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LARGE EDDY SIMULATION OF N-HEPTANE PREMIXED FLAME IN LOW TEMPERATURE IGNITION REGIME

Shenghui Zhong[1,2#], Ning Zhang[1#], Mehdi Jangi[3], Fan Zhang[1*], Zhijun Peng[1,4], Xue-Song Bai[2]
1 State Key Laboratory of Engines, Tianjin University, 135 Yaguan Rd, 300350Tianjin, China
2 Department of Energy Sciences, Lund University, PO Box 118, SE-221 00 Lund, Sweden
3 Department of Mechanical Engineering, University of Birmingham, B15 2TT Birmingham, United Kingdom
4 Faculty of Creative Arts, Technologies and Science, University of Bedfordshire, Luton, LU1 3JU, United Kingdom
#: have the equal contribution.
*Corresponding author: fanzhang_lund@tju.edu.cn.

ABSTRACT

This paper presents a Large Eddy Simulation (LES) study of the effect of low temperature chemistry on the structure and propagation of n-heptane/air turbulent premixed flame with transport Probability Density Function (t-PDF) model based on the Eulerian Stochastic Fields (ESF) method. The computation process is accelerated by conjugating ESF method with Chemistry Coordinate Mapping (CCM) approach. Initial n-heptane/air mixtures at an equivalence ratio of 0.6, a constant pressure of 1 bar and temperature of 600 K, 650 K and 700 K in a new RATS burner configuration are considered. The studied cases cover three regimes of combustion, a Chemical Frozen (CF) regime, a transition (TRA) regime and a Low Temperature Ignition (LTI) regime. The results showed that low temperature chemistry of n-heptane has a significant effect on the enhancement of turbulent flame speed. Also, CO emission widely exists in post flame zone in CF condition, whereas, it is quickly oxidized in reaction zone under LTI condition.

Keywords: low temperature ignition, premixed flame propagation, Eulerian Stochastic Fields, LES method.

1. INTRODUCTION

Combustion will be the main energy conversion approach in the transport sector for decades to come [1]. In order to meet the increasingly strict emission regulation, advanced combustion concepts in internal combustion (IC) engines, e.g. Reactivity Controlled Compression Ignition (RCCI), Partially Premixed Combustion (PPC), and Gasoline Compression Ignition (GCI) [2, 3], are being developed for higher thermal efficiency and lower emissions. Such advanced IC engines involve high pressure and large hydrocarbon fuels where low temperature combustion (LTC) process plays an important role. One novel RCCI concept based on single fuel has been studied recently [4]. In the experiments [4], the fuel was first reformed (through LTC) and then injected in the intake stroke to the cylinder. Then, the unreformed fuel is directly injected to the cylinder. The LTC reformed and unreformed fuels have different reactivity and their interaction has the potential of achieving improved engine efficiency and emission reduction. The underlying physics of the LTC on turbulent combustion is still unknown [5].

The cases presented in this paper are based on the experiment of RATS burner by Won et al. [6], who studied the combustion of n-heptane/air premixed mixtures that are partially reformed inside the burner through LTC. They found that the rate of combustion, i.e. the turbulent flame speed, is highly sensitive to the reformed gas mixtures. This paper is aimed to replicate the combustion process using high fidelity numerical simulations, and to gain insights into the physics of LTC flames.

2. NUMERICAL METHOD AND CASE SETUPS

2.1 Numerical method

The numerical simulation is based on large-eddy simulation (LES) and transported probability density function (t-PDF) based on Eulerian Stochastic Fields (ESF). The sub-grid scale stress tensor is modeled by Smagorinsky turbulence model. The ESF method is used to model the sub-grid turbulence-chemistry interaction with eight stochastic fields. The method is based on direct integration of finite rate chemistry, which is accurate for combustion process sensitive to the chemical kinetics, however, at the expense of high computational cost. To efficiently in-

tegrate the chemical reaction rates in LES a chemistry coordinate mapping (CCM) approach is adopted [7]. CCM can provide up to 30 times of reduction of computation time for the integration of the chemical kinetic rate. The speedup of CCM is more significant when large number of mesh points is needed in the computation, e.g. in LES, with regard to specific cases.

