highly-refined unstructured grid as shown in Fig. 2. A quarter of the burner was used for computation since it has a double symmetry. The choice of mesh size was based on a mesh independent test whose results are shown in Fig. 3. The predicted temperature profile at 5 cm from bed bottom under oxy-fuel condition is significantly different when using a mesh that consists of 100000 cells as compared to that of 200000 cells. The difference in temperature profiles is negligible for mesh that consists of 200000, 300000 and 400000 cells, respectively. Therefore, a mesh with 200000 cells was used for all the cases computed.

Oxidizer enters the domain through inlet boundary located at the bottom. The concentration of oxygen and N<sub>2</sub>/CO<sub>2</sub>/Ar was set in accordance to the required predesigned conditions. In the first set of experiments, O<sub>2</sub> concentration by volume was varied between 21 % and 50 % with diluent as either N<sub>2</sub> or CO<sub>2</sub>. In addition, four mixtures were designed to separate the effects of CO<sub>2</sub> environment. The four mixtures were denoted by letters A, B, C and D and their composition by volume was 21 % O<sub>2</sub>/79 % N<sub>2</sub>; 21 % O<sub>2</sub>/22.5 % CO<sub>2</sub>/56.5 % Ar; 40 % O<sub>2</sub>/60 % CO<sub>2</sub>; and 40 % O<sub>2</sub>/47 % CO<sub>2</sub>/13 % Ar, respectively. The inlet mass flux for the mixture for all the tests was 0.1 kg/m<sup>2</sup>/s. The temperature for each of the mixture at the inlet was 295 K. Top boundary was the outlet boundary with temperature and gases concentration gradient set to zero using Neumann boundary condition. A stationary wall with no-slip conditions was considered; the tangential velocity at the wall was explicitly set to zero. The model includes terms to account for heat transfer by radiation and convection at the wall. Emissivity of the surface and coefficient of heat transfer were 0.8 and 10 W/m<sup>2</sup>.K, respectively.

### 3. Results and discussion

Measured temperature profiles at various distances from bed bottom for wood combustion in 21 % oxygen in N<sub>2</sub> and CO<sub>2</sub> are presented in Figs. 4(a) and (b), respectively. The graphs show that the temperature profile at any given height in both environments exhibits similar behavior. They all have two peaks. When the flame front reaches an ignition point, the temperature rises rapidly to the first peak. Then it decreases gradually to another point and finally rises to the second peak.

Combustible pyrolysis products such as CH<sub>4</sub>, tar, H<sub>2</sub> and CO are oxidized through exothermic reactions which generate heat, subsequently increasing the temperature. The exothermic

Table 3. Biomass kinetic model.

| Drying   |                                 | Rate expression   |      |          | Source |
|--|---------------------------------|---|------|----------|--------|
| R(1) Wet wood $\rightarrow$ Dry wood + H <sub>2</sub> O (g)  |                                 | $R_{dry} = Y_b \rho_{b, wet} 1.610^{27} \exp(-25000 / T_s)$ |      |          | [27]   |
| Pyrolysis  |                                 |   |      |          |        |
| Reaction   | $K_i = A_i T^n \exp(-E_i / RT)$ |   |      | Source   |        |
|  | $A_i$ (s <sup>-1</sup> )        | $E_i$ (kJ/mol)  | $n$  |          |        |
| R(2) Dry wood $\rightarrow$ Gas  | $111 \times 10^9$               | 177   | 0    | [28]     |        |
| R(3) Dry wood $\rightarrow$ Tar  | $9.28 \times 10^9$              | 149   | 0    | [28]     |        |
| R(4) Dry wood $\rightarrow$ Char   | $30.5 \times 10^9$              | 125   | 0    | [28]     |        |
| R(5) Tar $\rightarrow \gamma_i \text{Tar}_{inert} + \gamma_{CO} \text{CO} + \gamma_{CO_2} \text{CO}_2 + \gamma_{H_2} \text{H}_2 + \gamma_{CH_4} \text{CH}_4$ | $9.55 \times 10^4$              | 93.37   | 0    | [29, 30] |        |
| Homogeneous gas-phase reactions  |                                 |   |      |          |        |
| Reaction   | $K_i = A_i T^n \exp(-E_i / RT)$ |   |      | Source   |        |
|  | $A_i$ (s <sup>-1</sup> )        | $E_i$ (kJ/mol)  | $n$  |          |        |
| R(6) 2CO + O <sub>2</sub> $\rightarrow$ 2CO <sub>2</sub>   | $2.24 \times 10^{12}$           | 167.36  | 0    | [29, 30] |        |
| R(7) CH <sub>4</sub> + 2O <sub>2</sub> $\rightarrow$ CO <sub>2</sub> + 2H <sub>2</sub> O   | $11.6 \times 10^{13}$           | 202.5   | 0    | [29, 30] |        |
| R(8) 2H <sub>2</sub> + O <sub>2</sub> $\rightarrow$ 2H <sub>2</sub> O  | $2.19 \times 10^9$              | 109.2   | 0    | [29, 30] |        |
| R(9) Tar + 2.9O <sub>2</sub> $\rightarrow$ 6CO + 3.1H <sub>2</sub>   | $9.2 \times 10^6$               | 80.2  | 0    | [29, 30] |        |
| R(10) CO + OH $\rightarrow$ CO <sub>2</sub> + H  | $4.76 \times 10^7$              | 0.293   | 1.3  | [31]     |        |
| R(11) H + O <sub>2</sub> $\rightarrow$ O + OH  | $2.65 \times 10^{16}$           | 71.347  | -0.7 | [31]     |        |
| R(12) H <sub>2</sub> + O <sub>2</sub> $\rightarrow$ OH + OH  | $2.51 \times 10^{12}$           | 163.075   | 0    | [32]     |        |
| R(13) H <sub>2</sub> O + CO $\rightarrow$ CO <sub>2</sub> + H <sub>2</sub>   | 2.78                            | 12.55   | 0    | [27, 28] |        |
| R(14) CO <sub>2</sub> + H <sub>2</sub> $\rightarrow$ H <sub>2</sub> O + CO   | 93.69                           | 46.594  | 0    | [27, 28] |        |
| Heterogeneous reactions  |                                 |   |      |          |        |
| Reaction   | $K_i = A_i T^n \exp(-E_i / RT)$ |   |      | Source   |        |
|  | $A_i$ (s <sup>-1</sup> )        | $E_i$ (kJ/mol)  | $n$  |          |        |
| R(15) $\Omega \text{C} + \text{O}_2 \rightarrow 2(\Omega - 1)\text{CO} + (2 - \Omega)\text{CO}_2$  | $2.54 \times 10^{-3}$           | 74.8  | 0    | [29, 30] |        |
| R(16) C + CO <sub>2</sub> $\rightarrow$ 2CO  | $1.81 \times 10^{-2}$           | 130   | 0    | [29, 30] |        |
| R(17) C + H <sub>2</sub> O $\rightarrow$ CO + H <sub>2</sub>   | $1.81 \times 10^{-2}$           | 130   | 0    | [29, 30] |        |

