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A numerical investigation on NO_X formation in counterflow *n*-heptane triple flames

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Abstract

The formation of NO_X in counterflow *n*-heptane/air triple flames was investigated by numerical simulation. Detailed chemistry and complex thermal and transport properties were employed. The results indicate that a triple flame produces more NO and NO_2 than the corresponding premixed flames due to not only the appearance of the diffusion flame but also the interaction between different flame branches. The relative contributions of different routes to NO formation in the premixed flame branches change with the variation of the equivalence ratio, but the thermal mechanism always dominates in the diffusion flame branch. The interaction between flame branches is enhanced with the decrease of the distance between them. Both heat and radical exchange between flame branches contribute to the interaction. A new feature that does not exist in methane/air triple flame was observed in *n*-heptane/air triple flames, i.e. when the rich mixture equivalence ratio is higher, there are two peaks of CH concentration on the rich side of the diffusion flame branch, which leads to that some NO is formed beside the diffusion flame branch by the prompt route.

Keywords: Triple flame; NO_X; Laminar flame; Stratified combustion; Premixed flame

1. Introduction

Triple flames are of great importance for both industrial applications and fundamental combustion research. They play a significant role in flame attachment, lift-off, ignition and re-ignition processes of non-premixed systems. Many theoretical and experimental studies have been devoted to the structure and propagation of triple flames from various viewpoints [1–8]. However, fewer studies on NO_X formation in triple flames have been reported.

On the other hand, the formation of NO_X in combustion processes is of considerable practical interest because of the need to control pollutant formation. There have been many studies on the mechanism of NO_X formation. Miller and Bowman [9] presented an excellent review of NO_X formation mechanism. Based on the chemistry presented in this review paper, the formation of NO_X in methane/air double flames and two-dimensional laminar jet diffusion flames were respectively investigated by Nishioka et al. [10] and Ju and Niioka [11]. The effect of radiation heat loss on NO_X formation in counterflow flames was studied by several groups [12–16]. Atreya et al. [17] investigated the effect of change in flame structure on the formation of NO_X. An investigation on NO formation in an axisymmetric laminar diffusion flame was presented by Smooke et al. [18]. Naik and Laurendeau [19,20] studied NO formation in counterflow partially-premixed and non-premixed flames under sooting oxy-fuel and high pressure conditions. Sohn et al. [21] reported a study on the effects of pressure and air-dilution on NO formation in laminar counterflow diffusion flames of methane in high temperature air combustion. Xue and Aggarwal [22] and Bertra et al. [23] studied NO formation in *n*-heptane/air partially premixed flames. Naha and Aggarwal [24] investigated fuel effect on NO_X emissions in double flames. It has been quite clear from these studies that NO_X formation in a flame is closely related to the flame structure.

A triple flame consists of a diffusion flame embedded between a fuel lean and a fuel rich premixed flame. The structure of a triple flame is different from those of either the correspond-

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ing premixed flames, or traditional diffusion flames. Furthermore, because of the coexistence of the three flame branches, there are interactions among them that may affect the formation of NO_X in a triple flame. Our previous study [25] on NO_X formation in methane/air triple flames showed that NO_X formation in triple flames differs from in either premixed or diffusion flames.

n-heptane is a relatively heavy hydrocarbon fuel that is generally used to simulate diesel combustion. Study of NO_X formation in *n*-heptane triple flames is of help in understanding the mechanism of NO_X formation in diesel combustion. The purpose of the present paper is to numerically investigate NO_X formation in *n*-heptane/air triple flames. The discussion first focus on the results for two typical triple flames that exhibit the most significant features of triple flames. Then the effect of the variation in the equivalence ratio of the lean or rich mixture is examined. Finally the formation of NO_2 and N_2O is briefly discussed.

2. Numerical model

The flame configuration studied is an axisymmetric counterflow laminar flame. The governing equations can be found elsewhere [26]. The calculations were carried out with a code revised from that of Kee et al. [27]. Upwind and center difference schemes were used for the convective and diffusion terms, respectively, in all the governing equations. Adaptive refinement of meshes was done to obtain grid independent result. The pressure and the fresh mixture temperature were, respectively, 1 atm and 300 K. Radiation heat transfer was calculated by an optically thin method [28]. The distance between the two opposed jets was kept as 4.0 cm in all the simulations.

