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# Large eddy simulation of *n*-heptane spray combustion in partially premixed combustion regime with linear eddy model

Gang Xiao [a], Ming Jia [b], Tianyou Wang [a, *]

[a] State Key Laboratory of Engines, Tianjin University, Tianjin 300072, China
[b] School of Energy and Power Engineering, Dalian University of Technology, Dalian 116024, China

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ABSTRACT

Spray combustion of *n*-heptane in a constant-volume vessel under engine-relevant conditions was investigated using linear eddy model in the framework of large eddy simulation. In this numerical approach, turbulent mixing was traced by an innovative stochastic approach instead of the conventional gradient diffusion model. Chemical reaction rates were calculated with the consideration of the sub-grid scale spatial fluctuations of reactive scalars. Turbulence-chemistry interactions were represented by the separated treatments of the underlying processes including turbulent stirring, chemical reaction, and molecular diffusion. The model was validated against the experimental data of ignition delay times, chemiluminescence images, and soot images from Sandia National Laboratories. Numerical results showed that the ignition process changed from the temperature-controlled regime to the mixing-controlled regime as the initial ambient temperature increased from 800 K to 1000 K. The premixed flame and the diffusion flame coexisted, while the gross heat release rate was found to be dominated by the premixed flame. The temperature fluctuation was mainly observed around the spray jet due to the cooling effect of the fuel vaporization. The fluctuations were more significantly smoothed out by the high-temperature flame than the low-temperature flame. The mean temperature would be over-predicted if the sub-grid temperature fluctuation was neglected.

## 1. Introduction

Chemical energy stored in hydrocarbon fuels is one of the most important sources of industrial power. Most of IC (internal combustion) engines are operated with liquid fuel spray combustion, through which the fuel is burned and the chemical energy stored therein is released [1,2]. The requirement for high efficient and clean IC engines motivates the in-depth understanding of spray combustion. Many sub-processes are observed in spray combustion, such as the liquid fuel injection and atomization, droplet interaction and evaporation, fuel-gas mixing, chemical reaction, and soot formation and oxidation [3]. These processes are strongly coupled with each other, making it a challenge to deeply understand them by experiments. Accordingly, three-dimensional CFD (computational fluid dynamics) simulation is necessarily employed to provide insights.

LES (Large eddy simulation) is a promising tool to capture the inherently unsteady turbulence. LES aims to directly resolve the eddies with length scales beyond the filter size $\Delta$, since the large-scale eddies are believed to dominate the dynamics of the turbulence. The SGS (sub-grid scale) eddies are supposed to be universal, and are taken into account by turbulence models [4]. For turbulent flows with chemical reaction, LES offers the advantages in capturing the crucial turbulent mixing process before and/or during the chemical reaction process [5]. However, the time and length scales of chemical reactions are respectively far smaller than the time step and grid size in numerical simulations. Therefore, the filtered chemical source term needs to be addressed by the combustion model in LES.

Most combustion models are customized for specific combustion regimes in order to facilitate the implementation and/or speed-up of the computation [3]. It is necessary to choose the combustion model according to the combustion regime. It should be pointed out that chemical reaction only takes place when the fuel and the oxidizer are mixed at the molecular level, hence the combustion regimes are fundamentally consistent and only

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[*] Corresponding author. No. 92, Weijin Road, Nankai District, Tianjin 300072, China. Tel.: +86 (0)22 27403434; fax: +86 (0)22 2740 6890.
*E-mail address:* wangtianyou@tju.edu.cn (T. Wang).

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categorized by the ways through which the mixture is formed. In HCCI (homogeneous charge compression ignition) engines, the fuel and air have been well mixed before ignition, and the combustion process is kinetically controlled by the temperature, pressure, and compositions of the mixture [6]. Therefore, direct integration of the chemical source term without using the sub-grid combustion model is capable to reproduce the premixed combustion in HCCI engines. Kong et al. [7,8] implemented CHEMKIN into a CFD code to investigate HCCI combustion. Although the ignition timings were well reproduced over a wide range of engine conditions, the gross HRR (heat release rates) were inaccurately predicted if the effects of turbulent mixing on reaction rates were unconsidered. As for conventional diesel engines, the fuel is injected near top dead center where the in-cylinder temperature and pressure are high. Due to the low volatility and high cetane number of diesel, only a small part of the liquid fuel is premixed with air before auto-ignition [9]. The fuel-air mixing process mainly takes place in the reaction zone, and the combustion is mixing-controlled because the chemical timescale is much smaller than the mixing timescale [6]. In order to consider the non-equilibrium chemical effects, the combustion model of characteristic timescale was employed by Kong et al. [10] and Rao [11] to bridge the gap between the actual state and the chemical equilibrium state. Satisfactory results were obtained, but the model coefficients must be adjusted for different cases according to the experimental data.