Table 4. Rate expression for the reactions.

| Reaction | Rate expression   | Reaction | Rate expression                                      |
|----------|---|----------|--|
| R(2)     | $w_b = K_2 \rho_{b, dry}$   | R(10)    | $R_{CO} = K_{10} [\text{CO}] [\text{OH}]$            |
| R(3)     | $w_b = K_3 \rho_{b, dry}$   | R(11)    | $R_H = K_{11} [\text{O}] [\text{OH}]$                |
| R(4)     | $w_b = K_4 \rho_{b, dry}$   | R(12)    | $R_{H_2} = K_{12} [\text{H}_2] [\text{O}_2]$         |
| R(5)     | $w_{Tar} = K_5 \rho_{Tar}$  | R(13)    | $R_{H_2O} = K_{13} [\text{H}_2\text{O}] [\text{CO}]$ |
| R(6)     | $R_{CO} = K_6 [\text{CO}] [\text{O}_2]^{0.25} [\text{H}_2\text{O}]^{0.5}$ | R(14)    | $R_{CO_2} = K_{14} [\text{CO}_2] [\text{H}_2]$       |
| R(7)     | $R_{CH_4} = K_7 [\text{CH}_4]^{0.7} [\text{O}_2]^{0.8}$                   | R(15)    | $w_{char, O_2} = K_{15} P_{O_2} S_{a, char}$         |
| R(8)     | $R_{H_2} = K_8 [\text{H}_2] [\text{O}_2]$                                 | R(16)    | $w_{char, CO_2} = K_{16} P_{CO_2} S_{a, char}$       |
| R(9)     | $R_{Tar} = K_9 [\text{Tar}]^{0.5} [\text{O}_2]$                           | R(17)    | $w_{char, H_2O} = K_{17} P_{H_2O} S_{a, char}$       |

reactions occur concurrently with pyrolysis and drying of wood particles, which are endothermic reactions and cause decrease in temperature after the first peak. When pyrolysis and drying processes are completed, exothermic reactions dominate and temperature rises again to the second peak. After the second peak, the temperature gradually decreases until the end of combustion. During this phase, a wood particle has completely been devolatilized, leaving a pure char that under-

goes oxidation and gasification with H<sub>2</sub>O and CO<sub>2</sub>. It is deduced that gasification, which is endothermic, is more pronounced than exothermic process (oxidation), hence the temperature decrease.

Figs. 4(a) and (b) also show that at corresponding height, air-fuel peak temperature is higher than oxy-fuel temperature by about 200 K. This is a result of the combination of both chemical and thermal effects. Lower temperatures are seen in

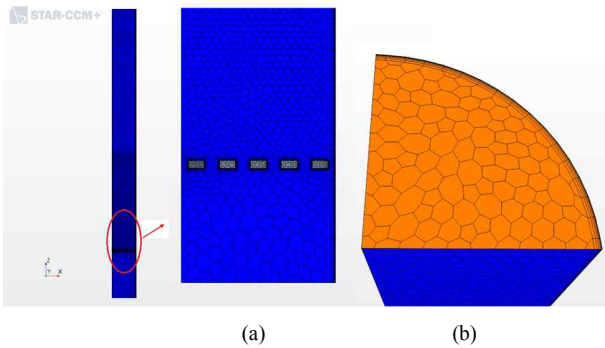


Fig. 2. Computational mesh for the fixed bed: (a) Highly refined mesh in fuel bed and grate; (b) prismatic layers near the wall.

