

# Effects of fuel decomposition on the minimum ignition energy of n-decane/air

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## 1 Introduction

In scramjet combustion chamber, it is common to cool the engine with the inboard fuel in order to reduce the weight of cooling system and to get additional heat [1]. During the cooling process, the hydrocarbon fuels undergo pyrolysis through endothermic reactions. Consequently, the liquid heavy hydrocarbons decompose into light gaseous species including hydrogen, methane, ethylene, and butane [2]. It was found that the pyrolysis occurs in the preheat zone within a temperature range of 1050-1450 K [3] and the typical time scale for the overall decomposition process is less than 1 ms [2,4]. Though extensive studies have been conducted to characterize the process of the fuel decomposition [2,4,3,5,6], there are only a few studies on how fuel decomposition affects ignition and flame propagation. Smolke et al. [3] assessed the effects of n-dodecane decomposition on its mass burning rate and extinction strain rate. They found that the mass burning rate is only slightly increased by fuel decomposition while the density-weighted extinction strain rate is notably more sensitive to fuel decomposition under fuel-lean and stoichiometric conditions. Zhong and Peng [7] found that cracking of endothermic hydrocarbon fuel cannot greatly increase the laminar flame speed and thereby it cannot dramatically improve the combustion characteristic in practical combustor. However, to the authors' knowledge, the effects of fuel decomposition on the transient forced ignition process have not been studied before. Ignition is one of the most fundamental combustion processes [8]. Understanding of ignition is important not only for fundamental combustion research but also for fire safety control and the optimization of high performance engines. Since the decomposed small fragments have shorter ignition delay and larger mass diffusivity, it is expected that fuel decomposition has a great impact on forced ignition. This motivates the present work, which aims to investigate numerically the effects of fuel decomposition on the minimum ignition energy (MIE).

Besides, it is well known that fuel-stratified combustion has the advantages in improving the flame stability [9] and extending lean flammability [10]. Recently, Wang et al. [11] have demonstrated that fuel stratification can greatly promote the forced ignition and reduce the MIE in fuel-lean n-decane/air mixtures. This is because the ignition kernel develops much more easily in fuel-lean mixture with lower Lewis number. As mentioned before, fuel decomposition also helps to reduce the Lewis number. Therefore, the

combination of fuel decomposition and fuel stratification is expected to further promote forced ignition. This is also investigated in the present work.

In this study, one-dimensional numerical simulation considering detailed chemistry and transport is conducted to investigate the transient forced ignition process in n-decane/air mixture. The objective is to assess the effects of fuel decomposition on heated kernel induced ignition in homogenous and fuel-stratified mixtures. N-decane is chosen as the targeted fuel since it is popularly used as a component in surrogate jet fuel. Meanwhile, fuel-lean n-decane/air mixture is difficult to be ignited.

## 2 Numerical model and methods

The in-house code A-SURF [12-14] is used to simulate 1D transient forced ignition process. The conservation equations for unsteady, compressible, reactive flow are solved in A-SURF using finite volume method. To resolve the moving flame front, an adaptive mesh is used and the moving reaction zone is always fully covered by the finest mesh with the size of 15.6  $\mu\text{m}$ . More details on governing equations and numerical schemes can be found in Refs. [12-14]. The pyrolysis and oxidation of n-decane are modeled using the high-temperature mechanism of Chaos et al. [15], which contains 54 species and 382 elementary reactions. The initial temperature of  $T_0=400$  K, pressure of  $P_0=1$  atm, and flow velocity of  $u_0=0$  cm/s are uniformly distributed in the whole computational domain of  $0 \leq r \leq 25$  cm. The  $T_0$  value is chosen to ensure n-decane is fully vaporized over the whole equivalence ratio range of 0.7-1.4. Zero flow speed and zero gradients of mass fractions and temperature are enforced at the spherical center ( $r=0$ ) and wall boundary ( $r=25$  cm). In simulation, the combustible mixture is centrally ignited by a heated kernel produced by a temporally and spatially dependent energy deposition. The energy deposition is achieved by including the following source term in the energy equation [16]:

$$q_{ig}(r, t) = \begin{cases} \frac{E_{ig}}{\pi^{1.5} r_{ig}^3 \tau_{ig}} \exp\left[-\left(\frac{r}{r_{ig}}\right)^2\right] & \text{if } t < \tau_{ig} \\ 0 & \text{if } t \geq \tau_{ig} \end{cases} \quad (1)$$

where  $E_{ig}$  is the total ignition energy deposited into the mixture,  $\tau_{ig}$  represents the duration of energy deposition and  $r_{ig}$  is the ignition kernel radius. The MIE is obtained by the method of trial and error with relative error below 2%. Previous studies [8,17] showed that the MIE is affected by both  $\tau_{ig}$  and  $r_{ig}$ . Similar to our previous work [11], the duration of ignition energy deposition and the ignition kernel radius are fixed to be  $\tau_{ig}=0.5$  ms and  $r_{ig}=0.5$  mm, so that lean mixture with  $\phi=0.7$  can be successful ignited.

