Combustion and Flame 192 (2018) 101–119

Contents lists available at ScienceDirect

Combustion and Flame

journal homepage: www.elsevier.com/locate/combustflame

# Soot formation modelling for *n*-dodecane sprays using the transported PDF model

Muhammad A. Chishty[a,*], Michele Bolla[a], Evatt R. Hawkes[a,b], Yuanjiang Pei[c], Sanghoon Kook[a]

[a] School of Mechanical and Manufacturing Engineering, The University of New South Wales, Sydney, NSW 2052, Australia
[b] School of Photovoltaic and Renewable Energy Engineering, The University of New South Wales, Sydney, NSW 2052, Australia
[c] Energy System Division, Argonne National Laboratory, Argonne, IL 60439, United States

ARTICLE INFO

*Article history:*
Received 23 February 2017
Revised 24 April 2017
Accepted 18 January 2018
Available online 20 March 2018

*Keywords:*
Transported probability density function
Spray A
Engine Combustion Network
Soot modelling
Turbulence–chemistry interactions
Diesel engines

ABSTRACT

Soot formation in an *n*-dodecane spray flame under diesel engine conditions, known as Spray A, is modelled with the transported probability function (TPDF) method. The approach employs an acetylene-based two-equation soot model coupled with a Reynolds-averaged turbulence model and a Lagrangian discrete phase spray model. The aims are to evaluate, in the context of soot, the predictive capability of the model, the effects of turbulence–chemistry interactions (TCI), and various available chemistry mechanisms. TCI effects are evaluated by comparisons between the TPDF model and simulations using a well-mixed model neglecting turbulent fluctuations. Five test cases having variations in ambient temperature and oxygen concentration are considered.

Five chemical mechanisms are first compared to experiments in terms of their ignition delay (ID) and lift-off length (LOL) under ambient $O_2$ and temperature variations. Three relatively new mechanisms exhibit good ID performance (with both TCI approaches), while two short mechanisms also provide good LOL performance in conjunction with the TPDF approach. The two short mechanisms are considered for further comparisons. The auto-ignition process is analysed by comparing TPDF simulations with measurements from schlieren and 355 nm planar laser-induced fluorescence, detecting $CH_2O$ and polycyclic aromatic hydrocarbons, with overall good qualitative agreement, though with some differences on low-temperature reactivity.

The experimental comparisons for soot consider transient soot mass and KL in the baseline condition, and steady state soot volume fraction (SVF) fields and total soot masses for all five ambient conditions. In terms of comparisons to experiment, the transient stage of the soot mass development is not well captured. An analysis of the transient KL in the baseline case shows the soot-containing region is larger in the experiment than the model, with soot extending in the experiment much closer to the jet boundary, suggesting that the model underestimates gradients around the jet head. During the steady period, however, the SVF agrees quite well. The soot models with both chemistry and TCI approaches were able to reproduce the overall soot trends with varying ambient temperature and oxygen, though the effect of the ambient temperature on the soot mass was under-predicted, in particular in its variation from 900 to 1000 K. TCI effects on soot were in overall terms relatively minor, in part due to compensating errors. Neglecting TCI showed generally higher peak soot amounts, narrower soot distributions, and more downstream soot onset and soot peak locations. These differences between the models are explained with the help of a detailed analysis of the soot phenomena.



## 1. Introduction

Diesel engines are known for their high thermal efficiency but also for high pollutant emissions (mainly $NO_x$ and particulate) due to the existence of hot and rich regions in the cylinder. Reducing these emissions while maintaining or improving fuel economy are the main challenges in designing new engine combustion strategies. These challenges are proving difficult to overcome, due in part to trade-offs between different pollutants and fuel economy, and in part to the complexity of the in-cylinder spray, combustion, and pollutant formation phenomena. Computational models of combustion are playing an increasing role in meeting

* Corresponding author.
*E-mail addresses:* m.chishty@unsw.edu.au, muhammadaqibchishty@gmail.com (M.A. Chishty).

https://doi.org/10.1016/j.combustflame.2018.01.028
0010-2180/

these challenges by enabling shorter design cycles and improved solutions.

Historically, these models were validated against basic data such as pressure traces and engine-out emissions. In the last two decades, driven by increasingly stringent emission legislations, a significant improvement of experimental diagnostics has provided the chance for further development and a more quantitative validation of numerical methods for diesel engine combustion. In particular, the international collaborative forum known as the Engine Combustion Network (ECN) provides a platform to develop and validate numerical models used for supporting the design of advanced combustion engines [1]. Currently, one main focus lies on diesel-relevant spray flames, initially with *n*-heptane (Spray H) and more recently with *n*-dodecane (Spray A). The analysis is very comprehensive, including inner nozzle flow, near field fuel atomisation, fuel-air mixing, ignition, flame stabilisation, and soot formation.