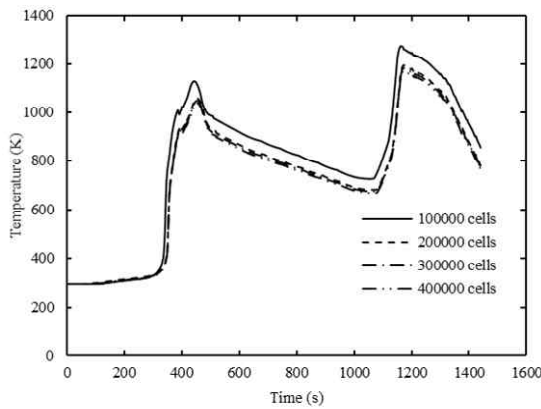
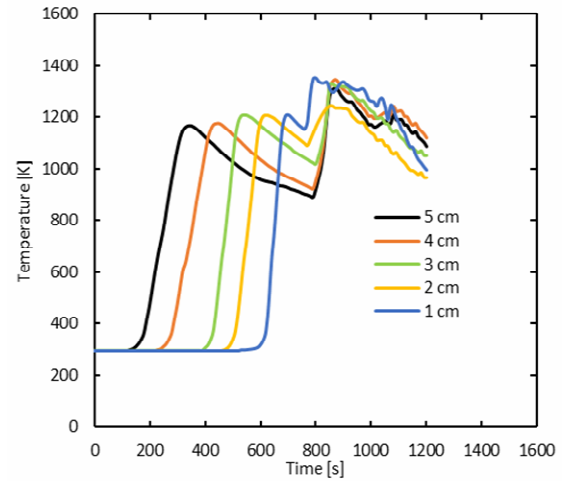


Fig. 3. Predicted temperature profiles at 5 cm from the bed bottom for wood combustion in 21 % O<sub>2</sub>/79 % CO<sub>2</sub> mixture for different mesh sizes.

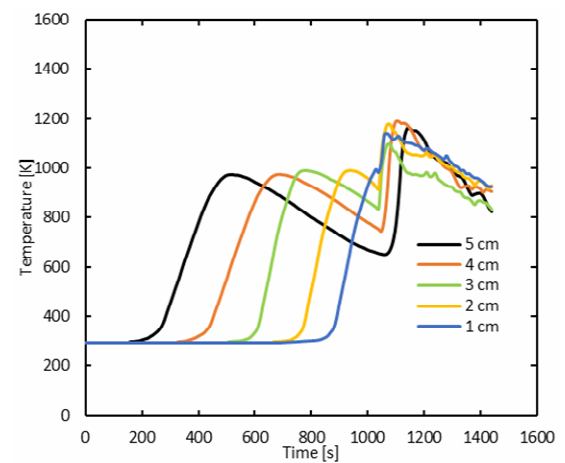
oxy-fuel environment because CO<sub>2</sub> has higher heat capacity than N<sub>2</sub>. Furthermore, chemical effect through endothermic reaction of CO<sub>2</sub> with char contributes in lowering the temperature of oxy-fuel environment.

The individual contribution of various effects of CO<sub>2</sub>, namely, chemical, thermal and oxygen concentration effects are evaluated through CFD-DEM modeling. The model results are validated by comparing them with experimental values. Shown in Fig. 5 are measured and predicted temperature profiles at 5 cm from bed bottom for air-fuel and oxy-fuel environments both at 21 % O<sub>2</sub> concentration. The accuracy of model data was good with deviation of most points from measured values being within 10 %.

Presented in Fig. 6 are predicted temperature profiles at 5 cm from the bed bottom for wood combustion in different combustion atmospheres. It is observed that peak temperature occurrence time comes much earlier in N<sub>2</sub> atmosphere than in CO<sub>2</sub> atmosphere. This is an indication that combustion rate is slower in CO<sub>2</sub> environment. For oxy-fuel combustion, peak temperature value is directly proportional to O<sub>2</sub> concentration. In addition, its occurrence time increases as O<sub>2</sub> concentration is decreased. Peak temperature of oxy-fuel atmosphere, which is equivalent to that of standard air-fuel condition, occurs at about 40 % O<sub>2</sub> concentration. However, its occurrence time is



(a) 21 % O<sub>2</sub>/79 % N<sub>2</sub> mixture



(b) 21 % O<sub>2</sub>/79 % CO<sub>2</sub> mixture

Fig. 4. Measured temperature profiles at various distances from the bed bottom for wood combustion in different combustion atmospheres.

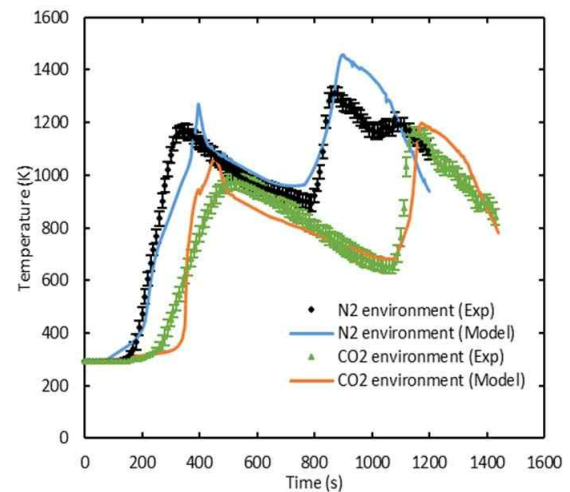


Fig. 5. Measured and predicted temperature profiles at 5 cm from the bed bottom for wood combustion in 21 % O<sub>2</sub>/79 % N<sub>2</sub> and 21 % O<sub>2</sub>/79 % CO<sub>2</sub> mixtures. Error bars are the standard deviations.