Potential and plug flow assumptions were alternately used in the literature for the free stream conditions in the simulation of counterflow flames. They usually generated similar qualitative results [29]. As a pure numerical study, the potential flow assumption was employed in this paper.

The reaction mechanism for the oxidation of *n*-heptane was one developed at the University of California, San Diego [30]. This mechanism has been validated by Li and Williams [31]. The nitrogen chemistry used was taken from GRI-Mech 3.0 [32], since it has been shown to offer reasonable prediction for NO formation at various flame conditions [20,33]. The combined mechanism consists of 303 elementary steps and 61 species. The thermal and transport properties were calculated by algorithms given in [34,35].

3. Results and discussion

The simulations were carried out for both triple and premixed flames for the sake of comparison. A counterflow triple flame (CFTF) was formed when a lean and a rich *n*-heptane/air mixture were respectively issued from the opposed nozzles, while a counterflow premixed flame (CFPF) was formed when the same mixtures were issued. A stretch rate of 60 s^{-1} was specified for all flames. This was an arbitrary choice. However, effect of the variation in stretch rate will be briefly discussed. In Figs. 1–9, the lean mixtures come from the left side, and the rich mixtures from the right side. The equivalence ratio is represented by ϕ.

3.1. Heat release rate distribution

To easily understand the characteristics of NO_X formation in triple flames, the heat release rate distribution of two typical counterflow *n*-heptane/air triple flames (Flames 1 and 2) is presented in Fig. 1. The equivalence ratios of the lean and rich *n*-heptane/air mixtures are 0.7 and 1.3 for Flame 1, and 0.7 and 2.0 for Flame 2. The reason to choose these two flames is that they both show typical triple flame structure, but the interaction among different flame branches varies for them.

The structure of triple flames is clearly illustrated. There are three heat release regions for each flame. The left one is due to the combustion of the lean mixture, while the right one is due to the rich mixture. These two heat release regions are named lean and rich premixed flame branches. Between these two flame branches, there is a relatively weak heat release region, named diffusion flame branch, which is because of the reaction of the excess oxygen from the lean mixture and the excess burning components from the rich mixture. Although not shown, the simulation indicated that similar to methane/air triple flames [25], all the fuel of the rich mixture is decomposed in the rich premixed flame, while the oxygen from the lean mixture can penetrate to the diffusion flame branch. The burning components transported from the rich premixed flame to the diffusion flame are some intermediate species, like CO and H_2. The diffusion branch of Flame 1 is located around the stagnation plane, while that of Flame 2 is located on the left side of the stagnation plane. The heat release rate in the diffusion flame branch of Flame 2 is higher than that of Flame 1, and the distance between the diffusion and rich premixed flame branches in Flame 2 is shorter than that in Flame 1. These are caused by the higher equivalence ratio of the rich mixture in Flame 2 than in Flame 1, leading to more burning components, such as H_2 and CO, are burnt in the diffusion flame branch of Flame 2.

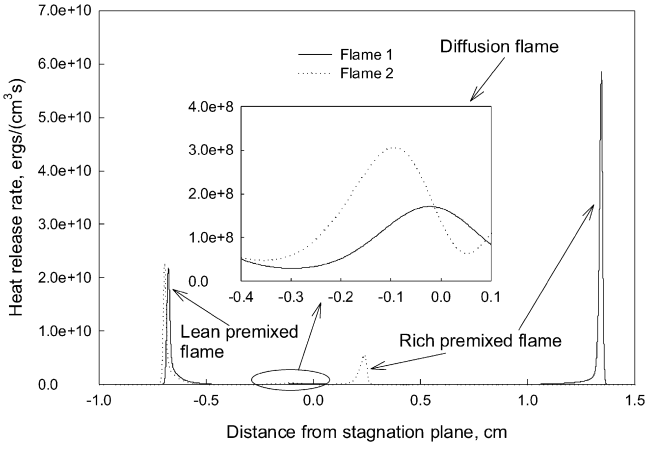

Fig. 1. Heat release rate distributions of two typical triple flames. Flame 1: $\phi_{lean} = 0.7$, $\phi_{rich} = 1.3$; Flame 2: $\phi_{lean} = 0.7$, $\phi_{rich} = 2.0$.