The skeletal n-heptane mechanism from Lu [8], including 68 species and 283 elementary reactions, is used. This mechanism has been used in previous numerical simulations and considered to be reliable.

The open source CFD code, OpenFOAM, is used to solve the governing equations for turbulent reacting flows. The code is based on finite volume method with a second-order scheme for spatial discretization and an implicit second-order backward Euler scheme for the time integration.

nous turbulence field generated using LEMOS [9] is superimposed on a power law velocity profile as the inlet velocity. The turbulence intensity is set as 12.5% of the bulk velocity, and the integral scale is 2.5 mm for all cases to mimic the turbulent inlet field in experiment [6]. Three initial temperatures of the fuel/air mixture are considered in this study, 600K (case 1), 650K (case 2) and 700K (case 3). Under this temperatures LTC takes place in the fuel/air mixture inside the burner before entering into the computation domain. In order to take into account the chemical reactivity inside the burner, numerical simulation is carried out using Chemkin-Pro for the homogenous ignition process of the mixture under constant pressure and the three temperature conditions. The species composition and temperature from the ignition simulations is used in LES as the inlet boundary condition, which is reasonable since species and temperature is al-

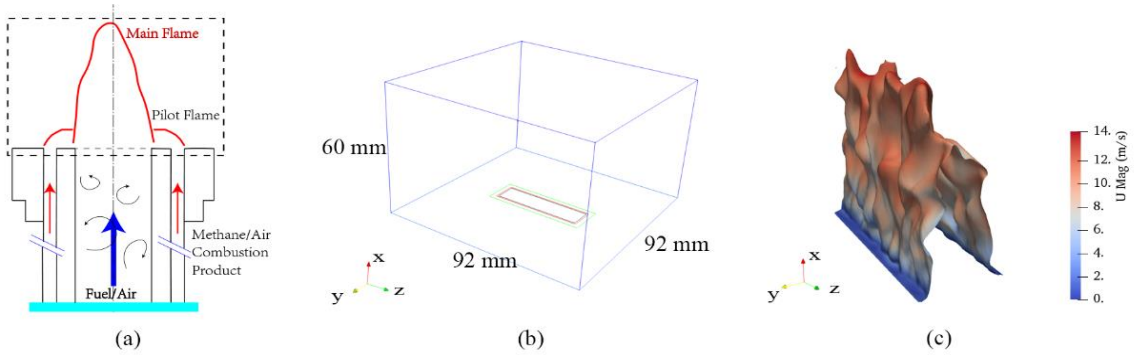

Fig 1 (a) A schematic diagram of RATS burner. (b) A schematic description of the computational domain. (c) An illustration of flame, presenting an instantaneous of temperature isosurface of 1490 K.

2.2 Case setups

Figure 1 presents the schematic diagrams of RATS burner, the simulation domain and an instantaneous isosurface of temperature, respectively. The computational domain is a cuboid with a size of 60 mm × 92 mm × 92 mm. The inlet is a rectangular with the length for two sides of 40 mm × 10 mm. The inlet is discretized using uniform grids made of 160 × 40 mesh cells. The top and the lateral boundaries are prescribed as pressure outlet conditions, with zero gradient boundary condition for the variables. In the streamwise x-direction, 120 cells are used and the total number of CFD cells is 2,304,000. To ensure flame stability the products of a pilot stoichiometric methane/air flame are prescribed at the pilot inlet with a uniform constant velocity of 4.5 m/s. A homogemost uniform after long time mixing in the pipe. The bulk velocity of fuel/air mixture is 10 m/s, the equivalence ratio is 0.6 and the residence time in the pipe is 63.75 ms (which is used in the ignition simulations). The max Courant number is limited to 0.15 and the max time step is 1 ms to ensure the stability of calculation. In order to quantitatively describe the LTC effect on the flames, a turbulent flame speed is calculated based on the mass flow conservation.

$$S_T = U_0 W / P_{avg} \quad (1)$$

where W is the inlet width, and P_{avg} is the flame surface length. The flame surface is defined as an iso-surface of temperature, corresponding to the maximum gradient of OH mass fraction in 1D freely propagation flame condition.

