STUDIES ON THE IGNITION OF N-DECANE/TOLUENE BINARY FUEL BLENDS

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Summary In the present work, the ignition of n-decane/toluene binary fuel blends was investigated by numerical simulation considering detailed chemistry and transport. The emphasis was spent on assessing the kinetic and transport effects. Two different systems were investigated: a homogeneous flame configuration to examine the kinetic ignition prohibition, and a non-premixed counterflow configuration to examine the effect of transport. The kinetic and transport effects involved in these two systems were analyzed.

INTRODUCTION

Binary fuel blends are widely utilized in internal combustion engines as well as in the development of surrogate fuel models [1]. Aromatics addition into alkanes can simultaneously reproduce the C/H ratio and other combustion properties of practical fuels and thereby provides a new way to develop accurate surrogate fuel models. In the present work, the ignition properties of n-decane/toluene binary fuel blends were systematically studied by numerical simulation considering detailed chemistry [2] and transport.

NUMERICAL MODELS AND SPECIFICATIONS

The effects of adding toluene on the ignition of n-decane was investigated in two different systems, a homogeneous flame configuration to examine the kinetic ignition prohibition, and a non-premixed counterflow configuration to examine the effect of transport. The ignition time of homogeneous mixtures at constant pressure and enthalpy was calculated by using CHEMKIN-SENKIN. For the non-premixed simulations, the quasi-steady temperature and species distributions of counterflowing n-decane/toulene (500 K at the boundary) and hot air jets (1400 K at the boundary) were determined under a frozen flow constraint. At time zero, chemical reactions were allowed in the pre-calculated frozen flow field. Ignition time was recorded when the first increase in the temperature field exceeded 400 K, indicating thermal runaway. Simulations were conducted using an unsteady potential counterflow flame code described by Ju et al. [3]. To further examine the effect of flow residence time on ignition enhancement, the stretch rate in the frozen flow configuration was varied from low stretch to that near the ignition limit.

RESULTS AND DISCUSSIONS

Homogeneous ignition process

In order to examine the kinetic effects of toluene addition on the ignition of n-decane, the homogenous ignition process of stoichiometric n-decane/toluene/air mixtures at constant pressure and enthalpy was investigated. Figure 1 shows the ignition delay time as a function of the blending ratio, α, which is equal to the volumetric fraction of toluene in the binary fuel blends. The ignition is shown to be prohibited by toluene addition. When toluene fraction is relatively small (α<0.6, n-decane dominating regime), the ignition delay time is slightly affected. However, when toluene takes up a larger part of the mixture (α≥0.6, toluene dominating regime), the ignition delay time increases exponentially with the blending ratio.

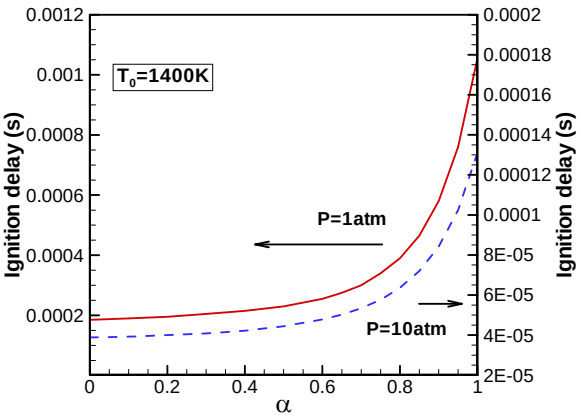

Fig.1 Ignition delay time as a function of the toluene addition level α.

In order to understand the kinetics involved in ignition of the binary fuel blends, sensitivity analysis and reaction path analysis were conducted. We found that the increase of the ignition delay by toluene addition is mainly caused by the following two reactions:

$C_6H_5CH_3+H \rightarrow C_6H_5CH_2+H_2$

$C_6H_5CH_3+OH \rightarrow C_6H_5CH_2+H_2O$

In the homogenous ignition system, a large amount of H and OH radicals is consumed by toluene and thus the radical pool development is strongly affected by toluene addition.

