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Roles of CO_2 and H_2O in premixed turbulent oxy-fuel combustion

Shenghui Zhong[a], Fan Zhang[a,*], Zhijun Peng[a,*], Fuqiang Bai[b], Qing Du[a]

[a] State Key Laboratory of Engines, Tianjin University, 135 Yaguan Rd, Tianjin 300350, China
[b] Internal Combustion Engine Research Institute, Tianjin University, Tianjin 300072, China

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ABSTRACT

A series of Two-Dimensional Direct Numerical Simulation (2-D DNS) cases are performed to investigate the effects of CO_2 and H_2O on premixed turbulent oxy-fuel combustion (case oxy-H_2O, case oxy-CO_2) in a constant vessel. A DNS solver for low Mach reacting flow is developed based on open source code OpenFOAM. The chemical effects of CO_2 and H_2O are isolated by a pair of artificial species. 2-D DNS results shows the flame surface of oxy-CO_2 case trends to be wrinkled with small convex and concave structures due to a lower laminar flame speed and a smaller effective Lewis number. Moreover, the response of flame surface to the curvature is different with corresponding dilute agent. Owing to the high binary diffusion coefficient between H_2O and H, the negative curvature effect on fast diffusing species, e.g. H and H_2, are enhanced in oxy-H_2O, and results in a higher burning velocity. The effects of CO_2 on H transport are contrary to the effects of H_2O and the oxidation process is slowed due to the elementary reaction $CO_2 + H \Leftrightarrow CO + OH$, which result in a more uniform Heat Release Rate (HRR) distribution on flame surface. In addition, chemical reaction pathway analysis is performed to elucidate the chemical effects of CO_2 and H_2O. It is found that CO_2 and H_2O will cool down the temperature of burnt region compared with N_2. Finally, an alternative solution is raised to counteract the negative effect of CO_2 on flame speed, which should be useful in the development and design of oxy-fuel combustion.

1. Introduction

As it has been evidenced that CO_2 has a serious effect on global warming, the reduction of CO_2 emissions has been a major topic in energy and environment area in recent years. Oxy-fuel combustion due to its potential to reduce the CO_2 emissions dramatically by the way of Carbon Capture and Storage (CCS) has attracted significant attention [1–4]. Meanwhile, it produces zero emissions of NO_x by replacement of CO_2 and H_2O (water steam) to N_2 as existing in traditional air/fuel mixture. This solves the problem of the tradeoff between NO_x and soot, as well. As a consequence, oxy-fuel combustion provides a practical way to the environmental-friendly clean combustion model.

However there is still a long way to put forward an application of oxy-fuel combustion mode in the current power plant due to two main challenges: (1) to fit oxy-fuel combustion into the current power plant and (2) to maintain a high thermal efficiency while keeping a low level of energy consumption in the process of tail gas treatment with CCS [3]. It has been shown that with high level of CO_2-stream impurities more energy will be consumed in order to capture and storage CO_2 [5]. The impurities are mainly from redundant O_2 or fuel due to the incomplete combustion and also the remaining nitrogen and argon which is hard to remove completely from the air in the pre-combustion process. Therefore, it motivates stoichiometric oxy-fuel combustion. The feasibility of oxy-fuel combustion in gas turbines has been investigated extensively with regard to the application of integrated gasification combined cycle with CCS [2]. Liu et al. [6] found that if the mixture is not supplied properly, the flame can be unstable, and there exists a tradeoff between flame stability and extremely high flame temperature. The same phenomenon is also found in Nemitallah's work [7] for which the results showed that increasing the fraction of O_2 in the oxidizer will improve the flame stability and increase the flame temperature. Kutne [8] studied partially premixed mixture of $CH_4/O_2/CO_2$ with O_2 fractions 20–40% and equivalence ratios of 0.5–1 by experiments and found that the flame shape and stabilization are primarily effected by the O_2 fraction compared to the equivalence ratio, and oxy-fuel combustion has a larger heat loss than conventional combustion. Besides the high flame temperature, it was reported by Di Benedetto [9,10] that high oxygen fraction could lead to an anomalous pressure peak in a constant vessel, which has been attributed to the onset of superheating water vaporization explosion at the vessel walls.

