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Modelling of diesel spray flames under engine-like conditions using an accelerated Eulerian Stochastic Field method

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ABSTRACT

This paper aims to simulate diesel spray flames across a wide range of engine-like conditions using the Eulerian Stochastic Field probability density function (ESF-PDF) model. The ESF model is coupled with the Chemistry Coordinate Mapping approach to expedite the calculation. A convergence study is carried out for a number of stochastic fields at five different conditions, covering both conventional diesel combustion and low-temperature combustion regimes. Ignition delay time, flame lift-off length as well as distributions of temperature and various combustion products are used to evaluate the performance of the model. The peak values of these properties generated using thirty-two stochastic fields are found to converge, with a maximum relative difference of 27% as compared to those from a greater number of stochastic fields. The ESF-PDF model with thirty-two stochastic fields performs reasonably well in reproducing the experimental flame development, ignition delay times and lift-off lengths. The ESF-PDF model also predicts a broader hydroxyl radical distribution which resembles the experimental observation, indicating that the turbulence–chemistry interaction is captured by the ESF-PDF model. The validated model is subsequently used to investigate the flame structures under different conditions. Analyses based on flame index and formaldehyde distribution suggest that a triple flame, which consists of a rich premixed flame, a diffusion flame and a lean premixed flame, is established in the earlier stage of the combustion. As the combustion progresses, the lean premixed flame weakens and diminishes with time. Eventually, only a double-flame structure, made up of the diffusion flame and the rich premixed flame, is observed. The analyses for various ambient temperatures show that the triple-flame structure remains for a longer period of time in cases with lower ambient temperatures. The present study shows that the ESF-PDF method is a valuable alternative to Lagrangian particle PDF methods.

1. Introduction

To comply with the increasingly stringent regulations that aim to reduce emitted harmful pollutants from diesel engines, the implementation of alternative fuels and new engine combustion technologies such as low-temperature combustion (LTC) has become the main focus of both the automotive and maritime engine industries. With the use of alternative fuel and/or LTC, the associated combustion modes are expected to be different from that of conventional diesel combustion in the same operating strategy, which may be varying from a classical diffusion-controlled combustion to a partially premixed reacting system where ignition, premixed reaction front and diffusion flame can co-exist and interact with each other [1]. It is necessary to couple advanced experimental and numerical tools for the investigation and understanding of the auto-ignition, flame stabilisation/propagation and emissions formation. The experimentation using laser diagnostics and high-speed photography incorporated with optically accessible combustion chambers [2–8] and engines [9] is a promising approach to provide a more comprehensive understanding of the in-cylinder phenomena. The optical measurements also serve as an important asset for validating newly developed turbulent combustion models. These models, once validated, can arguably provide a qualitative picture of the missing data and be used to infer characteristics of flame structures that cannot yet be measured [10]. The validated model can also be used to simulate and elucidate in-cylinder events of engines which are not optically accessible, expanding on the limited details from experimental exhaust measurements in a more cost-effective manner [11,12].

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Table 1
Numerical studies on the ECN sprays performed in year 2013 to 2016.

Investigator(s)	Framework	Type of fuel combustion	TCI closure	Soot model
Jangi et al. [1]	URANS	*n*-Heptane	ESF	–
Pei et al. [10,21]	URANS	*n*-Dodecane	L-tPDF	–
Pang et al. [12,29,43]	URANS	Diesel, *n*-Heptane	WSR	Four-step
D'Errico et al. [13]	URANS	*n*-Dodecane	WSR + PDF	–
Pei et al. [19,20]	URANS	*n*-Heptane	L-tPDF	–
Bhattacharjee and Haworth [22]	URANS	*n*-Heptane, *n*-Dodecane	L-tPDF	–
Bolla et al. [23–25]	URANS	*n*-Heptane, Diesel	CMC	Four-step
Irannejad et al. [27]	LES	*n*-Heptane	FMDF	–
Lucchini et al. [28]	URANS	*n*-Dodecane	ESF	–
Wang et al. [30]	URANS	*n*-Dodecane	WSR	Five-step
Gong et al. [31]	LES	*n*-Dodecane	WSR	Two-step
Chishty et al. [32]	URANS	*n*-Dodecane	L-tPDF	Four-step
Frassoldati et al. [33]	URANS	*n*-Dodecane	mRIF	–
Cheng et al. [34]	URANS	Biodiesel	WSR	Four-step
Poon et al. [35]	URANS	Diesel	WSR	Four-step
Vishwanathan and Reitz [36]	URANS	Diesel	WSR	Five-step
D'Errico et al. [37]	URANS	*n*-Dodecane	WSR, mRIF	–
Gong et al. [38]	URANS	*n*-Heptane	ESF	–
Gallot-Lavallée and Jones [39]	LES	*n*-Heptane	ESF	–
Pandurangi et al. [40]	URANS	*n*-Dodecane	CMC	Four-step
Wehrfritz et al. [41]	LES	*n*-Dodecane	FGM	–
Jangi et al. [42]	URANS	*n*-Heptane	WSR	Two-step
Bolla et al. [44,45]	URANS	*n*-Dodecane	L-tPDF	Four-step