Fuel decomposition is studied in a homogeneous adiabatic and isobaric process following the same methodology proposed by Smolke et al. [3]. The pyrolysis of homogeneous  $\text{nC}_{10}\text{H}_{22}$ /air mixtures is modelled under isobaric and adiabatic conditions at the same atmospheric pressure but a high initial temperature of  $T_{P,0}=1300$  K. During the transient homogeneous pyrolysis process, the species concentrations evolve and are frozen at a certain value of fuel decomposition fraction,  $C$ , which is defined as the percentage of fuel decomposed. The frozen mixture is then cooled to a temperature  $T_1$  to match the enthalpy of the initial undecomposed  $\text{nC}_{10}\text{H}_{22}$ /air mixture at  $T_0=400$  K [3]. The frozen mixture at  $T_1$  is used as the initial states for heated kernel ignition simulated by A-SURF.

We also consider forced ignition process in fuel-stratified mixture: the ignition kernel develops in a fuel-decomposed mixture and then it propagates into n-decane/air mixture without fuel decomposition. The molar fraction distribution for the  $i^{\text{th}}$  specie is specified by the following hyperbolic tangent function:

$$X^i(r, t = 0) = \frac{X_{in}^i + X_{out}^i}{2} - \frac{X_{in}^i - X_{out}^i}{2} \tanh\left(\frac{r - R_S}{\delta}\right) \quad (2)$$

where  $X_{in}^i$  and  $X_{out}^i$  are respectively the inner and outer molar fractions of the  $i^{\text{th}}$  species;  $R_s$  represents the stratification radius; and  $\delta$  denotes the mixing layer thickness. The molar fractions in the inner zone are determined by fuel decomposition fraction  $C$  and its temperature  $T_{in}$  is calculated based on the constant total enthalpy. In all simulations, the mixing layer thickness is fixed to  $\delta=0.04$  mm and thereby fuel stratification is characterized only by three parameters,  $C$ ,  $\phi$  and  $R_s$ , where  $\phi$  is the equivalence ratio.

### 3 Results and discussion

#### 3.1 Pyrolysis of n-decane in an isobaric homogeneous system

We first model the oxidation of n-decane/air under isobaric and adiabatic conditions.

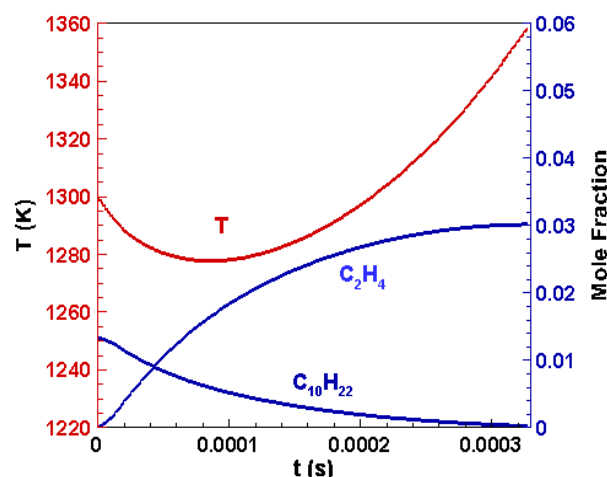


Figure 1. Evolution of temperature and molar fractions of  $C_2H_4$  and  $nC_{10}H_{22}$  during homogeneous ignition of  $nC_{10}H_{22}$ /air with  $\phi=1.0$ ,  $T_{P,0}=1300$  K and  $P=1$  atm.

