Modelling *n*-dodecane spray and combustion with the transported probability density function method

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ABSTRACT

An *n*-dodecane spray in temperature and pressure conditions typical of diesel engines, known as Spray A, is modelled by the transported probability density function (TPDF) method coupled with a time-dependent Reynolds-averaged $k-\epsilon$ turbulence model and a Lagrangian discrete phase model of the liquid spray. To establish a baseline for comparisons, non-reacting cases are first studied. Good results are obtained for the vapour penetration, the mean and variance of fuel mixture fraction, and velocity profiles, with variations in ambient density and injection pressure. These comparisons are more extensive than previous studies due to new experimental data being available. Reacting cases are then investigated for a number of ambient conditions and injection parameters, employing a reduced chemical kinetic model. The chemical mechanism incorporates an OH* sub-mechanism (Hall and Petersen, 2006) which enables a direct comparison with experimental measurements of the lift-off length that are based on OH* chemiluminescence. To assess the importance of interactions between turbulence and chemistry, the results from the PDF model are compared to the measurements and to those from a well-mixed model that ignores turbulent fluctuations. Variations of ambient temperature, ambient oxygen concentration, ambient density, and injection pressure are considered. In all cases the PDF model with the EMST mixing model and $C_\phi = 1.5$ shows an excellent agreement with the experimental lift-off length and presents improved results compared with the well-mixed model. Ignition delay is however over-predicted by both the PDF method and well-mixed models. Available shock tube data suggests that this may be due to the chemical kinetic model over-predicting ignition delay at higher pressures.

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1. Introduction

To reduce pollutant emissions and improve fuel economy, further improvements of the combustion process in diesel engines are required. Several advanced strategies to achieve these improvements involve changes of the ambient conditions including pressure, oxygen concentration and temperature, changes of the injection parameters such as the number, timing, and pressure of injections, and changes of the in-cylinder flow by altering, for example, swirl or bowl geometry. Computational models of diesel combustion can be a valuable tool to seek improvements in this large design space, especially given the stringent performance constraints imposed by emissions legislation and consumer expectations.

In this context, the predictive capability of a model is obviously important, but the environment of a real engine is not a good starting point for validation since it is difficult to control precisely and measurements are limited. Extensive databases for validation of combustion models are available for canonical atmospheric flames, e.g., the references in Ref. [1]. One good example is from the series of International Workshops on Measurement and Computation of Turbulent Non-premixed Flames (TNF workshops) [2], where jet flames [3–5], piloted jet flames [5–7] and bluff-body flames [8], etc., were extensively studied to serve the purpose of validation of combustion models. However these too are not ideal as the ambient conditions are vastly different from those in a diesel engine. For example, the higher pressures experienced in a diesel engine influence the kinetics significantly, and change the regimes of turbulence–chemistry interactions (TCI) by altering parameters

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such as the Reynolds and Damköhler numbers. Owing to a large injection velocity of the order of 500 m/s, flames in diesel engines are substantially lifted from the nozzle, typically 200–500D [9,10], where D is the nozzle diameter, which results in more substantial mixing prior to the flame compared with a typical atmospheric pressure laboratory lifted flame where the lifted length is limited to roughly 5–100D. Thus, there is a need to test models in the applicable conditions while retaining a canonical and well controlled experiment in which comprehensive measurements are possible.

Recently, efforts have been made to fill this gap via an international collaboration of national laboratories, universities and industry known as the Engine Combustion Network (ECN) [11]. The ECN provides a collaborative platform for experimentalists and modellers to develop and validate computational models to aid in the design of advanced combustion engines. The main focus to date has been on spray flames in diesel engine conditions. Currently, more than 16 research groups worldwide have been involved in modelling the ECN spray flame datasets with different models in different computational codes. N-heptane was considered as the first target for experiments and modelling due to the availability of tractable chemical kinetic models. A comprehensive list of n-heptane modelling studies can be referred to Ref. [12]. More recently, a new dataset with fuel of n-dodecane, named Spray A, was made available through the ECN to promote coordinated studies of a canonical spray flame in conditions relevant to practical diesel engines. Comprehensive experimental data are available, and parametric variations include variations of ambient temperature, ambient density, ambient oxygen concentration and injection pressure for both non-reacting and reacting conditions.