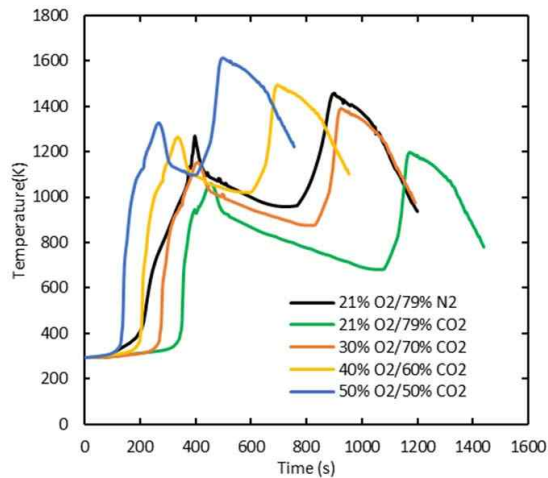


Fig. 6. Predicted temperature profiles at 5 cm from the bed bottom for wood combustion in different combustion atmospheres.

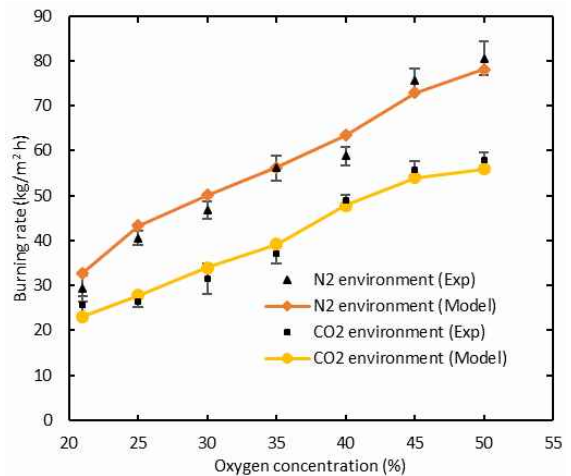


Fig. 8. Measured and predicted burning rates for fuel bed of wood combustion in  $N_2$  and  $CO_2$  environments. Error bars are the standard deviations.

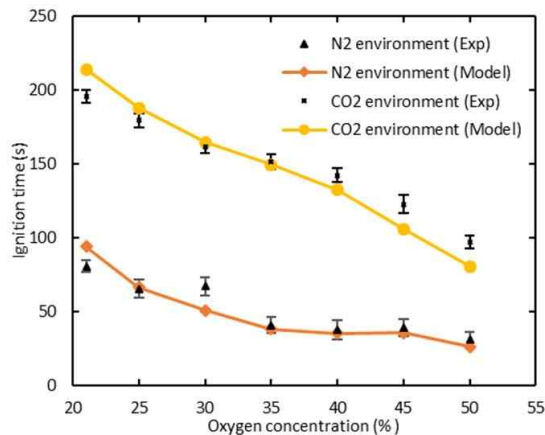


Fig. 7. Measured and predicted ignition time for fuel bed of wood combustion in  $N_2$  and  $CO_2$  environments. Error bars are the standard deviations.

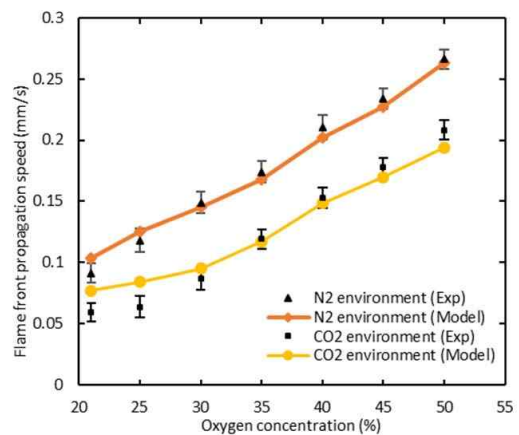


Fig. 9. Measured and predicted flame front propagation speed for fuel bed of wood combustion in  $N_2$  and  $CO_2$  environments. Error bars are the standard deviations.

slightly earlier than in air-fuel condition.

The time taken for the reaction front to start at the top surface of the fuel bed was defined as ignition time. Presented in Fig. 7 is ignition time for wood combustion in both oxy-fuel and air-fuel environments. The graph shows that at any given oxygen concentration, ignition time in oxy-fuel environment is almost twice that of corresponding air-fuel condition. Retarded ignition in  $CO_2$  environment could be attributed to its high specific heat capacity and low  $O_2$  diffusivity in it. In both cases, ignition time gradually decreases as oxygen concentration is increased.

