DNS study of the ignition of n-heptane fuel spray under high pressure and lean conditions

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Abstract. Direct numerical simulations (DNS) are used to investigate the ignition of n-heptane fuel spray under high pressure and lean conditions. For the solution of the carrier gas fluid, the Eulerian method is employed, while for the fuel spray, the Lagrangian method is used. A chemistry mechanism for n-heptane with 33 species and 64 reactions is adopted to describe the chemical reactions. Initial carrier gas temperature and pressure are 926 K and 30.56 atmospheres, respectively. Initial global equivalence ratio is 0.258. Two cases with droplet radii of 35.5 and 20.0 macrons are simulated. Evolutions of the carrier gas temperature and species mass fractions are presented. Contours of the carrier gas temperature and species mass fractions near ignition and after ignition are presented. The results show that the smaller fuel droplet case ignites earlier than the larger droplet case. For the larger droplet case, ignition occurs first at one location; for the smaller droplet case, however, ignition occurs first at multiple locations. At ignition kernels, significant \( \text{NO} \) is produced when temperature is high enough at the ignition kernels. For the larger droplet case, more \( \text{NO} \) is produced than the smaller droplet case due to the inhomogeneous distribution and incomplete mixing of fuel vapor.

1. Introduction

Fuel spray combustion is one of the most important phenomena in gas turbine and internal combustion engine. With the development of computer technology and advanced numerical computing methodology, it has become accessible to use direct numerical simulation to investigate turbulent combustion [1-4]. Due to the limitation of computer resources, however, it is still very challenging to simulate a three-dimensional turbulent combustion flame using detailed chemistry. With the support of INCITE Program (Innovative and Novel Computational Impact on Theory and Experiment), Chen [5] is performing the first direct numerical simulation of a three-dimensional turbulent nonpremixed flame with detailed chemistry aimed at understanding extinction and reignition issues. Previous three-dimensional simulations usually adopted one-step or simple reaction mechanism [6]. For the sake of simplicity, most DNS studies did not consider fuel droplets or fuel spray in the simulations. However, evaporation of fuel spray has a very important impact on processes of turbulence mixing, ignition and combustion. In our previous study [7], direct numerical simulations were performed to study the autoignition process of n-heptane fuel spray in a turbulent field using a detailed chemistry mechanism. The initial gas pressure was 6 atmospheres and the initial temperature varied from 1100 K to 1300 K. Initial global equivalence ratio varied from 0.5 to 1.5. Effects of initial gas temperature and initial...
global equivalence ratio were studied. We found that with the increase of initial temperature, the
autoignition occurs earlier. With the increase of the initial equivalence ratio, however, autoignition
occurs later due to a larger decrease in gas phase temperature caused by fuel droplet evaporation.
Therefore, evaporation cooling plays an important role in the autoignition of fuel spray.

In this study, we extend our DNS study to investigate the ignition of n-heptane fuel spray under
high pressure and lean conditions. Initial carrier gas temperature and pressure are 926 K and 30.56
atmospheres, respectively. Initial global equivalence ratio is 0.258. We adopt a chemistry mechanism
for n-heptane with 33 species and 64 reactions including NOx reaction mechanism, which was
developed at the Engine Research Center (ERC) in the University of Wisconsin-Madison [8]. Two
cases with droplet radii of 35.5 and 20.0 macrons are simulated. Evolutions of the carrier gas
temperature and species mass fractions are presented. Contours of the carrier gas temperature and
species mass fractions near ignition and after ignition are presented. The objective is to understand the
autoignition of fuel spray under high pressure, lower temperature and lean conditions.

2. Numerical method
The gaseous phase numerical simulations are performed using a parallel code for turbulent reacting
flows, called S3D, which was developed at Sandia National Laboratories, Livermore [9]. Fourth-order
explicit Runge-Kutta time integration and eighth-order finite differencing are used.

Fuel droplets are treated in a Lagrangian manner and assumed to be spherical, with constant
density. Droplet rotation, distortion and direct inter-droplet interactions are neglected. The drag force
is calculated using the Stokesian drag law and the evaporation is calculated according to the infinite
heat conductivity model inside the fuel droplet [10].

Two-way coupling between phases is taken into account through the exchange of mass, momentum
and energy. More details such as the governing equations for both phases can be found in our previous
studies [7, 11]. To alleviate numerical stiffness in the chemical reactions, the implicit VODE solver
[12] is used for gas phase reaction source terms in a time splitting method. The reaction rates are
calculated using Chemkin-III [13] with the chemistry mechanism for n-heptane with 33 species and 64
reactions [8].

