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Methane combustion in various regimes: First and second thermodynamic-law comparison between air-firing and oxyfuel condition

Yaming Liu [a], Sheng Chen [b, c, d, *], Shi Liu [a], Yongxin Feng [a], Kai Xu [a], Chuguang Zheng [b]

[a] *Electric Power Research Institute of Guangdong Power Grid Company, Guangzhou 510080, China*
[b] *State Key Laboratory of Coal Combustion, Huazhong University of Science and Technology, Wuhan 430074, China*
[c] *Institute for Modelling and Simulation in Fluodynamics, Nanoscience and Industrial Mathematics "Gregorio Millán Barbany", Universidad Carlos III de Madrid, Leganes 28911, Spain*
[d] *Faculty of Engineering, The University of Nottingham, University Park, Nottingham NG7 2RD, UK*

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ABSTRACT

MILD oxyfuel combustion has been attracting increasing attention as a promising clean combustion technology. How to design a pathway to reach MILD oxyfuel combustion regime and what can provide a theoretical guide to design such a pathway are two critical questions that need to be answered. So far there has been no open literature on these issues. A type of combustion regime classification map proposed in our previous work, based on the so-called "Hot Diluted Diffusion Ignition" (HDDI) configuration, is adopted here as a simple but useful tool to solve these problems. Firstly, we analyze comprehensively the influences of various dilution atmosphere and fuel type on combustion regimes. The combustion regime classification maps are made out according to the analyses. In succession, we conduct a comparison between the map in air-firing condition and its oxyfuel counterpart. With the aid of the second thermodynamic-law analysis on the maps, it is easy to identify the major contributors to entropy generation in various combustion regimes in advance, which is crucial for combustion system optimization. Moreover, we find that, for the first time, a combustion regime classification map also may be used as a safety indicator. With the aid of these maps, some conclusions in previous publications can be explained more straightforwardly.

1. Introduction

Although industrial and academic communities always pursue to develop a more efficient way to generate heat and power, combustion is still playing a predominant role in energy conversion of most daily and industrial applications, not only in current stage but also in the visible future [1]. Combustion usually faces two main challenges: (1) to improve the efficiency of combustion processes and (2) to reduce air pollutant products by combustion processes. The former is extremely important for industries as it contributes to their operational costs while the public pays high attention on the latter as it concerns our well-being. Unfortunately, there is a tradeoff between these two respects as in general it is difficult to eliminate air pollution while maintaining a high combustion efficiency. To overcome this difficulty, some innovative combustion technologies are inspired recently. Among them, two, namely MILD (Moderate or Intense Low oxygen Dilution) combustion [2] and oxyfuel combustion [3], attract increasing attention.

Compared with the conventional combustion technologies, MILD combustion is a type of "slow" reaction as the reactants are diluted to moderate the oxidization rates of fuels. Consequently, the peak temperature of combustion will decrease and the temperature distribution will become even, which can eliminate thermal NO_x production effectively [2]. Meanwhile, it was found that unburnt hydrocarbon products also could be reduced significantly by MILD combustion [4]. It is an interesting feature as few available combustion technologies can satisfy, simultaneously, the requirements of low NO_x emission and low unburnt hydrocarbon production. More excitingly, it was observed that fuel nitrogen translation also could be suppressed in MILD condition [5]. Due to its intrinsic advantages, MILD combustion is regarded as a promising clean

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* Corresponding author. Faculty of Engineering, University of Nottingham, UK.
E-mail address: shengchen.hust@gmail.com (S. Chen).