A comparison of burning rates for wood combustion in  $N_2$  and  $CO_2$  burning conditions is presented in Fig. 8. At the same  $O_2$  concentration, the burning rate in  $CO_2$  burning atmosphere is less than in  $N_2$  burning atmosphere. The burning rate of wood particles in oxy-fuel condition is lowered by the aforementioned  $CO_2$  effects, which contribute differently as will be discussed later. Thermal diffusivity of  $CO_2$  is less than that of

$N_2$  by about 35 % [34]. In addition,  $CO_2$  absorbs radiative heat more than  $N_2$ . The overall effect of these thermal properties of  $CO_2$  is a decrease in burning rate as seen in Fig. 8. Furthermore, the burning rate in oxy-fuel environment is also decreased by chemical effect of  $CO_2$  through Boudouard reaction R(16), which is endothermic. On the other hand, the role played by dilution is clearly demonstrated in Fig. 8. In both cases, burning rate is directly proportional to  $O_2$  concentration. More  $O_2$  concentration enhances oxidation of combustible pyrolysis products and char, hence releasing more heat and increases the burning rates.

Illustrated in Fig. 9 is the flame front propagation speed for wood combustion in oxy-fuel and air-fuel burning atmospheres. For all oxygen concentrations,  $CO_2$  burning atmosphere had lower propagation speed as compared to  $N_2$  burning atmosphere. Furthermore, as oxygen concentration increased flame propagation speed also increased. Flame speed is directly linked to the burning rate. Therefore, the factors which

reduce the burning rates in oxy-fuel environment as discussed in the preceding paragraph are also responsible for the reduced flame speed.

The species and temperature profiles along axial length of the fixed bed when the flame front is at 4 cm from the grate for 21 % O<sub>2</sub>/79 % CO<sub>2</sub>, 30 % O<sub>2</sub>/70 % CO<sub>2</sub>, 40 % O<sub>2</sub>/60 % CO<sub>2</sub> and 50 % O<sub>2</sub>/50 % CO<sub>2</sub> are presented in Figs. 10(a)-(d). The flame structures are similar in profile but differ in magnitude. The flame front for the mixture with high O<sub>2</sub> concentration, 50 %, reaches 4 cm plane at 191 s, which is earlier than those for 40 %, 30 % and 21 % that reached the plane at 275 s, 360 s and 482 s, respectively. This is because flame speed increases as O<sub>2</sub> concentration is increased. As shown in Figs. 10(a)-(d) and Table 5, the amount of tar and CH<sub>4</sub> is high at the reaction zone of 21 % O<sub>2</sub> concentration mixture and decreases gradually for 30 %, 40 % and 50 % O<sub>2</sub> concentration mixtures. The graphs show that the mixture with 21 % O<sub>2</sub> concentration is operating under fuel rich conditions and does not have enough O<sub>2</sub> to oxidize these species through reactions R(7) and R(9). On the other hand, the graphs show that the mixtures with 30 %, 40 % and 50 % O<sub>2</sub> concentration are operating under fuel lean conditions and have excess O<sub>2</sub> in their reaction zones. Thus, reduced amount of tar and CH<sub>4</sub> are observed in these mixtures as compared to those of 21 % O<sub>2</sub> concentration mixture. Consequently, since these reactions are exothermic, a high amount of heat is released as O<sub>2</sub> concentration is increased. This is seen in the peak temperatures attained by these mixtures, Fig. 6. The high amount of heat released increases the heating rates for the particles in the bed and explains the higher flame front propagation speed and burning rates for high O<sub>2</sub> concentration mixtures. High heat energy also accelerates the ignition of the particles for mixtures with high O<sub>2</sub> concentration.

Figs. 10(a)-(d) and Table 5 show that the amount of CO is highest in the reaction zone of the mixture with 30 % O<sub>2</sub> concentration. The mixtures with 21 %, 40 % and 50 % O<sub>2</sub> concentration have almost the same amount of CO in their reaction zone. Unlike tar and CH<sub>4</sub> whose sole source is devolatilization of the wood particles, CO is produced from devolatilization process, oxidation of tar through reaction R(9) and char gasification with CO<sub>2</sub> through reaction R(16). CO is consumed by oxidation reaction R(6). For a mixture with high O<sub>2</sub> concentration, excess O<sub>2</sub> brings an antagonistic effect to the amount of CO where there is a tendency for high consumption through oxidation reaction R(6) and high production by oxidation of tar through reaction R(9) as compared to that of a mixture with low O<sub>2</sub> concentration. However, for mixtures with high O<sub>2</sub> concentration, the production of CO through char gasification could be less than that of low O<sub>2</sub> concentration mixture because of low amount of CO<sub>2</sub>. The overall effect of these reactions is that there is an increase in CO production as O<sub>2</sub> concentration is increased up to a peak point, then it starts to decrease.