Note: L-tPDF denotes the Lagrangian particle transported PDF model. The two-step soot model represents the Hiroyasu–Nagle and Strickland-Constable (NSC) model which describes soot formation and oxidation [48]. The four-step soot model denotes that developed by Leung et al. [18] where soot nucleation, surface growth, coagulation and oxidation are accounted for. The five-step model considers PAH condensation on top of the four-step soot model [36].

With the aim to achieve more accurate predictions of combustion and emissions formation processes, it is now widely accepted that a more comprehensive chemistry should be incorporated into multi-dimensional computational fluid dynamics (CFD) studies [13], instead of semi-global or global reaction mechanisms. In particular, the presence of low-temperature chemistry is essential to simulate the first stage (cool-flame) ignition [14] since the cool flame behaviour may then influence the second stage (high-temperature) ignition. Also, radicals such as oxygen atom (O) and hydroxyl (OH) should be present since they are pertinent species for the formation of nitric oxides (NO_x) [15] and sulphur oxides (SO_x) [16]. For detailed soot modelling, reactions of aromatics and Polycyclic Aromatic Hydrocarbon (PAH) are required [17]. Otherwise, for semi-empirical soot models, acetylene (C_2H_2) has to be taken into account in the combustion chemistry [18]. Prior to implementing a combustion chemistry with CFD codes, a common practice is to validate the reaction pathways and the associated rate constants under conditions of interest using measurements obtained from shock tube, plug flow and flame speed experiments.

In addition to the validated combustion chemistry, turbulence–chemistry interaction (TCI) closure strategies become an important subject and various numerical studies have proven that TCI affects the computation of ignition delay time, lift-off length and reacting zone thickness [19–24]. Furthermore, an advanced turbulent combustion model should also have the capability to capture multiple combustion modes, which may occur in the engines as aforementioned [1,10,26]. Numerous TCI closure approaches have been developed for the modelling of turbulent spray combustion under engine–relevant conditions. The coupling of TCI closure approaches and chemical kinetic models is often validated using the data provided by Engine Combustion Network (ECN) [2]. Modelling of the ECN spray flames have been performed in both the unsteady Reynolds-averaged Navier–Stokes (URANS) and Large Eddy Simulation (LES) frameworks. Detailed summaries of these works until year 2013 can be found in Refs. [19,22] and the references therein. The research is currently being pursued in multiple streams, including focuses on chemical kinetics, TCI effects and the combustion physics. Those performed in 2013 and onwards are summarised in Table 1. The commonly used TCI closure approaches include Flamelet Generation Manifold (FGM), multiple Representative Interaction Flamelet (mRIF), Conditional Moment-Closure (CMC) and probability density function (PDF). The 'simplest TCI closure' has also been frequently used, *i.e.* the mean chemical source term is directly evaluated using the mean temperature and composition neglecting turbulent fluctuations. In the literature, this approach is referred by different names, for example, direct integration, perfectly-stirred reactor or well-stirred reactor (WSR). This type of model will henceforth be addressed as WSR in this article. In order to simulate the multiple combustion modes, D'Errico et al. [37] proposed to combine different models, *i.e.* WSR and PDF.

The conventional CMC method has been successfully applied to various non-premixed combustion in the past; however, its application to premixed flames remained a challenge, due to the modelling of the progress variable [26,46]. An algebraic model was proposed by Azmin et al. [46] to address this limitation and the results suggested that the CMC, which considered a second conditioning variable, may be applied across the regimes of premixed combustion. However, this is yet to be validated in spray flame simulations. Alternatively, Wright et al. [26] implemented a fully elliptic first-order CMC model for spray autoignition simulations under diesel engine-like conditions. De Paola et al. [47] also employed the same method for diesel engine simulations. Their works showed that the single model can predict the autoignition, diffusion flame mode as well as certain features of the premixed mode such as flame propagations in the spray combustion [26]. The CMC model was also used to simulate *n*-heptane and diesel fuel spray combustion in the Sandia combustion chamber [23–25,40].

The transported PDF method is a more sophisticated TCI closure approach that solves the transport equation for the one-point, one-time Eulerian joint PDF of velocity and composition or alternatively composition only. The main advantage of the transported PDF method, as compared to the previous TCI closure strategies, is that no closure problems arising from averaging of one-point nonlinear chemical reaction rate terms in the governing equations. The