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combustion technology in this century [2]. Until now, numerous research has been published on MILD combustion. The majority of them may fall into five categories. The first one tries to classify different combustion regimes by a map, which can straightforwardly illustrate the relationship between various combustion regimes. De Joannon et al. discussed how to classify combustion regimes in a number of different combustion configurations [6–8]. In their work the influences of various combustion pressures were also investigated. In order to classify combustion regimes more conveniently, some of the present authors [9] proposed to adopt the effective equivalence ratio of reactants and the temperature of oxidant flow as the coordinate axes, instead of those used in Refs. [6,7], to plot the map, as these two parameters can be obtained directly from practical combustion systems. The above studies all are based on the so-called counter-flow combustion configuration. Recently, Wang et al. [10] investigated the combustion regimes of a co-flow configuration. They observed that in co-flow combustion there was a quasi-MILD regime which was similar with MILD combustion but did not share the same features of MILD combustion. More recently, Evans et al. [11] proposed a new approach, based on the initial/final temperature and the effective activation energy of reaction, to classify combustion regimes. Their effort provided an insight into classification of different types of combustion. The second category focuses on the special reaction structures of MILD combustion. Szego et al. [12] reported the profiles of temperature and concentration inside a lab-scale furnace operated in MILD combustion condition. Their work paid high attention on how to form MILD combustion stably. A so-called jet in hot coflow (JHC) burner was designed in Ref. [13]. The temporally and spatially resolved measurements of reactive scalars were carried out with the aid of this equipment. As it can prevent atmosphere to affect the fine reaction structures of MILD combustion within the core zone, the JHC burner has been widely used in the MILD combustion research community, especially for MILD combustion simulation. The influences of different fuels on reaction structures of MILD combustion also have been reported [14,15]. It was found that MILD combustion was highly flexible to various fuels. As MILD combustion is a kind of “bulk” combustion, therefore the furnace chamber shape would influence MILD combustion more significantly, as compared with traditional combustion modes. Recently some of the present authors discussed such topic [16]. The results demonstrated that a larger divergence angle of a furnace would be better to establish MILD combustion. The publications on reaction structures of MILD combustion are too many to be listed here. A detailed review on it has been presented in Refs. [2,17]. The efforts on simplified reaction mechanisms of MILD combustion constitute the third category, which is indispensable for industrial-scale simulation. Kim et al. [18] compared different global reaction mechanisms for MILD combustion simulation. As their study was based on the so-called “Sandia Flame-D” which is not a typical MILD combustion research prototype, the conclusions drawn in Ref. [18] were questionable. Some of the present authors also made a comprehensive comparison between several popularly used global reaction mechanisms, with the aid of the JHC configuration [19]. It was observed that these global reaction mechanisms all could predict the major concentrations sufficiently accurately, except carbon monoxide. Based on the analyses, the same authors proposed a new global reaction mechanism for MILD combustion research [20]. Compared against the GRI-Mech3.0, Hamdi et al. [21] proposed a 5-step and a 9-step reduced reaction mechanism for natural gas MILD combustion simulation. They claimed that the latter was better for NO_x and CO prediction. Nitrogen translation pathways in MILD combustion condition were also investigated [22–26]. Some studies revealed that the NNH and N_2O routes were the most important pathways in NO formation in MILD condition [27–31]. The next category covers the aerodynamics of MILD combustion. Historically, MILD combustion can be looked as a variant of High Temperature Air Combustion (HiTAC) [2]. Consequently, in the early stage of MILD combustion research, preheating of reactants was regarded as one of the necessary conditions to establish MILD combustion. Later, it was found that aerodynamics played a predominant role on sustaining MILD combustion and a MILD regime might be formed in a furnace even without preheating [32]. In succession, it was reported, compared with traditional combustion modes, molecular diffusion could not be ignored in the MILD combustion regime investigated in Ref. [33]. The latest research concentrates in the effect of aerodynamics on reaction rates of fuels in MILD regime, namely the so-called turbulence-chemistry interaction [34,35], as it has been widely accepted that most popularly used models for turbulence-chemistry interaction were not suitable for MILD combustion simulation [9]. The above research all are based on the first thermodynamic-law analysis. Recently, a number of studies starting from the second thermodynamic-law begin to emerge. In this paper they are classified as the last category. In Ref. [36] it was revealed that the exergy efficiency of a lab-scale furnace operated in MILD combustion regime is significantly higher than that under conventional combustion conditions. The same authors showed this conclusion could hold water for different fuels [37]. A comparison of entropy generation between different combustion regimes was made by the present authors [9]. It was observed that the maximum exergy loss in hydrogen-air MILD combustion regime depended closely on a number of operational parameters.

At first, the oxyfuel combustion technology was developed to address the global warming challenge due to the intensive man-made CO_2 emissions [3,38]. Soon, it was observed that some air pollutant products also could be suppressed in oxyfuel condition [39]. Numerous studies have been published during the past decades on different aspects of oxyfuel combustion, such as burner design [40,41], reaction mechanisms [42,43], techno-economic assessment [44,45] and so on. A number of review papers are also available [39,46,47]. A latest review on numerical modeling of oxyfuel combustion is presented in Ref. [48]. The oxyfuel combustion technology is regarded as one of the most promising options in the near future to restrict CO_2 concentration in the atmosphere [3]. Until now, some pilot-scale demonstrations have been built up and a number of commercial-scale units are under consideration [49].

To remedy some shortcomings of the “standard” oxyfuel combustion technology, recently a so-called MILD oxyfuel conception was proposed [20,50–53]. The MILD oxyfuel combustion is an organic combination of MILD and oxyfuel technologies, namely to establish and sustain a MILD combustion regime in CO_2/O_2 atmosphere [20]. Originally, the present authors proposed this new conception to utilize biogas with a higher efficiency [20,51]. Later, it was extended to different fuels [50,52,53]. The fine structures of MILD oxyfuel combustion have been investigated with the aid of numerical simulation [20,51–53] and its feasibility has also been proven by experimental studies [50]. However, as a recently emerging research area, a lot of efforts are still required to deepen our insight into it. For example, from the viewpoint of industrial practice, it is impossible to reach a MILD oxyfuel regime directly. According to our experimental experience, a safe pathway to establish and sustain a MILD oxyfuel regime in a furnace may be: air-firing → oxyfuel combustion → MILD oxyfuel regime [54]. However, how to design a safe and effective transition pathway is still an open question. More important, we should answer what can be used as a theoretical guide to design such a transition pathway for practical applications. Unfortunately until now nobody has focused on these critical problems. After a careful consideration, a