Modelling studies of Spray A performed to date are summarised in Table 1. Luo et al. [13] developed a 106-species skeletal mechanism for n-dodecane and validated against Spray A using unsteady Reynolds-averaged Navier–Stokes (RANS) in conjunction with a well-mixed model to treat turbulence–chemistry interactions. Overall good agreement was obtained for the predictions of ignition delay and lift-off length, however, the sensitivity of lift-off lengths with respect to the ambient temperatures was over-estimated. D'Errico et al. [14] implemented a multiple-flamelet representative interactive flamelet (mRIF) model in conjunction with a RANS solver to study Spray A at different ambient temperature and oxygen conditions. A β form was assumed for the scalar PDFs and good agreement was obtained. The results from the mRIF model were also compared to those from a well-mixed model. Significant improvements were found when considering the TCI effect. Kundu et al. [16] used the same mRIF approach to conduct a more comprehensive study of Spray A at different ambient conditions. Different forms of scalar PDFs were also evaluated. The most relevant study for the present work is Bhattacharjee and Haworth [17], who applied a RANS implementation of the transported probability density function (TPDF) approach and compared results using this method to a well-mixed model which ignores turbulence–chemistry interactions. It was reported that the TPDF model gave much better results than the well-mixed model.

Similar to Refs. [12,17,20], the present study focuses on modelling diesel spray combustion using the transported probability density function (TPDF) method [21]. The principal advantage of this method is that it treats the source term exactly without approximation. This is expected to provide significant advantages in the modelling of finite rate processes such as ignition and pollutant formation. Another feature of the model is that it is not specific only to premixed or non-premixed combustion, which is expected to be an advantage considering that diesel combustion is widely agreed to involve both premixed and non-premixed modes [22,23]. Finally, the TPDF model also makes no assumption about the relative timescales associated with mixing and chemical reaction. This too may prove to be an advantage considering the intense mixing expected near the nozzle where relatively slow, low temperature chemistry is active, and the transition to a fast-chemistry, mixing-controlled mode of combustion downstream.

Most previous applications of the PDF model have focussed on atmospheric pressure gas-phase laboratory flames, with substantial success [24–32]. A few studies have considered multi-phase problems where a Lagrangian-particle-based method was used to treat the spray while the gas-phase was treated with the TPDF approach [33–37]. An excellent review of recent progress in PDF methods can be found in Ref. [38]. However, few works have considered applications of the model in engine-relevant conditions, and thus further work is needed in this direction.

In previous studies [12,20], we modelled an n-heptane spray injection and combustion in a constant volume chamber with high pressure and high temperature ambient conditions (spray H). Ref. [20] treated the spray simply by approximating it as a gaseous jet, while Ref. [12] employed a Lagrangian discrete phase spray model. In the latter work, comprehensive evaluations of the mixing model, mixing constants, and chemical mechanisms were conducted. Excellent agreement was obtained for the spray structure in non-reacting cases and for lift-off length and ignition delay in reacting cases, given appropriate choices for mixing constant, mixing model and chemical mechanism. It was also demonstrated that the PDF model significantly improved the predictions compared to a well-mixed model which ignores turbulence–chemistry interactions.

The present work extends the previous study of Spray H (n-heptane) to Spray A (n-dodecane), and is among the first modelling works considering Spray A. The objectives of the present study are to quantify and understand the model performance, determine how this is affected by the mixing model, and evaluate the effects of turbulence–chemistry interactions on the results. The latter objective will be achieved by comparing the PDF model results to a well-mixed model which ignores turbulence chemistry interactions. Such an approximation is attractive because of its simplicity and low computational cost, but expected to result in significant errors if turbulent fluctuations are non-negligible. Several previous works [39–50] have demonstrated such approaches are able to predict at least qualitative trends, but systematic comparisons with more advanced (and expensive) approaches number very few.

Apart from considering a different fuel, two other aspects are also new compared with the earlier studies of spray H. First, compared with the n-heptane dataset, a wider range of experimental parametric variations about Spray A are available, enabling more comprehensive testing of the model. The data include variations of temperature, oxygen concentration, ambient density, and injec-

Table 1
Summary of modelling studies of Spray A.

Groups	Formulations	Chemical mechanisms	TCI model
Luo et al. [13]	URANS	106-species [13]	Well-mixed
D'Errico et al. [14,15]	URANS	106-species [13], 88-species, 104-species [15]	mRIF
Kundu et al. [16]	URANS	103-species [19,18], 106-species [13]	mRIF
Bhattacharjee and Haworth [17]	URANS	103-species [19,18]	Composition PDF
Pei, Hawkes et al., this work	URANS	88-species	Composition PDF