3. Initial parameters
A two-dimensional square domain of 2.0 cm by 2.0 cm and a grid with 192 by 192 points are used in
the simulations (\(\Delta x = 105 \mu m\)). Initial thermodynamic parameters for the gaseous phase and fuel
droplets are obtained by averaging the computational results from KIVA3V. The initial gas pressure is
30.56 atmospheres. Initial gas temperature is 926 K. The global equivalence ratios based on liquid fuel
and fuel vapor is 0.258. Initial mass fraction of each species is uniformly distributed, which is also
obtained from KIVA3V. For the KIVA3V run, the compression ratio is 16.5:1, and the engine speed is
821 rpm. The stroke size is 16.58 cm and the bore size is 13.72 cm. The turbulent gas velocity field is
initialized by specifying a von Karman isotropic energy spectrum in Fourier space. The initial
fluctuating velocity \(u'\) is 1.8 m/s.

The initial mean temperature of droplets is 300 K. Initial droplet radius is 35.5 \(\mu m\) for one case and
20.0 \(\mu m\) for the other case. Initial droplet locations are determined through a uniform distribution over
the whole domain. The initial mean droplet Reynolds number is around 65.

4. Computational results
Evolutions of temperature and mass fractions of some important species are shown in figures 1 and 2
for both cases of \(r_d=35.5 \mu m\) and \(r_d=20.0 \mu m\), respectively. The figures show that fuel spray evaporates
first to produce more fuel vapor. For the case of \(r_d=20.0 \mu m\), the mass fraction of \(\text{C}_7\text{H}_{16}\) reaches the
peak value much earlier than the case of \(r_d=35.5 \mu m\) due to its higher evaporation rate (higher total
droplet surface area). At the same time, fuel vapor is decomposed into intermediate species like \(\text{C}_3\text{H}_4\)
and \(\text{C}_6\text{H}_6\). This decomposition process usually absorbs some heat. Then intermediates species are
converted into \(\text{CO}\) and \(\text{H}_2\text{O}\) to release more heat than the decomposition process, which leads to the
slight increase of gas temperature. When temperature reaches around 1400 K, ignition occurs. Due to
the rapid reactions, a large amount of CO$_2$ and H$_2$O are produced to release most of the heat. For the case of $r_e=20.0$ µm, global ignition occurs at $t=2.57$ ms. This is much earlier than the case of $r_e=35.5$ µm, which ignites at around $t=2.89$ ms.

For the case of $r_e=35.5$ µm, temperature contours near and after ignition are shown in figure 3. The plots show that there is only one significant ignition kernel for this case. At later time ($t=2.75$ ms), the ignition kernel spreads out. At $t=2.85$ ms, this ignition kernel becomes even bigger, and at the same time, more independent ignition kernels appear. At $t=3.55$ ms, ignition has taken place over most part of the computational domain. However, we can see that the temperature distribution is very nonuniform over the whole domain.

For the case of $r_e=20.0$ µm, temperature contours near and after ignition are shown in figure 4. Different from the case of $r_e=35.5$ µm, ignition occurs at multiple locations at $t=2.49$ ms. At $t=2.57$ ms, these ignition kernels spread out and more new ignition kernels appear. At $t=2.64$ ms, ignition has taken place over most of the computational domain. Compared with the case of $r_e=35.5$ µm at $t=3.55$ ms, the temperature distribution at $t=2.99$ ms for the case of $r_e=20.0$ µm is more uniform. Due to the uniformity distribution, the spreading speed of the ignition kernels for the case of $r_e=20.0$ µm is much lower than the bigger droplet size case.
Mass fraction contours of species NO after ignition for both cases are shown in figure 5. We can clearly see that significant NO is produced when temperature is high enough at the ignition kernels (also see figures 3-4). For the case of $r_d=35.5 \mu m$, more NO is produced than the smaller droplet case, which was caused by the inhomogeneous distribution and incomplete mixing of fuel vapor.
Figure 5   NO mass fraction contours after ignition for both cases of \( r_d = 35.5 \, \mu\text{m} \) (left) and \( r_d = 20.0 \, \mu\text{m} \) (right)

5. Conclusions
Direct numerical simulations are used to investigate the ignition of n-heptane fuel spray under high pressure, lower temperature and lean conditions. Initial carrier gas temperature and pressure are 926 K and 30.56 atmospheres, respectively. Two cases with droplet radiuses of 35.5 and 20.0 \( \mu\text{m} \) are simulated. The results show that the smaller fuel droplet case ignites earlier than the larger droplet case. For the larger droplet case, ignition occurs first at one location. For the smaller droplet case, however, ignition occurs first at multiple locations. Significant NO is produced when temperature is high enough at the ignition kernels. For the larger droplet case, more NO is produced than the smaller droplet case due to the inhomogeneous distribution and incomplete mixing.

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