Burning rate, ignition of fuel particles and flame front propagation speed are all influenced by thermal behavior of

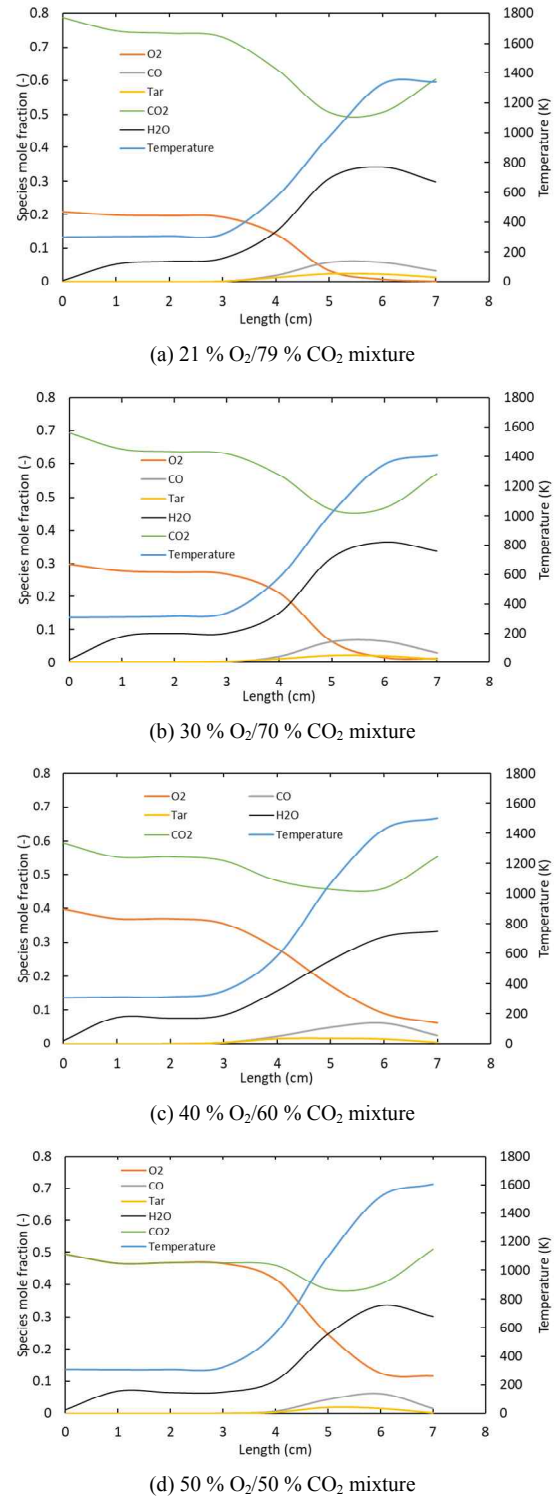


Fig. 10. Species and temperature profiles along axial length of the bed for different O<sub>2</sub>/CO<sub>2</sub> mixtures when the flame front is at 4 cm from the grate.

the bed. Apart from heat of combustion through chemical reactions discussed in the preceding paragraphs, flame temperature at a given point is also determined by heat flux distribution in the bed, which is mostly by radiation. H<sub>2</sub>O and CO<sub>2</sub> are the main products of combustion that participate in radi-

Table 5. Peak values of major combustible species and temperature profiles for wood combustion in different O<sub>2</sub>/CO<sub>2</sub> mixtures.

| Temperature/<br>species mole<br>fraction (-) | O <sub>2</sub> /CO <sub>2</sub> mixture |                     |                     |                     |
|--|---|---------------------|---------------------|---------------------|
|  | 21 % O <sub>2</sub>                     | 30 % O <sub>2</sub> | 40 % O <sub>2</sub> | 50 % O <sub>2</sub> |
| Temperature (K)                              | 1338                                    | 1406                | 1499                | 1605                |
| Tar  | 0.02427                                 | 0.02164             | 0.01605             | 0.01837             |
| CO   | 0.05839                                 | 0.06488             | 0.06013             | 0.06124             |
| CH <sub>4</sub>                              | 0.00819                                 | 0.00769             | 0.00542             | 0.00684             |

tion. The presence of high amount of CO<sub>2</sub> in an oxy-fuel environment makes it more emissive than air-fuel environment. As depicted by the flame temperatures in Figs. 6 and 10, a large amount of heat energy is released in the fuel bed with a high O<sub>2</sub> concentration mixture. In this study, the heat energy contribution from different sources has not been separated. Therefore, an increase in heat energy cannot be explicitly linked to a particular source. Though, in the region of intense combustion, heat contributed by combustion is more dominant; the contribution by radiation heat flux is only 10-15 % [35].

Wood combustion in four different mixtures of O<sub>2</sub> and Ar/CO<sub>2</sub>/N<sub>2</sub> was numerically simulated so as to separate the various effects of CO<sub>2</sub> on burning rate of wood. For all the cases, temperature profiles at 5 cm from fuel bed were considered. A method of adjusting the flame temperature using Ar, which was initially proposed by Du et al. [15] and previously used by other researchers [14, 16, 17], was implemented in this study. The compositions of the four mixtures are specified in Sec. 2.2. Furthermore, other properties of the different mixtures such as mass fraction of the constituents, combined heat capacity and oxygen diffusion coefficient are provided in Table 6. These properties were evaluated and compared at room temperature (298 K), ignition temperature (500 K) and flame temperature (1400 K). Combustion of wood in mixtures A, B and C was designed to have the same peak temperatures, as shown in Fig. 11. A large amount of Ar in mixture B was to increase the peak temperature, which is low when CO<sub>2</sub> alone is used as a diluent. As shown in Table 6, this mixture has a lower specific heat capacity. This enabled the mixture to have the same peak temperature as that of mixture A and C. The peak temperature of wood combustion in mixture D was higher than for the other three by 167 K.

