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Effects of partial premixing on NO production in methanol/dimethyl ether counterflow flames

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ABSTRACT

In this study, the effects of partial premixing on NO production in methanol/dimethyl ether counterflow flames were investigated through the simulation of counterflow flames. Two types of partially premixed counterflow flames were computed: methanol-side premixed counterflow flames and dimethyl ether-side premixed counterflow flames. These two types of flames were both air-side partially premixed ones because the strategy of partial premixing was to add excessive air into one side of counterflow to produce the lean fuel/air mixture while remaining the fuel stream on the other side. The computation results showed that there were two flame reaction zones in these air-side partially premixed flames. For both types of flames, NO was primarily produced in the non-premixed flame zone through the formation routes of thermal and prompt NO and the destruction pathway of reburn NO. In the premixed flame zone, the reactions related to NO were not active, but the NO_2 reactions could be promoted with partial premixing. For both types of flames, with the increase in the premixing equivalence ratio, the peak concentrations of NO and its peak production rates were decreased, but the integrated NO production and NO emission index showed the significantly different variations. All studied flames presented the decreased NO production when their strains increased.

1. Introduction

The damaging roles of nitric oxide (NO) have been well recognized. It is one of the most important factors in the production of photochemical smog and the destruction of the ozone layer of atmosphere. The excessive NO emission causes serious pollution. Combustion of fossil fuels is a primary source of NO emission, the regulation of NO is therefore a hot topic in combustion community. Non-premixed combustion is the most common fuel utilization style, but it also presents a significant drawback: high yields of NO and soot in flame. Partial premixing is derived from non-premixed combustion and has been considered as an effective approach of lowering NO and even soot emission while keeping the high efficiency of non-premixed flame [1]. Counterflow flame, also called as opposed-flow flame is an optimal model for the theoretical investigation of non-premixed flame (NF). Counterflow flame is generally stabilized between two opposed jets of fuel and oxidizer, and owns the convenience in getting the numerical solution due to its one-dimensional flame feature [2]. Partially premixed flames (PPFs) can be easily obtained on the basis of counterflow flame configure by adjusting the components of fuel and oxidizer jets. PPF remains one-dimensional flame feature as well. Therefore, the counterflow flame configure had also been extensively adopted in the fundamental studies on PPF.

A PPF is characterized by the hybrid flame containing multiple reaction zones [1]. The common structure of a PPF consists of three forms, i.e. "double", "triple" and "edge" flame. In most of cases, a counterflow PPF can be commonly described as a double flame containing two reaction zones, namely, a premixed zone and non-premixed zone. These double-flame zones of PPFs are spatially separated from each other, but synergistically coupled through thermochemical and fluid-dynamic interactions between them. These flame zones of PPFs are merged together or separated from each other, according to the variations in the partial premixing level, the global strain rate of flame, and even fuel types, and consequently the flame shows the fickle features which are different from those of non-premixed or premixed flame [1,3]. The interactions within multiple reaction zones of PPFs have been identified as one of the most important factors for flame structure variations. The effects of partial premixing on non-premixed flames, such as broadening the flammability [4], improving the stability [5–7], and lowering soot emissions [8,9], have been well addressed.

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The effects of partial premixing on NO formation have been extensively discussed as well [10]. Barlow et al. [11] made a numerical and experimental investigation on NO formation in laminar counterflow partially premixed methane/air flames and found that the heat radiation largely determined the accuracy of NO prediction. Blevins and Gore [12] computed the structures of partially premixed methane/air counterflow flames at low strain rates and indicated that these PPFs showed two NO formation regions, which respectively corresponded to two CH peak concentrations in flame. Mungekar and Atreya [13] reported that, for partially premixed methane/air flames, the peak concentration and emission index of NO were increased firstly and subsequently decreased with the progressive partial premixing, and that the critical equivalence ratio of partial premixing was about 2.2. Ravikrishna and Laurendeau [14] measured and computed NO distribution in partially premixed methane/air flames respectively with Laser-induced Fluorescence technique and flame modeling and found that, under high partial premixing levels, NO produced in the premixed flame zone was primarily prompt NO and that the contribution of thermal NO accounted for a large proportion of NO production in the non-premixed flame zone. Aggarwal and his co-workers [15–17] made a series of studies on NO formation in PPFs, explored the effects of the premixing equivalence ratio, fuel type and flame strain rate, and suggested that, in PPFs, NO production mainly involved thermal NO mechanism and prompt NO mechanism and that the NO reburn mechanism was the key reaction route for NO destruction. The results also indicated that that the relative contributions of thermal NO and prompt NO to NO production were strongly influenced by the equivalence ratio of premixed stream, but not sensitive to the variation in the strain rate of flame.

