# A Numerical Study on NO Formation in Counterflow n-Heptane Triple Flames

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## Introduction

Many studies have been devoted to the structures and propagation of triple flames. However, fewer studies on  $NO_X$  formation in triple flames have been reported.

It has been shown that  $NO_X$  formation in a flame is closely related to the flame structure. Our recent study on  $NO_X$  formation in methane/air triple flames showed that the mechanism of  $NO_X$  formation in a triple flame is different from in either a premixed or a diffusion flame, due to the specific structure of a triple flame.

n-Heptane is a relatively heavy hydrocarbon fuel that is generally used to simulate a diesel combustion. The purpose of the present paper is to numerically investigate NO, the dominant component of  $NO_x$ , formation in n-heptane triple flames. The discussions first focus on the results for two typical triple flames that exhibit the most significant features of triple flames. Then the effects of the variation in the equivalence ratio of the lean or rich mixture and the stretch rate will be examined.

### **Numerical Model**

The flame configuration studied is an axisymmetric counterflow laminar flame. The potential boundary conditions were used. Upwind and center difference schemes were employed for the convective and diffusion terms, respectively, in all the governing equations. The pressure and the fresh mixture temperature were, respectively, 1 atm and 300 K. The reaction mechanism for the oxidation of n-heptane is one developed in UCSD [1]. The nitrogen chemistry used was taken from GRI-Mech 3.0 [2].

It has been known that NO can be formed through the thermal, the  $N_2O$  intermediate, the NNH intermediate, and the prompt routes, based on the initiation reactions by which molecular nitrogen is converted to atomic nitrogen or other intermediate species containing the nitrogen element. The method to identify the relative contributions of these four routes to the NO formation in a flame was described in [3]. The same method was used in this paper.

#### **Results and Discussion**

The simulations were carried out for both triple and premixed flames for 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<sup>-1</sup> was specified for all flames,

except for the discussion of the stretch rate effect. In all the plots, the lean mixtures come from the left side, and the rich mixtures from the right side. The equivalence ratio is represented by  $\phi$ .

Figure 1 shows the distributions of NO mole fractions in the first studied CFTF (Flame 1) obtained by the four different NO mechanisms [3] and in the corresponding CFPFs obtained by the full NO chemistry. Because of the symmetry, only halves of the CFPFs are displayed. It is observed that NO (full NO) starts to appear and increases rapidly on both outer edges of the CFTF. With the stagnation plane being gradually approached from two sides, the NO concentration gradually increases, and finally rises quickly. The maximum NO concentration is reached near the stagnation plane.

Figure 2 illustrates the NO formation rates in Flame 1 and the corresponding CFPFs. There are three main NO formation regions in the CFTF. These regions correspond to the three flame branches. The left and right ones are, respectively, the lean and rich premixed flame branches. Between them, there is a diffusion flame branch located around the stagnation plane.

In the premixed flame branch regions, the differences in the NO concentrations and formation rates between the CFTF and the corresponding CFPFs are negligible. However, the differences in the stagnation plane region become significant. In this region, the CFPFs almost do not produce NO, while the CFTF does significantly. This indicates that a triple flame produces more NO than the corresponding premixed flames due to the appearance of the diffusion flame branch.

The prompt route contributes most NO in the rich premixed flame branch of the CFTF. However, in the diffusion flame branch, the thermal mechanism dominates. In the reaction zone of the lean premixed flame branch, the NNH intermediate route is the most significant one.

Figures 3 and 4 display the distributions of NO mole fractions and formation rates in the second studied CFTF (Flame 2) and the corresponding CFPFs. Some new features are observed. For this CFTF, the NO concentration and production rate are higher than those of the corresponding CFPFs not only in the stagnation plane region, but also in the rich premixed flame branch region. The NO formation region in the rich premixed flame branch is further away from the stagnation plane than that in the corresponding rich CFPF. These differences are caused by the fact that the rich mixture of this CFTF is richer than that of Flame 1. Therefore the rich premixed flame branch in Flame 2 is closer to the diffusion flame branch than in Flame 1. The shorter distance enhances the interaction, caused by the radical and heat exchanges, between the diffusion and rich premixed flame branch of this CFTF is higher than that of the corresponding CFPFs. Therefore the interaction between the different flame branches in a triple flame is a very important feature that can enhance the NO formation and combustion intensity.

Figure 5 shows NO emission indices in different CFTFs. The equivalence ratio of the lean mixture ( $\phi_{lean}$ ) in Fig. 5a is 0.7, while that of the rich mixture ( $\phi_{rich}$ ) in Fig. 5b is 1.3. It is demonstrated that the variation of either  $\phi_{lean}$  or  $\phi_{rich}$  affects the formation of NO. When  $\phi_{lean} = 0.7$ , the NO emission index first decreases, then slightly increases and finally decreases again, with the increase of  $\phi_{rich}$ . The slight increase of NO formation when  $\phi_{rich}$  is increased from 1.3 to 1.4 is caused by the increase of prompt NO in the rich premixed flame branch. The final decrease is because of the reduced combustion intensity in the rich premixed flame branch for higher  $\phi_{rich}$ .

When  $\phi_{rich} = 1.3$ , the NO emission index first reduces, and then slightly increases again, with the decrease of  $\phi_{lean}$ . The first decrease is due to the reduction in the combustion intensity in the lean premixed flame branch. The final increase is because the contribution of the lean premixed flame branch to the NO formation in a CFTF is sharply reduced and the formation of NO in a

CFTF is actually dominated by that in its rich premixed and diffusion flame branches with the further decrease of  $\phi_{\text{lean}}$ .

The relative contributions of different routes to NO formation also change with the variation of either  $\phi_{lean}$  or  $\phi_{rich}$ . This is mainly caused by the variation in the relative contributions in the premixed flame branches. However, simulations indicated that the thermal route always dominates in the diffusion flame branch of a CFTF.

Figure 6 shows the effect of stretch rate on NO formation in CFTFs with  $\phi_{\text{lean}} = 0.7$  and  $\phi_{\text{rich}} = 1.3$ . It is indicated that the NO formation in a CFTF is reduced with the increase of stretch rate. This is caused by the decrease in the flame thickness, when the stretch rate is increased. Although the simulation was only conducted for a pair of specific lean and rich mixtures, it is reasonable to expect that this conclusion is valid for most CFTFs.

## Conclusions

A triple flame produces more NO than the corresponding premixed flames due to the appearance of the diffusion flame branch and the interaction between 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.

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#### **References:**

- 1. Williams, F.A., http://maeweb.ucsd.edu/~combustion/cermech/.
- 2. Gregory P. Smith et al., <u>http://www.me.berkeley.edu/gri\_mech/</u>.
- 3. Guo, H., Smallwood, G. J., Liu, F., Ju, Y., and Gülder, Ö. L., Proc. Comb. Inst. 30 (2005) 303-311.







Fig. 2 NO formation rates in the triple flame with  $\phi_{\text{lean}} = 0.7$  and  $\phi_{\text{rich}} = 1.3$ .



Fig. 3 Mole fraction of NO in the triple flame with  $\phi_{lean} = 0.7$  and  $\phi_{rich} = 1.6$ .



Fig. 4 NO formation rates in the triple flame with  $\phi_{\text{lean}} = 0.7$  and  $\phi_{\text{rich}} = 1.6$ .



Fig. 5 The effect of the equivalence ratio of rich or lean mixture on NO emission index.



Fig. 6 Effect of stretch rate on NO formation.