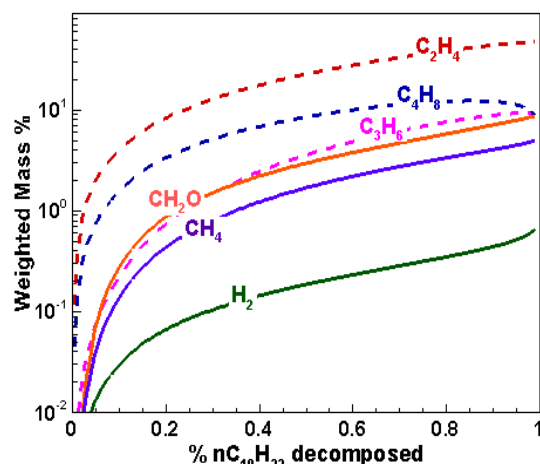


Figure 2. Mass percentages of key products computed for  $nC_{10}H_{22}$  decomposition with  $\phi=1.0$ ,  $T_{P,0}=1300$  K and  $P=1$  atm.

According to previous studies [3,18], n-decane initially decomposes through C-C fission, and then converts to  $C_2H_4$  through  $\beta$ -scission via alkyl radicals. As the reaction progresses, more  $C_2H_4$  is produced with H-abstraction of OH radicals from the fuel. As shown in Fig. 1, the typical time for complete decomposition of n-decane is around 0.3 ms at the cracking temperature of  $T_{P,0}=1300$  K. In the early stage, the temperature decreases due to the endothermic decomposition of large hydrocarbon molecules. With the growth of radical pool, the overall behavior of the system is dominated by exothermic oxidation which leads to the temperature rise. In consistent with previous work [4], Fig. 2 shows that the decomposed products are mainly  $CH_4$ ,  $H_2$ , and small alkene fragments. The mass fractions are normalized by the initial mass fraction of  $nC_{10}H_{22}$ . Being the most abundant intermediate, the weighted mass of  $C_2H_4$  is about one magnitude larger than other products. After fuel decomposition, lighter and more energetic fragments appear in the mixture. On the other hand, the temperature decreases due to endothermic reactions. These two factors are coupled and compete with each other.

#### 3.2 Heated kernel induced ignition in a homogenous mixture

In this subsection, the effects of fuel decomposition on ignition are investigated for heated kernel induced ignition in a homogenous mixture. In order to quantify the effects of fuel decomposition on ignition, the

MIEs are calculated for different values of equivalence ratio and fuel decomposition fraction. The results are summarized in Fig. 3. It is seen that for stoichiometric  $nC_{10}H_{22}$ /air mixture, fuel decomposition has little effect on the MIE, and the MIE remains nearly constant. However, substantial reduction in the MIE is observed for the fuel-lean mixture with  $\phi=0.7$ : for 90% n-decane decomposition, the MIE decreases to only about 10% of that for the case without fuel decomposition. Therefore, fuel decomposition can greatly promote ignition for fuel-lean  $nC_{10}H_{22}$ /air mixture. Besides, it is noticed that there exists a lower limit of MIE around 0.75 mJ. Once the MIE decreases to this limit, further increase in fuel decomposition does not help to reduce the MIE. This lower limit may correspond to the energy required to heat the mixture to the so-called crossover temperature above which the radical pool can be quickly built up.

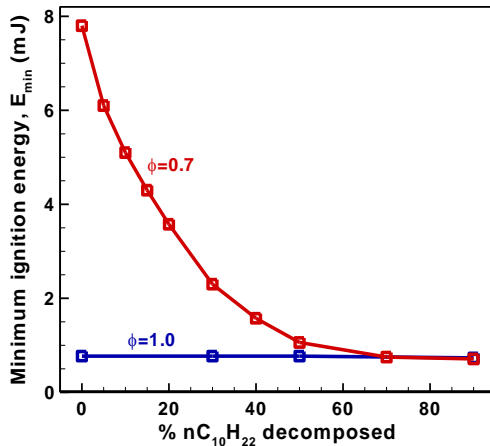


Figure 3. Change of the MIE with the fuel decomposition fraction.

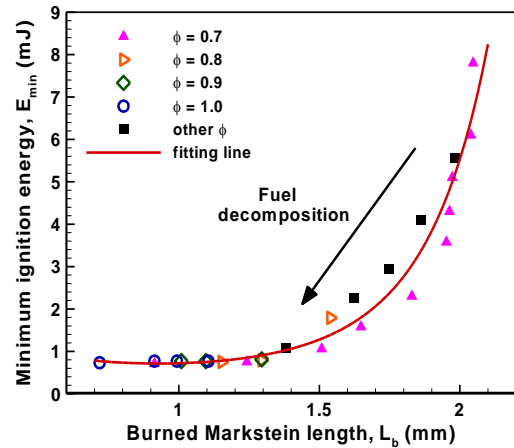


Figure 4. Change of the MIE with the burned Markstein length.