3. RESULTS AND DISCUSSION

Figure 2 shows the comparison between direct long exposure photos of n-heptane/air turbulent flame in the experiment [6] and time-average temperature distribution of from LES for the three run cases. A well-defined flame cone is identified after sufficient time on average. The flame height decreases with the increase of the initial mixture temperature, which is shown in both the experiments and simulations. Owing to the high initial temperature, LTC occurs first before the intense high temperature oxidization if the residence time (τ_r = 63.75 ms in the present case) is longer than the first ignition delay time (τ_{1st} = 488.83, 65.60 and 14.39 ms for Case 1, 2 and 3 respectively). In experimental study, the turbulent flame speed was calculated based on the time-average OH PLIF images in a range of equivalence ratios and temperatures which is fitted to two polynomials. Three regimes of combustion were suggested from the experiments, low temperature ignition (LTI), conventional flame (CF), and transition from LTI to CF. As shown in Fig. 3, the upper polynomial line represents the LTI regime and the lower is CF regime. For comparison, the LES and the experimental results are shown in the figure. It is found that the same tendency of transition from LTI to CF regime is predicted when decreasing the initial temperature of the fuel/air mixture inside the burner.

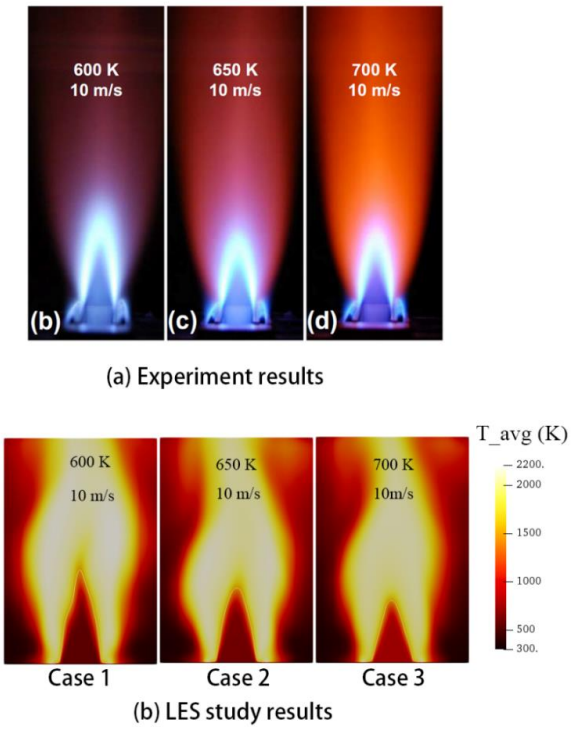

Fig 2 (a) Direct long exposure photos of n-heptane/air turbulent flames of experiment [6]. (b) Temperature time-average distribution of LES study.

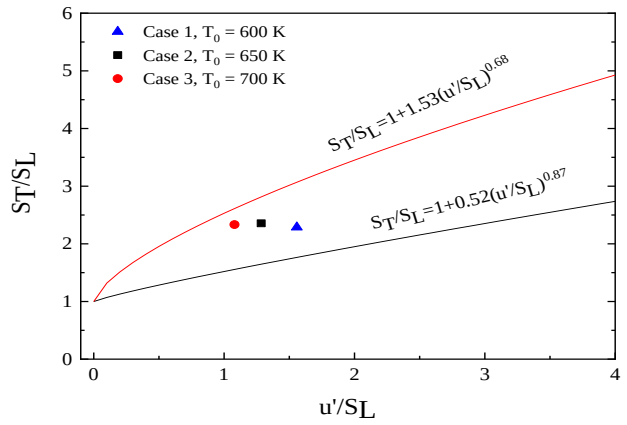

Fig 3 Comparison on the turbulent flame speed between experimental results (lines) and simulation results (scatters). The upper line denotes the turbulent flame speed in LTI regime, and the lower line represents the CF condition.