There are three common ways to stabilize a PPF: adding some amount of oxidizer into fuel stream, premixing fuel into oxidizer or premixing at both streams. For most of PPFs, partial premixing is generally applied on the fuel side by adding a certain amount of oxidizer into the fuel stream because the procedure is handy for treating both gaseous and liquid fuels. Gaseous fuels can be freely mixed with air and the entrainment caused by high pressure spray is a common way to achieve the premixing of liquid fuels with oxidizer. The PPFs with fuel-side premixing generally have two reaction zones. One is the rich premixed flame (RPF) near the fuel stream, and the other is the non-premixed flame (NF) near the oxidizer stream. Recently, the study on PPFs with partial premixing on the oxidizer side has also attracted adequate attention. Especially for liquid fuels, adding some volatile and active fuels into the oxidizer stream is a promising combustion technology widely used in compression ignition engines and has an euphonious name of reactivity charge compression ignition (RCCI) [18]. The flame in a RCCI engine can be considered as a PPF stabilized between a rich premixed stream caused by the entrainments of high pressure spray and a lean premixed mixture of active fuel and air previously mixed in the air inlets of engine. The flame structure generally consists of a rich premixed flame and a diffusion flame at the fuel spray side as well as a lean premixed reaction zone near the air side. The literature review indicated that the pioneering study on the effects of air-side premixing on PPFs might be done by McNesby et al. [19]. They comparatively studied the different behaviors of ethane/air counterflow flames with fuel-side and air-side ethanol premixing, and found that a lean premixed flame (LPF) was aroused on the oxidizer side with the addition of air-side premixing. The existence of LPF could promote OH production in flame and consequently lead to the significant reduction of soot emissions of non-premixed ethane/air flames. Wada et al. [20] and Park and Chang [21] studied the structures of counterflow flames with air-side premixing as well and confirmed the importance of LPF and the interactions between LPF and NF.

Previous studies were mostly focused on the counterflow PPFs with partial premixing on the fuel side, but the characteristics of PPFs with partial premixing on the oxidizer side were seldom reported. The flame behaviors are closely related to the interactions between different flame zones. In order to understand air-side partial premixing combustion and NO chemistry in RCCI engines, it is necessary to explore the flame dynamics between lean premixed flames and non-premixed flames. In this work, dimethyl ether and methanol were selected as the studied fuels because both of them were coal-based fuels and their emissions in combustion were low [22]. The combination of dimethyl ether and methanol in combustion can improve the cleaning utilization level of coal, reduce atmospheric pollutions, and enhance the energy security in China. The counterflow flames were stabilized between two opposing jets, one containing a lean premixed fuel/air mixture and the other being pure fuel stream. We computed the structure of partially premixed flames of dimethyl ether (DME)/methanol in counterflow with the validated fuel/air chemistries. This investigation primarily focused on the influences of the partial premixing at methanol-side and dimethyl ether-side on NO formation characteristics in terms of some significant parameters of PPFs, such as the equivalence ratio of premixed stream and the global flame strain.

2. Flame modeling methodology

In the study, the counterflow flame model was used to compute the structure of PPFs. The physical model of counterflow flame is basically an axisymmetric laminar diffusion flame. As shown in Fig. 1, two streams, one stream containing a lean premixed fuel/air mixture and the other stream containing pure fuel, go reversely from two identical tube burners. These two axisymmetric jets intersect together at a specific position between the two burners, and then radially expand. The stagnation plane (SP) is the intersection plane between the two jets. At the SP, the axial velocities of both streams are decreased to zero. After the counterflow streams are ignited, two flames can be observed. One is a lean premixed flame close to the premixing side and the other is a non-premixed one near the side of the fuel stream. All the premixed mixtures of the studied PPFs were lean. The premixing procedure was just like adding a small amount of fuel into the oxidizer side of a non-premixed counterflow flame. These flames were air-side partially premixed ones.

The governing equations for partially premixed counterflow flames consists of the steady state continuity equation of gas and the conservation equations for mass, momentum, chemical species, and energy. The numerical solutions for them were conducted with OPPDIF code on the basis of Newton iteration methodology [23]. The numerical iteration of OPPDIF is initiated on a coarse mesh of flame temperature, to yield the velocity distribution in flame, by resolving the steady state continuity equation and momentum conversation equations of gas. With the temperature and velocity distributions of flame, the conservation equations for mass, chemical species, and energy can be resolved, to complete the first-round iteration and yield the species structures and an updated temperature profile of flame. The next round

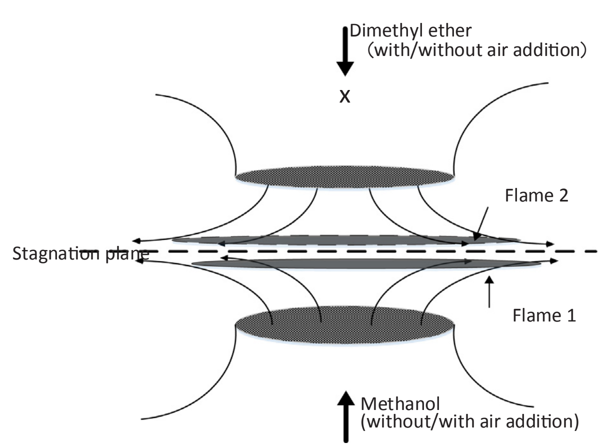

Fig. 1. Schematic diagram of the partially premixed counterflow flames.