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Numerical analysis of ignition and flame stabilization in an n-heptane spray flame

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ABSTRACT

Unsteady Reynolds-averaged Navier–Stokes (URANS) and large-eddy simulations (LES) of an n-heptane spray flame have been performed with efficient chemistry calculation via dynamic adaptive chemistry and uniformly random distribution parallelization. Predictions for such key parameters as ignition delay time and flame lift-off length are validated against the experimental data from the engine combustion network. The transient, convection, diffusion and chemical reaction terms in species transport equations are analyzed to gain insight into flame stabilization mechanisms, showing the dominant effects from the auto-ignition process. The influence of the turbulence–chemistry interaction on the ignition and flame stabilization is studied for two cases with different initial ambient temperatures by reconstructing probability density function of mixture fraction. For the case with an initial ambient temperature of 1000 K, the analysis shows the fluctuation in mixture fraction is significant, but it has negligible influence on the ignition process. For the case with an initial ambient temperature of 850 K, the turbulence–chemistry interaction plays a significant role on ignition and consequently the stabilization process. In addition, large eddy simulations with a third-order Monotone Upstream-centered Schemes for Conservation Laws are performed for a series of cases with different oxygen concentrations. The results show that LES predict the instantaneous flame dynamics and flame lift-off lengths more accurately than URANS.

1. Introduction

Understanding and accurate modeling of spray combustion process are essential for efficiency improvement and emissions reduction in diesel engines. The process is inherently complex, as it is a transient phenomenon involving liquid breakups, two-phase turbulent flows, mixing and ignition at elevated pressures. Multi-dimensional computational fluid dynamics of reactive flows has become an indispensable and effective tool for probing the multiscale physicochemical processes involved in diesel spray combustion, parts of which are difficult to access in experiments, e.g. the three-dimensional composition distributions. For practical importance, some key combustion characteristics such as ignition delay time and flame lift-off length (LOL) have to be determined accurately, which have crucial influence on the emissions of the system since it represents the balancing between chemistry and mixing. The present study targets at the well-documented constant volume combustion chamber experiment, often denoted as the "Spray H" [1], from the Sandia National Laboratories, with experimental data being available from the engine combustion network (ECN) [2]. Both URANS and LES are performed and analyzed to gain insights into the flame stabilization and the influence of the turbulence–chemistry interaction (TCI) on the auto-ignition process.

A number of numerical studies with detailed chemistry [3–15] have been reported to investigate the importance of the chemical kinetic and TCI on the auto-ignition process and flame stabilization in the "Spray H" flame. For example, Pei et al. [4] implemented the transported probability density function (PDF) method into the standard unsteady Reynolds-averaged $k-\varepsilon$ model to simulate the "Spray H" without spray modeling, utilizing a 29-species skeletal mechanism. The study showed that, compared to the experimental data, the transported PDF simulations considering TCI are more accurate than the well stirred reactor (WSR) model with TCI neglected. Bhattacharjee and Haworth [5] performed a more systematic study of this flame using the URANS/transported PDF

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method with a 40-species mechanism and a secondary breakup model. It indicates that the importance of TCI rises at low initial ambient temperatures and low oxygen levels. Large eddy simulations of the "Spray H" have been reported recently [6–8]. Som et al. [6] compared results of URANS and LES with two chemical kinetic mechanisms with 42 and 68 species, respectively. The study demonstrated the advantages of LES for predicting the instantaneous behavior of the flame, while predictions for the global parameters such as ignition delay time and quasi-steady LOLs by URANS and LES are close to each other.

Dynamic adaptive chemistry (DAC) [16–19] has recently gained significant interests to accelerate combustion simulations with detailed chemistry through on-the-fly mechanism reduction to avoid computating the species and reactions that are locally "inactive", i.e. having negligible impact on the kinetics at the local cell and time instance. To minimize the computational overhead, a fast method is required for on-the-fly mechanism reduction. The direct relation graph (DRG) [20,21] and its variations, such as DRG-EP [22], Path Flux Analysis (PFA) [23] and decoupled species and reaction reductions methods [24], have been demonstrated to meet this criterion. DAC is now commonly applied to speed up turbulent combustion simulations, e.g. those for IC engines [18,25–26], and has combined with in situ adaptive tabulation (ISAT) to further improve the computational efficiency [27–29].

In this study, both URANS and LES of "Spray H" have been performed with detailed chemistry and primary and secondary breakup models [30]. The 92-species detailed mechanism employed consists of an updated 387-reaction n-heptane mechanism [31] and a 13-reaction sub-mechanism [32]. The major contributions of this study include: (1) the efficient implementation via dynamic adaptive chemistry (DAC) and uniformly random distribution parallelization (URDP) for detail chemistry in spray flame simulations; (2) a third-order Monotone Upstream-centered Schemes for Conservation Laws (MUSCL) in finite volume method for improved numerical accuracy; (3) for the first time, the species transport budgets analysis which compares different terms being employed for investigating the flame stabilization process in spray flame; (4) and a detailed analysis of the effects of TCI on flame stabilization by reconstructing the probability density function of mixture fraction.