Markstein length is an indicator of the sensitivity of the flame responses. Large value of Markstein length implies strong stretch effects on the flame propagation. Figure 4 shows the MIE as a function of Markstein length,  $L_b$ , for different values of equivalence ratio and fuel decomposition. The MIE is shown to decrease exponentially as  $L_b$  decreases. It is also noticed that the results with different equivalence ratios and fuel decomposition fractions collapse onto a single curve. Therefore, the MIE can be quantified by  $L_b$ . Both the increase in fuel decomposition and equivalence ratio result in a lower  $L_b$  and lower MIE. Therefore, the combination of fuel decomposition and fuel stratification is expected to further promote forced ignition, which is investigated in the following subsection.

### 3.3 Heated kernel induced ignition in a fuel-stratified mixture

As mentioned above, fuel stratification is characterized by the following three parameters: the stratification radius  $R_s$ , the equivalence ratio  $\phi$  and the fuel decomposition fraction  $C$  in the inner zone. Since the effect of equivalence ratio has been discussed in detail in previous studies [19,20,11], the equivalence ratio is fixed to be  $\phi=0.7$  and the emphasis is placed on assessing and interpreting the influence of the other two parameters. Figure 5 depicts the change of the MIE with the extent of fuel decomposition in the inner zone. The largest extent of fuel decomposition considered here is  $C=50\%$ . Similar to the homogenous case, reduction in the MIE was observed due to fuel stratification. For a fixed stratification radius, the MIE decreases with the fuel decomposition. It is noted that the case of  $R_s=0.0$  mm corresponds to the homogenous

mixture without fuel decomposition, and therefore the MIE is constant with  $E_{min}=7.9$  mJ. The case of  $R_S=\infty$  corresponds to the homogenous case with fuel decomposition. Therefore, the results for  $R_S=\infty$  are the same as those shown in Fig. 3 for homogenous mixtures. Figure 5 shows that for small value of stratification radius, e.g.  $R_S=2.5$  mm, the MIE decreases linearly with fuel decomposition and the largest reduction occurs to  $C=50\%$  with  $E_{min}=5.9$  mJ (only around 25% lower than that for  $C=0$ ). When the stratification radius is increased to  $R_S=4.5$  mm, the results are close to those for homogenous mixtures with  $R_S=\infty$ . Therefore, in order to promote the heated kernel induced ignition, only the fuel around the initial ignition kernel needs to be decomposed.

#### 4 Conclusions

In this work, 1D numerical simulation is conducted to investigate the effects of fuel decomposition and fuel stratification on the forced ignition in n-decane/air mixtures. The main conclusions are:

1. For homogeneous n-decane/air mixture, fuel decomposition can greatly promote the ignition of fuel-lean mixtures. With the increase of fuel decomposition, the MIE reduces greatly at fuel-lean case while it remains to be nearly constant for the stoichiometric case. There is a lower limit of the MIE, around which further increase in fuel decomposition does not reduce the MIE.
2. The combination of fuel decomposition and fuel stratification can further promote forced ignition. In order to promote the heated kernel induced ignition, only the fuel around the initial ignition kernel needs to be decomposed.

#### Acknowledgements

This work was supported by National Natural Science Foundation of China (Nos. 91741126, 51861135309).

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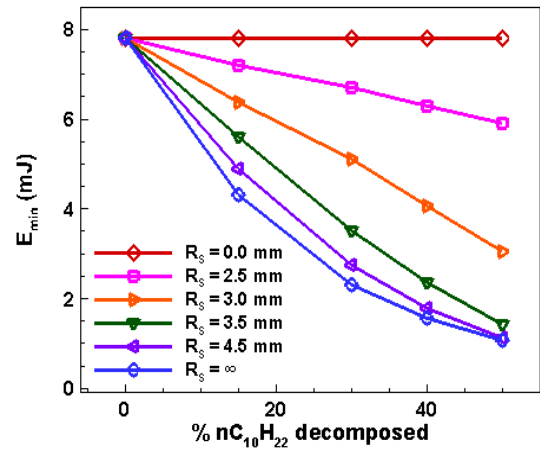


Figure 5. The MIE as a function of the fuel decomposition fraction for fuel-stratified  $nC_{10}H_{22}$ /air mixtures with different values of  $R_S$  and fixed values of  $\phi=0.7$ .

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