Non-premixed counterflow ignition process

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Numerical simulations of the non-premixed counterflow ignition process were conducted to examine the transport effects of toluene addition on the ignition of n-decane. The ignition delay time of the counterflow system at different stretch rates is plotted in Fig. 2. The results for the homogenous ignition process are also presented for comparison. It is seen that, at the same blending ratio of α, the ignition delay for the non-premixed counterflow system is about one-order larger than that of the homogenous system and it strongly depends on the stretch rate.

At a given stretch rate, the prohibition effect of toluene addition can be divided into two distinct regimes, namely the transport-limited regime and the kinetic-limited regime. With the increase of the stretch rate, the dividing point between these two regimes shifts towards lower toluene fraction, as indicated by the dash-dotted line in Fig.2. The ignition in these two regimes can be explained by the diffusive nature of couterflow systems [4].At a high stretch rate and high blending ratio, the short flow residence time (which is inversely proportional to the stretch rate) prevents the build-up of the radical pool, making ignition process very sensitive to kinetic effects. As a result, the non-premixed counterflow ignition is kinetically controlled and toluene addition significantly affects the ignition delay. On the other hand, at a low stretch rate and low blending ratio, the ignition is controlled by the characteristic transport time. Consequently, toluene addition has a much less influence on the ignition delay time in the transport-limited regime.

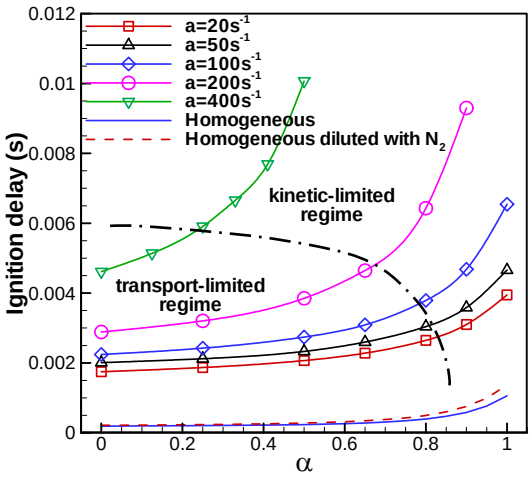

Fig.2 Ignition delay time as a function of α.

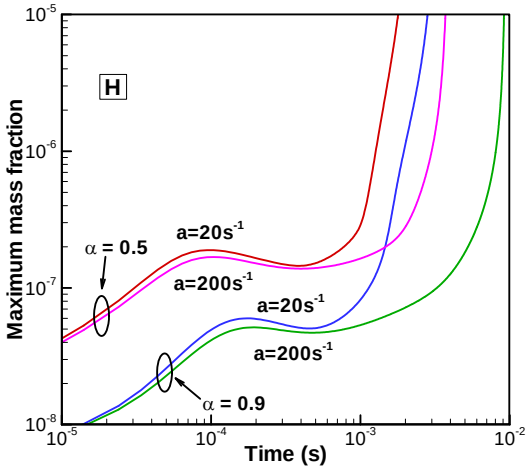

Fig.3 Evolution of the maximum mass fraction of H.

Figure 3 presents the evolution of the maximum mass fraction of H radical at different stretch rates and blending ratios. Although the initial H concentration is mainly affected by toluene addition, the later development of the H radical pool is strongly affected by the stretch rate. As shown in Fig.3, after 0.001s, the H concentration gap between systems of 50% and 90% toluene additions strongly depends on the stretch rate. On the other hand, a higher toluene addition increases the difference between the H concentrations of two systems with different stretch rates in the later stage of ignition as well.

CONCLUSIONS

The ignition of n-decane/toluene binary fuel blends was investigated by numerical simulation considering detailed chemistry and transport. Two different systems were investigated: a homogeneous flame configuration to examine the kinetic ignition prohibition, and a non-premixed counterflow configuration to examine the effect of transport. For the homogeneous ignition process, the ignition delay time was found to increase exponentially with the volumetric fraction of toluene in the binary fuel blends, which is due to the fact that a large amount of H and OH radicals is consumed by toluene. For the non-premixed counterflow ignition process, the ignition delay is found to be strongly affected by the stretch rate. Two ignition regimes, a kinetic limited regime and a transport limited regime, were observed. In the kinetic limited regime, small amounts of toluene addition cause a dramatic increase of ignition time. However, in the transport limited regime, ignition prohibition by toluene addition is much less effective.

References

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