The burning rates of wood combustion in the four mixtures were evaluated and presented in Fig. 12. Burning rate in mixture A was used as a datum. The difference in burning rates of combustion in mixture A and B is due to chemical effect because they have the same oxygen concentration and temperature values. Since temperature is the only similar parameter for combustion in mixture A and C, then the difference in their burning rate is due to a combination of oxygen concentration and chemical effect. Oxygen concentration effect is achieved when oxygen concentration is increased to 40 % while maintaining the same temperature in CO<sub>2</sub> environment (combustion

Table 6. Composition, combined heat capacity and O<sub>2</sub> diffusion coefficient of the four mixtures at different temperatures.

| Properties   | Gas mixtures    |       |       |       |       |
|--|-----------------|-------|-------|-------|-------|
|  | A               | B     | C     | D     |       |
| Mass fraction of components (-)  | O <sub>2</sub>  | 0.233 | 0.171 | 0.327 | 0.331 |
|  | CO <sub>2</sub> | 0.000 | 0.253 | 0.673 | 0.535 |
|  | N <sub>2</sub>  | 0.767 | 0.000 | 0.000 | 0.000 |
|  | Ar              | 0.000 | 0.576 | 0.000 | 0.134 |
| c <sub>p</sub> for the mixture (kJ/kg K)                                 | At 298 K        | 1.005 | 0.670 | 0.868 | 0.825 |
|  | At 500 K        | 1.030 | 0.725 | 1.006 | 0.939 |
|  | At 1400 K       | 1.209 | 0.826 | 1.255 | 1.147 |
| O <sub>2</sub> diffusion coefficient in the mixture (cm <sup>2</sup> /s) | At 298 K        | 0.209 | 0.184 | 0.156 | 0.164 |
|  | At 500 K        | 0.513 | 0.462 | 0.398 | 0.415 |
|  | At 1400 K       | 2.888 | 2.642 | 2.310 | 2.401 |

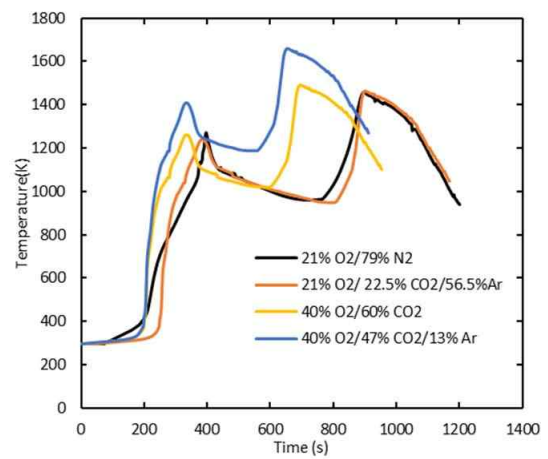


Fig. 11. Predicted temperature profiles at 5 cm from the bed bottom for wood combustion in four combustion environments.

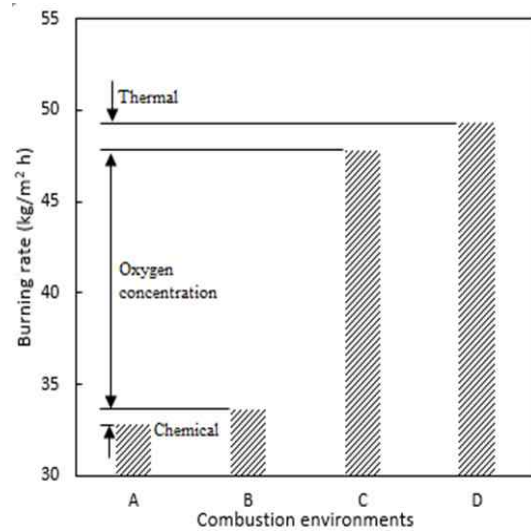


Fig. 12. Predicted separate effects of CO<sub>2</sub> on burning rates for wood combustion in four combustion environments.



tion in mixture B and C). Finally, the difference in burning rates for combustion in mixture C and D is due to thermal effect since they have the same oxygen concentration but different temperature values.

The individual contribution of CO<sub>2</sub> effects on burning rates of wood combustion is evaluated from Fig. 12. It was established that chemical, thermal and oxygen concentration influenced burning rate of wood by 5 %, 9 % and 86 %, respectively. It is evident that oxygen concentration is the most influential parameter in the burning rate. As oxygen concentration is increased, oxidation of char and combustible pyrolysis products is also enhanced. Therefore, more heat is generated and fuel burning rate is significantly improved. The influence of thermal and chemical is not very significant. Thermal effect is only 9 % and translate to a temperature change of 167 K. Chemical effect on the burning rate is quite small because the rate of the chemical reactions involving CO<sub>2</sub> consumption (R(14) and R(16)) is far much less compared to the rate of (R(6) and R(13)).

#### 4. Conclusions

The overall and separate effects of CO<sub>2</sub> burning atmosphere on the combustion properties of wood burning in a fixed bed were investigated through numerical modeling. Modeling was validated by comparison with measured data. The following are the key findings:

- The dilution effect is the most influential parameter on the burning rate of wood combustion in an oxy-fuel system. The influence of thermal and chemical is not very significant.
- Peak temperature of oxy-fuel atmosphere, which is equivalent to that of standard air-fuel condition, occurs at a higher O<sub>2</sub> concentration. However, its occurrence time is slightly earlier than in air-fuel condition.
- At any given oxygen concentration, ignition time in oxy-fuel is almost twice that of corresponding air-fuel condition. In both cases, ignition time gradually decreases as oxygen concentration is increased.
- At the same oxygen concentration, burning rate and flame propagation speed in CO<sub>2</sub> combustion environment was less than in N<sub>2</sub> combustion environment.