In recent decades, efficient and clean combustion strategies for engines, such as GDI (gasoline direct injection) and PCCI (premixed charge compression ignition), are typically under PPC (partially premixed combustion) regime [12–14]. By injecting the fuel well before top dead center in the cylinder, PPC generally gains longer ignition delay than the non-premixed combustion in CDC (conventional diesel combustion) engines, thus more fraction of the liquid fuel can be premixed before ignition. However, the fuel and air cannot be perfectly premixed due to the low volatility of diesel fuel and the relatively limited available time in the PPC regime. Therefore, PPC has the potential advantages for avoiding incomplete combustion, severe pollutant emissions, and excessive pressure rise rate [15]. PPC is of great research interest due to the difficulties in controlling combustion phrasing. Jia et al. [16–18] conducted full-cycle CFD simulations of diesel PCCI engines. It was found that the combustion process can be divided into the kinetically-controlled regime and the mixing-controlled regime depending on the operating conditions. In this perspective, PPC brought challenges to the combustion model, in which both chemical and mixing effects have to be considered simultaneously. The conventional combustion models that solve the chemical reaction rate indirectly based on mixture fraction or progress variable are no longer appropriate, since mixture fraction and progress variable fail to exactly represent the state of the mixture in the PPC regime. Banerjee et al. [19] and Hu et al. [20] proposed a map of diesel combustion regimes based on the local chemical and mixing conditions. The chemical reaction rate was divided into three categories including the kinetically-controlled reaction rate, the quasi-steady homogenous reaction rate, and the quasi-steady flamelet reaction rate. Zhang and Rutland [21,22] further proposed a MCDC (mixing controlled direct chemistry) model based on the computation of the chemical kinetics, thermo–chemical equilibrium state and SGS mixing effects.

The aforementioned combustion models provided satisfactory predictions on the HRR over a wide range of diesel operating conditions. However, the chemical reaction rate in these models was obtained by an empirical correction to some extent. In addition, the effects of the fuel-air mixing and the local fuel-air in-homogeneity on the chemical reaction rate were only described by the scalar dissipation rate at the grid scale without considering the SGS effects. Transported PDF (probability density function) model [23–25] is a powerful tool to characterize the partially premixed combustion without any *a priori* assumption about the combustion regimes. However, the transported PDF model is extremely complex and computationally expensive, especially when it is coupled with detailed chemical kinetics. Thus, it is difficult to apply the transported PDF model in three-dimensional LES of two-phase spray combustion, although Zhang and Haworth [26–29] employed the model in the framework of RANS (Reynolds Averaged Navier-Stokes). As a simplification, the presumed β-PDF model facilitates the closure of the chemical source terms in LES [30–33], whereas the experimental study of Tong [34] found that the bimodal form of the scalar filtered density function substantially deviated from $\beta$-function. Furthermore, the PDF models are weak in capturing SGS mixing effect [35].

Besides the filtered chemical source term, the SGS scalar transport equations are also needed to be closed by models. The eddy diffusivity model is widely adopted, which is derived based on the gradient diffusion hypothesis that the SGS scalar transport aligns with the gradient of the scalar at the grid scale. Moin et al. [36,37] proposed an improved model, in which the diffusion coefficients were obtained by a dynamic procedure. However, recent investigation revealed that the gradient diffusion hypothesis was invalid in the entire computational domain [38], and the counter-gradient diffusion phenomenon did occur in the PPC regime [39]. Furthermore, the eddy diffusivity model is incapable to capture the counter-gradient diffusion phenomenon. What's worse, the effects of the SGS turbulence on mixing cannot be well captured by the eddy diffusivity model, though the mixing process was strongly enhanced or even dominated by turbulence. The turbulence flow affects the mixing process by stirring the scalar field, especially in the sub-grid scale. As a result, the scalar field was found anisotropy, even at the smallest scale [40]. Note that the fluctuations of scalars, especially that of temperature, have direct and noticeable influence on the combustion process. DNS (Direct numerical simulation) of the auto-ignition of hydrogen/air [41,42] and $n$-heptane/air [43] revealed that ignition delay and HRR were strongly affected by the amplitude of the temperature fluctuations.

In summary, a satisfactory numerical approach employed for PPC simulation should be regime-independent. Moreover, the turbulence-chemistry interaction, the turbulent mixing effect, and the spatial fluctuations of scalars should be addressed. In the present work, the LEM (linear eddy model) originally developed by Kerstein [44–46] was employed to meet the above requirements. In the concept of LEM, turbulent stirring and molecular diffusion were resolved in one-dimensional domains embedded in the three-dimensional computational grid cells. Therefore, the SGS fluctuations in a grid cell can be easily evaluated. Unlike the eddy diffusivity model which perverted the nature of turbulent mixing [38], the effects of turbulence on the SGS scalar field were traced by an innovative stochastic approach that mimicked the behaviors of the SGS turbulent eddies. By rearranging the scalar values on proper time and length scales, the counter-gradient diffusion was automatically captured [47]. LEM has been used to study the scalar mixing in a wide range of Reynolds number and Schmidt number [47–50]. Moreover, Menon [51] extended LEM as a sub-grid combustion model for LES, yielding an approach called LES-LEM. In the LES-LEM approach, the chemical reaction was resolved in the one-dimensional LEM domains where SGS scalar fluctuations were described and evolved, so that the effects of scalar fluctuations on the chemical reaction rate can be considered. Moreover, the underlying processes including turbulent stirring, molecular diffusion, and chemical reaction were resolved separately, and their effects on the SGS scalar evolutions can be respectively evaluated in the LES-LEM model. Due to the direct treatment of the