Figure 4 shows snapshots of instantaneous distribution of temperature, mass fraction of C_7H_{16}, CH_2O, CO and OH from Case 1, 2, 3, respectively. Experimental results had shown that low temperature ignition occurs when the initial temperature in the range of 650 K to 700 K at a residence time of 63.75 ms. As shown in Figs. 4, Case 1 corresponds to the CF regime, while Case 3 represents LTI regime. Owing to the longer first-stage ignition delay time of Lu's chemical reaction mechanism, Case 2 is the transition state from CF regime to LTI regime instead of LTI regime as experiment suggested. Since after low temperature ignition, the larger hydrocarbon species are firstly decomposed to small hydrocarbon species, CH_2O is identified to represent the onset of low temperature ignition. As shown in Fig. 4, CH_2O appears in a thin layer in Case 1 which is typical for premixed flame in the laminar flamelet regime. In the LTI regime (Case 3), CH_2O appears in the entire cold region downstream the burner exit. This is accompanied with the decrease of C_7H_{16} in the cold region. Case 2 shows an intermediate level of C_7H_{16}, and an appearance of local broadening of the CH_2O in tip of the cold region, indicating that Case 2 is in the transition from CF to LTI regime. The LTC effect of the combustion process can be further identified from the CO and OH distribution. A small amount of CO is generated in the cold region of LTI case (Case 3), which is oxidized in the high temperature flame region where OH radicals exist. The consumption of CO is much quicker in

the LTI case than the CF case (case 1). For the CF case (Case 1) CO is mainly produced in the thin reaction zone as indicated by the CH_2O distribution, and CO oxidized in a thick oxidation layer downstream the CH_2O layer.

4. CONCLUDING REMARKS

LES with ESF-CCM combustion model is used to study turbulent premixed combustion of n-heptane/air mixture in the conventional flame (CF) regime, the low temperature ignition (LTI) regime and in the transition regime. The LES replicated the experimental observation of the increased turbulent flame speed with increasing initial temperature of the fuel/air mixture. In the CF region it is well known that the turbulent flame speed increases with increasing initial temperature of the reactant temperature by increasing the temperature of the flame. However, the increased turbulent flame speed in the LTI regime is due to a different mechanism. It is found that the fuel in the cold region upstream the flame is reformed due to LTC to combustion intermediates such as CH_2O and CO, which gives rise to a faster flame speed and faster CO oxidation.

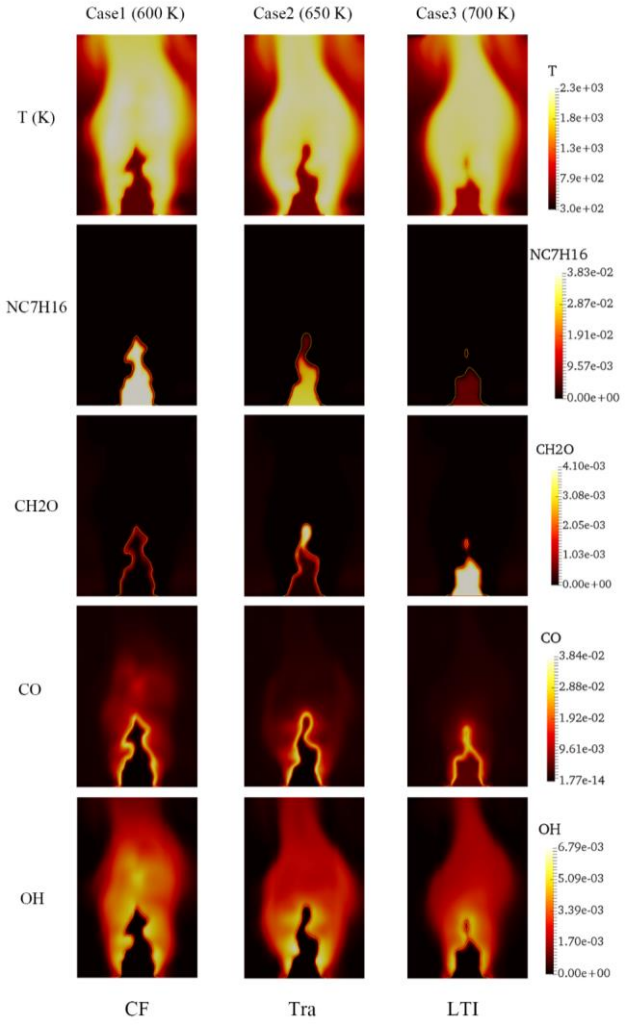

Fig 4 The instantaneous distributions of temperature, mass fraction of C_7H_{16}, CH_2O, CO and OH (from top to bottom rows) in CF, Tra and LTI regimes (from left to right column) in the middle 2-D plane, respectively.

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