From the modelling point of view, one currently debated question within the ECN community is whether a model for turbulent combustion under diesel-engine conditions needs to account for turbulence–chemistry interactions (TCI), i.e., whether or not turbulent fluctuations of temperature and species concentrations need to be explicitly accounted for. In recent years, there is a clear trend for modellers to progressively account for TCI (see e.g., [2–6] and references therein). In these studies, the performance of models including TCI was seen to be superior but also models without TCI were found to perform reasonably well in terms of global ignition and combustion related quantities [7–9]. Generally, when neglecting TCI an over-prediction of the flame lift-off length is observed, whereas the impact on the ignition delay was seen to be minor in a number of studies [5,10]. Other studies showed that ignoring TCI also caused over-prediction of ignition delay, in particular at lower ambient temperature [3]. Another trend is to employ large-eddy simulations, which resolve large-scale turbulent fluctuations and either neglect or model small-scale fluctuations [11,12].

On the other hand, the current situation of soot modelling in the context of ECN is not as mature as the combustion modelling part. In the last decade, soot-related simulation works comparing in-cylinder soot mass with experiments have been reported for optically accessible diesel engines, e.g., [13–17], and spray combustion in constant-volume vessels with various fuels; these include, for example diesel fuel [18,19], *n*-heptane [2,16,20–23], *n*-dodecane/*m*-xylene blends [21] and *n*-dodecane [12,24–26] fuels. Experimentally, recent advances compared to earlier ECN soot databases (e.g., [27,28]) have been reported for time-resolved soot measurements [29–31]. The advent of a more detailed soot measurements database has the potential to promote the development of advanced soot models for diesel engines.

At the ECN2 and ECN3 Workshops [1], first attempts to qualitatively assess soot model performance were presented. Only three modelling groups contributed to the comparison. Overall, one of the main barriers preventing a conclusive analysis for different soot modelling approaches was the significant over-prediction of the computed ignition delays and to a lesser extent the lift-off lengths, which affect the amount of time available for premixing and therefore soot. The same shortcoming has been observed at the recent ECN4 Workshop, where the focus of the analysis was devoted to the soot onset characteristic. The identified problems with chemical mechanisms available at the time of ECN3 led to the development of several alternative mechanisms. However, these mechanisms have not been comprehensively compared in terms of their ignition delays and lift-off lengths, which are arguably an essential starting point for obtaining good soot predictions. Also, differences in the flame structure resulting from the different mechanisms including important species involved in soot phenomena such as hydroxyl radicals and acetylene have not been compared.

In addition to the above-mentioned chemical mechanism effects, to date, the influence of TCI for soot modelling in diesel engine-relevant conditions has only been reported in few preliminary studies in a constant-volume chamber [9] and in a heavy-duty diesel engine considering engine-out soot [32]. Overall, TCI has been found to increase the soot oxidation rate, resulting into considerably lower soot mass in the exhaust [32].

The present work extends a previous study of Spray A [6,33], where the TPDF model has been comprehensively validated in terms of mixture formation, ignition, flame stabilisation and flame structure for various ambient conditions. The contributions of the present work are as follows. First, several of the available chemical mechanisms that have a manageable size are compared in terms of global indicators such as the ignition delay and lift-off length and in terms of the resulting flame structure. This comparison leads to the selection of two new short mechanisms that are able to predict the ignition delay and lift-off length quite well as candidates for further investigation of soot processes. Then, the TPDF model is coupled with a two-equation soot model widely used in the literature [34], which has seen successful application for various laboratory flames [3,34,35]. The results are comprehensively analysed with both candidate mechanisms.

The paper is organised as follows. The experimental and simulation details are briefly described in Section 2. The results are analysed according to the objectives outlined above in Section 3 and finally a summary and discussion are reported in Section 4.

## 2. Methodology

### 2.1. Experimental setup

The spray combustion experiments have been performed under the framework of the Engine Combustion Network [7]. In the present work, modelling results are validated against data from a constant-volume pre-burn combustion vessel operated at Sandia National Laboratories [29,36]. The experiments consider fuel injection into a high pressure and high temperature ambient environment. Liquid fuel is injected into the nominally quiescent ambient environment, evaporates, ignites and eventually there is a transition to a quasi-stationary flame that is lifted from the nozzle. Five test cases with different ambient temperatures and ambient oxygen mole fractions are considered here, as shown in Table 1. Measurements have been carried out with the spray A injector (210,370) with an effective orifice diameter of 90.8 µm.

Recent measurements of 355 nm planar laser-induced fluorescence (PLIF) from Ref. [36] - detecting the spatial distribution of formaldehyde and polycyclic aromatic hydrocarbons (PAH) - have been used to further validate the model in terms of the auto-ignition and soot precursor formation processes. Measurements of soot volume fraction and soot mass [7], performed with the diffused back-illumination extinction imaging (DBIEI) technique as described in [30], are used here for the validation of the soot model. This technique determines the optical thickness KL via ex-

**Table 1**
List of experimental specifications of test cases considered. The baseline spray A non-reacting and reacting case are shown in bold.

| $T_{amb}$ (K) | $O_2$ (%) | $P_{amb}$ (MPa) |
|---|---|---|
| **900** | **0/15** | **6.16/5.98** |
| 850 | 15 | 5.63 |
| 1000 | 15 | 6.62 |
| 900 | 13 | 6.04 |
| 900 | 21 | 5.91 |