The remainder of the paper is organized as follows. In Section 2, the computational model is presented including the flow solver, efficient chemistry implementation and detailed numerical settings. In Section 3, simulation results are presented with a detailed analysis on the lift-off and ignition characteristics. Conclusions are presented in Section 4.

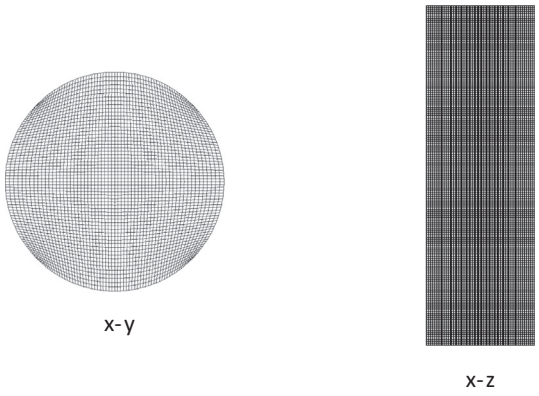

Fig. 1. The computational mesh.

Table 1
Experimental conditions.

Injected fuel	C_7H_{16}
Orifice diameter (mm)	0.1
Injection duration (ms)	6.8
Injection pressure (MPa)	150
Fuel mass (mg)	17.8
Fuel temperature (K)	373
O_2 (vol.%)	10–21%
Ambient density (kg/m^3)	14.8
Ambient temperature (K)	850/1000

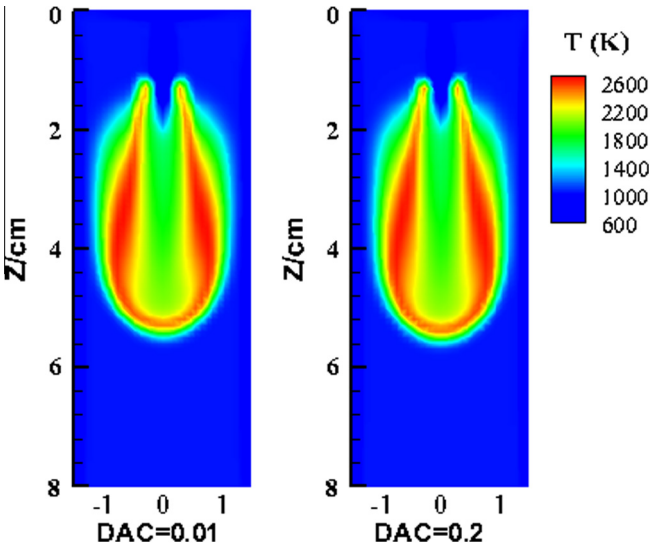

Fig. 2. Temperature distributions with two ε_{DAC} values of 0.2 and 0.01 at t = 2.0 ms ASI using URANS.

2. Model description

2.1. Flow solver

The program KIVA3V [33] has been enhanced with the LES capability and spray models [34] for studying the "Spray H". The numerical scheme is based on the Arbitrary Lagrangian–Eulerian method with the finite volume method. For the continuum phase in URANS, a $k-\varepsilon$ turbulence model is used with the model parameters $C_\mu = 0.085$, $C_{\varepsilon 1} = 1.42$, $C_{\varepsilon 2} = 1.68$, $C_{\varepsilon s} = 1.50$, $\mathrm{Pr}_k = 1.39$, and $\mathrm{Pr}_\varepsilon = 1.396$. For LES, a K-equation sub-grid turbulent kinetic energy model with $C_\mu = 0.067$ and $C_\varepsilon = 0.916$ has been implemented. The third-order MUSCL [35] is implemented to replace the Quasi-Second-Order Upwind (QSOU) scheme for convection to obtain improved accuracy.

For the dispersed phase, the discrete droplet model [33] is applied, with the droplet particles tracked by solving the droplet velocity, mass, and temperature equations using the Lagrangian method. The interactions between the two phases are described through a two-way coupling, i.e. "gas-to-liquid" and "liquid-to-gas". In "gas-to-liquid", the changes of the droplet velocity in the computation domain are attributed to the drag force $F_{i,d}$ on droplet and calculated by the relative velocity between the droplet and the gas. In the "liquid-to-gas" aspect, the effects of liquid motion on the gas phase are treated as the Lagrangian source terms in the Eulerian momentum equation. The Kelvin–Helmholtz and Rayleigh–Taylor model [30] is employed to predict the primary and secondary liquid breakups. The collision and coalescence model used is that proposed by O'Rourke [36]. Note that