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#### Nomenclature

*A* : Arrhenius pre-exponent factor [s<sup>-1</sup> (mol m<sup>-3</sup>)]

|                        |  |
|------------------------|--|
| <i>A<sub>s</sub></i>   | : Particle surface area [m <sup>2</sup> ]                                      |
| <i>c<sub>p</sub></i>   | : Specific heat [J kg <sup>-1</sup> K <sup>-1</sup> ]                          |
| <i>C<sub>1</sub></i>   | : Permeability [m <sup>2</sup> ]   |
| <i>C<sub>2</sub></i>   | : Inertia loss coefficient [m <sup>-1</sup> ]                                  |
| CFD                    | : Computation fluid dynamics   |
| <i>d</i>               | : Particle diameter [m]  |
| <i>D</i>               | : Diffusivity [m <sup>2</sup> s <sup>-1</sup> ]                                |
| DEM                    | : Discrete element method  |
| <i>E</i>               | : Activation energy [J mol <sup>-1</sup> ]                                     |
| <i>g</i>               | : Gravity [m s <sup>-2</sup> ]   |
| <i>G</i>               | : Incident radiative heat flux [W m <sup>-2</sup> ]                            |
| <i>h</i>               | : Enthalpy [J kg <sup>-1</sup> ]   |
| <i>h<sub>c</sub></i>   | : Convective heat transfer coefficient [W m <sup>-2</sup> K <sup>-1</sup> ]    |
| <i>H<sub>i</sub></i>   | : Enthalpy of formation of species <i>i</i> [J kg <sup>-1</sup> ]              |
| <i>J</i>               | : Diffusion mass flux [kg m <sup>-2</sup> s <sup>-1</sup> ]                    |
| <i>K</i>               | : Rate constant [s <sup>-1</sup> (mol m <sup>-3</sup> )]                       |
| <i>N<sub>g</sub></i>   | : Number of gas species [-]  |
| <i>p</i>               | : Pressure [Pa]  |
| <i>q<sub>R</sub></i>   | : Radiative heat flux [W m <sup>-2</sup> ]                                     |
| <i>Q<sub>a,p</sub></i> | : Particle absorption coefficient [-]  |
| <i>R</i>               | : Universal gas constant [J mol <sup>-1</sup> K <sup>-1</sup> ]                |
| <i>S<sub>a</sub></i>   | : Specific surface area [m <sup>-1</sup> ]                                     |
| <i>S<sub>E</sub></i>   | : Energy source term [J m <sup>-3</sup> s <sup>-1</sup> ]                      |
| <i>S<sub>M</sub></i>   | : Momentum source term [kg m <sup>-2</sup> s <sup>-2</sup> ]                   |
| <i>t</i>               | : Time [s]   |
| <i>T</i>               | : Temperature [K]  |
| <i>v</i>               | : Velocity [m s <sup>-1</sup> ]  |
| <i>w<sub>i</sub></i>   | : Rate of production of species <i>I</i> [kg m <sup>-3</sup> s <sup>-1</sup> ] |
| WSGGM                  | : Weighted-sum-of-gray-gas-model   |
| <i>Y</i>               | : Mass fraction [-]  |

#### Greek symbols

|            |  |
|------------|--|
| $\epsilon$ | : Turbulent dissipation rate [J kg <sup>-1</sup> s <sup>-1</sup> ] |
| $\theta$   | : Particle porosity [-]  |
| $\kappa$   | : Turbulent kinetic energy [J kg <sup>-1</sup> s <sup>-1</sup> ]   |
| $\lambda$  | : Thermal conductivity [W m <sup>-1</sup> K <sup>-1</sup> ]        |
| $\mu$      | : Viscosity [kg m <sup>-1</sup> s <sup>-1</sup> ]                  |
| $\rho$     | : Density [kg m <sup>-3</sup> ]                                    |
| $\sigma$   | : Stefan-Boltzmann constant [W m <sup>-2</sup> K <sup>-4</sup> ]   |
| $\tau$     | : Shear stress tensor [Pa]   |
| $\chi$     | : Region porosity [-]  |
| $\Omega$   | : Stoichiometric coefficient [-]                                   |

#### Subscripts

|            |                                   |
|------------|-----------------------------------|
| <i>b</i>   | : Biomass                         |
| <i>e</i>   | : Effective                       |
| <i>g</i>   | : Gas                             |
| <i>i</i>   | : <i>i</i> <sup>th</sup> reaction |
| <i>i,g</i> | : Gaseous species                 |
| <i>i,s</i> | : Solid-phase species             |
| <i>p</i>   | : Particle                        |
| <i>s</i>   | : Solid                           |

### Superscript

$g_s$  : Heterogeneous reaction  
 $n$  : Exponent

### Operators

$\nabla$  : Gradient operator  
 $\nabla \cdot$  : Divergence operator

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