Abbreviations: 1-D, One-Dimensional; 2-D, Two-Dimensional; CCS, Carbon Capture and Storage; DNS, Direct Numerical Simulation; HRR, Heat Release Rate; PDF, Probability Density Function; PISO, Pressure Implicit Split Operator; PRR, Pressure Rising Rate; ROP, Rate of Production

* Corresponding authors.
E-mail addresses: fanzhang_lund@tju.edu.cn (F. Zhang), pengzj@tju.edu.cn (Z. Peng).

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Apart from the practical application of oxy-fuel combustion, the effects of the dilute agents on laminar flame compared to air-fired condition are studied as well, such as the inhibition effect of CO_2 and H_2O since they have higher thermal heat capacity than N_2 resulting in lower adiabatic flame temperature, and laminar flame speed [11–16]. More fuel and less dilution are required to get similar combustion characteristics to air-fired condition. In addition to the thermal effect, it has been figured out that CO_2 has a significant chemical effects primarily through the chemical reaction of $CO_2 + H \Leftrightarrow CO + OH$ [14,15]. The competition of CO_2 for H through the most important chain branching reaction $H + O_2 \Leftrightarrow O + OH$ will slow down overall reaction rates and has a great impact on the production of CO in the reaction zone [16]. Recently the chemical effects of H_2O and CO_2 on flame temperature are studied using 1-D simulation of opposed diffusion flame with detail chemical kinetics mechanism GRI 3.0 by Song and Zou [17,18]. It showed that the overall chemical effects of CO_2 and H_2O are evident, and CO_2 has a passive effect on flame temperature while H_2O has a positive effect because reaction $H + O_2 + H_2O \Leftrightarrow HO_2 + H_2O$ is enhanced by providing sufficient HO_2. Different mole fractions of oxygen in the oxidizer lead to the diverse reaction paths. It is consistent with [19,20], where it is found that CO_2 has a stronger chemical effect than H_2O on laminar burning velocity. Xu [20] further investigated four pairs of artificial species in four isolated aspects: (1) thermal effects, (2) chemical effects, (3) transport effects and (4) radiation effects in a non-premixed laminar syngas flame. Mazas [21] studied the effect of H_2O on laminar burning velocity of oxygen-enriched flame. It is found that H_2O has a significant chemical effect in lean and near-stoichiometric conditions, but in high level oxygen condition H_2O can be considered as an inert dilution. Sebastian [22] presented an experimental laminar diffusion flame comparison study of oxy-CO_2 and air-fired condition. They found oxy-CO_2 leads to higher CO and H_2O concentrations and lower peak flame temperature. The effects of CO_2 dilution with mixtures of CH_4 and air on turbulent premixed flame were experimentally studied by Kobayashi [23,24], and they found the turbulent burning velocity and the smallest wrinkle scale in the flame front decrease with increasing CO_2 ratios.

As most of previous oxy-fuel combustion studies focus on the laminar flame condition, the characteristic of oxy-fuel combustion with turbulence is less investigated, especially by DNS method. Moreover, owing to the physical properties of dilutions in Table 1 and the chemistry effects of different dilutions, the interaction of turbulent-chemistry can be different. The investigation about turbulent premixed oxy-fuel combustion is significantly necessary. To the best of authors' knowledge, DNS study of oxy-fuel turbulent combustion is less investigated to date. DNS method is a powerful tool to study the interaction between chemistry and turbulence, which can also provide the detail information of the flame structure including the curvature and strain rate effects. The main object of the this research is by DNS method to figure out the roles of CO_2 and H_2O in oxy-fuel combustion and their effects on HRR, Flame Displacement Speed S_d and flame surface structure in oxy-fuel turbulent premixed combustion under suitable dilute ratio in a constant vessel. It is expected to provide a more comprehensive understanding of oxy-fuel combustion for better combustion performance in industrial combustors.

Table 1
Comparison of physicochemical properties at 1000 K, 0.1 MPa [17].

Gas	Density (mol/m^3)	C_v (J/mol·K)	C_p (J/mol·K)	Therm.Cond. (W/m·K)	ρC_p (J/m^3·K)	Therm. Diff (m^2/s)
H_2O	12.03	32.963	41.293	0.097085	496.754	0.000195
CO_2	12.025	46	54.322	0.070571	653.222	0.000108
N_2	12.023	24.386	32.703	0.065991	393.188	0.000168

2. Numerical method

2.1. Governing equations

A low Mach number reacting flow solver with detailed transport properties is developed in the open source code OpenFOAM [25], named as reactingDNSFoam. The detailed transport properties are calculated by the logarithm polynomial fitting method [26] as:

$$\ln M_i = \sum_{n=1}^{n} a_{n,i} (\ln T)^{n-1} \tag{1}$$

$$\ln D_{ij} = \left(\sum_{n=1}^{n} b_{n,ij} (\ln T)^{n-1} \right)^{*} p/p_{ref} \tag{2}$$

Here, M_i is i_{th} species viscosity or thermal conductivity, D_{ij} the binary diffusivity of i_{th} and j_{th} species. p is the pressure and p_{ref} denotes the standard atmosphere pressure. In this study, the third order polynomial fits (i.e., n = 4) is used, which can guarantee the fitting errors are well within one percent [26].

The conservation equations for total mass, momentum, chemical species and energy are solved in their compressible formulation. The conservation of total mass is given as:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = 0 \tag{3}$$

And the momentum equation reads:

$$\frac{\partial \rho \vec{v}}{\partial t} + \nabla \cdot (\rho \vec{v} \vec{v}) = -\nabla p + \nabla \cdot \mu (\nabla \vec{v} + (\nabla \vec{v})^T - \frac{2}{3} I \nabla \vec{v}) + \rho \vec{g} \tag{4}$$

where μ is mixture dynamic viscosity, and the semi-empirical Wilke formula is used to compute the μ. Only N − 1 chemical species equations are solved, and the diluent species (here is the species who possesses the maximum mass fraction) is obtained by writing $Y_d = 1 - \sum_{i=1}^{N-1} Y_i$ and absorbs all inconsistencies introduced by Eq. (5) [27].

$$\frac{\partial \rho Y_i}{\partial t} + \nabla \cdot (\rho \vec{v} Y_i) = \dot{\omega}_i - \nabla \cdot (\vec{J_i}) \tag{5}$$

$$\vec{J_i} = -\rho D_i \nabla Y_i \tag{6}$$

The reaction rate of i_{th} species $\dot{\omega}_i$ is computed by summing up the Arrhenius rates from all participant elementary reactions. $\vec{J_i}$ is the dilute approximate of diffusion flux of species i. And the D_i is the mass diffusivity of i_{th} species, which is calculated by:

$$D_i = \frac{\sum_{i \neq j}^{N} X_j M_j}{M \sum_{i \neq j}^{N} X_j / D_{ij}} \tag{7}$$

with X_i is mole fraction, while M_i and M denote the molecular weight of i_{th} species and mean molecular weight, respectively. The conservation equation of energy is formulated in terms of sum of sensible enthalpy and kinetic energy:

$$\frac{\partial \rho h_s}{\partial t} + \nabla \cdot (\rho \vec{v} h_s) + \frac{\partial \rho K}{\partial t} + \nabla \cdot (\rho \vec{v} K) = \nabla \cdot \left(\frac{\lambda}{C_p} \nabla h_s \right) + \dot{\omega}_T + \frac{dp}{dt} + \nabla \left(\rho \sum_{i}^{N} h_{ki} \vec{J_i} \right) \tag{8}$$

where h_s is the sensible enthalpy, and K is the kinetic energy $U^2/2$. λ and C_p are mixture thermal conductivity and heat capacity, respectively. Mixture heat capacity is calculated based on individual species mass fraction, and λ is defined as:

$$\lambda = \frac{1}{2} \left(\sum_{i=1}^{N} X_i \lambda_i + \frac{1}{\sum_{i=1}^{N} X_i / \lambda_i} \right) \tag{9}$$