Combustion and Flame 000 (2016) 1–16

Contents lists available at ScienceDirect

Combustion and Flame

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

An analysis of the structure of an *n*-dodecane spray flame using TPDF modelling

Yuanjiang Pei[a], Evatt R. Hawkes[b,c,*], Michele Bolla[c], Sanghoon Kook[c], Graham M. Goldin[d], Yue Yang[e], Stephen B. Pope[f], Sibendu Som[a]

[a] *Transportation Technology Research and Development Center, Argonne National Laboratory, Argonne, IL 60439, USA*
[b] *School of Photovoltaic and Renewable Energy Engineering, The University of New South Wales, Sydney, NSW 2052, Australia*
[c] *School of Mechanical and Manufacturing Engineering, The University of New South Wales, Sydney, NSW 2052, Australia*
[d] *Ansys Inc., Lebanon, NH, USA*
[e] *State Key Laboratory for Turbulence and Complex Systems, College of Engineering, Peking University, Beijing 100871, China*
[f] *Sibley School of Mechanical and Aerospace Engineering, Cornell University, Ithaca, NY 14853, USA*

ARTICLE INFO

Article history:
Received 14 May 2015
Revised 29 November 2015
Accepted 30 November 2015
Available online xxx

Keywords:
Spray A
Engine Combustion Network
Transported probability density function
Diesel
n-Dodecane

ABSTRACT

With a view to understanding ignition and combustion behaviours in diesel engines, this study investigates several aspects of ignition and combustion of an *n*-dodecane spray in a high pressure, high temperature chamber, known as Spray A, using data resulting from modelling using the transported probability density function (TPDF) method. The model has been validated comprehensively with good to excellent agreement in our previous work against all available experimental data including for mixture-fraction and velocity fields in non-reacting cases, and flame lift-off length and ignition delay in reacting cases. This good agreement encourages further investigation of the numerical model results to help understand the structure of this flame, which serves to complement the experimental information that is available, which is very limited due to the difficult experimental conditions in which this flame exists. For example, quantitative experimental measurements of local mixture-fraction, temperature, velocity gradients, etc. are not yet possible in reacting cases. Analysis of the model results shows that two-stage ignition is found to occur across the ambient temperature conditions considered: the first stage is rapidly initiated on the lean side where temperatures are high and sequentially moves to richer, cooler conditions. The first stage is extremely resilient to turbulence, occurring in a region of very low Damköhler number. The second stage of ignition occurs first in rich mixtures in a region behind the head of the fuel jet where mixture gradients are low, and appears to be influenced strongly by turbulence. Relative to a homogeneous reactor, it is delayed on the lean side but advanced on the rich side, suggesting entrainment and mixing from the early igniting lean regions into richer mixtures is an important moderator of the ignition process. The second-stage ignition front propagates at very high velocities initially, suggesting it is a sequential ignition moving according to gradients of ignition delay and/or residence time. The flame stabilises however on the lean side in a region of much lower velocity, where turbulent velocity fluctuations are sufficiently high such that turbulent transport influences the propagation. It stabilises in a region of low Damköhler number which implies that a competition of chemistry versus micro-mixing might also be involved in stabilisation. The stabilisation mechanism is investigated by an analysis of the transport budgets, showing the flame is stabilised by autoignition but moderated by turbulent diffusion. Further analysis of the flame index supports this stabilisation mechanism, and demonstrates the simultaneous existence of non-premixed and premixed combustion modes in the same flame. Analysis of the flow fields also reveals that local entrainment and dilatation are important flow features near the flame base.

1. Introduction

In the last two decades, significant progress has been made in using experimental techniques to understand the structure of diesel spray flames [1–7]. For example, in Dec's landmark paper [2], imaging techniques employing Mie scattering, Rayleigh scattering, chemiluminescence, polycyclic aromatic hydrocarbon (PAH) fluorescence,

* Corresponding author at: School of Photovoltaic and Renewable Energy Engineering, The University of New South Wales, Sydney, NSW 2052, Australia.
E-mail addresses: yuanjiang.pei@aramcoservices.com (Y. Pei), evatt.hawkes@unsw.edu.au (E.R. Hawkes).

http://dx.doi.org/10.1016/j.combustflame.2015.11.034
0010-2180/

and laser-induced incandescence were applied to develop a conceptual model of the structure of a diesel spray flame that was remarkably different to the physical pictures that were proposed before these techniques were available.

Many other works have followed and built upon this body of knowledge, e.g. see Ref. [7] for a review. For example, spray flames in a constant-volume combustion chamber under typical diesel engine conditions have been investigated in a forum known as the Engine Combustion Network (ECN) [8]. In particular, an *n*-dodecane spray flame, named Spray A has been a principal focus. Different facilities around the world have conducted experiments on Spray A conditions with different techniques to further understand spray flames under diesel engine conditions [9–14]. For example, in a constant-volume combustion vessel, Pickett et al. [10] investigated the relationship between vapor penetration and local fuel mixture fraction. Benajes et al. [11] characterised the ignition and lift-off length for Spray A in a constant-pressure flow rig. Pickett et al. [9] and Meijer et al. [14] reviewed the Spray A experiments in different high-temperature and high-pressure facilities in the ECN community. Some computational studies to investigate Spray A have also recently been reported [15–27], for example, using RANS-based transported probability density function (TPDF) method [15,23,26] and flamelet-type models [16–18] to demonstrate the importance of the effect of turbulence-chemistry-interaction (TCI) at diesel-engine conditions, and using large eddy simulation (LES)-type models [19–22,24,25] to demonstrate the capability of LES in simulating diesel spray.

Despite this substantial progress, the most detailed available experiments can still only provide a partial set of data – for example only one or two species would be simultaneously available, and these measurements are not quantitative. This stands in significant contrast to the situation with atmospheric pressure laboratory flames, where advanced experiments have been able to measure a large array of variables for some time: for example single point simultaneous measurements of all major species, some minor species, and temperature have been available for decades, e.g., [28–31], and more recently time- and space- resolved simultaneous measurements of some species and/or velocity and velocity gradients have become possible [32–34], with even some three-dimensional measurements also being reported [35,36]. Since such quantitative detail is not yet available in diesel engine conditions, much less is known about the details of ignition and combustion under these conditions than is known about these phenomena under atmospheric conditions.

In contrast, advanced models of turbulent combustion compute an approximation to the missing information, and therefore, once validated, can arguably suggest a qualitative picture of the missing data and infer characteristics of the flame structure which cannot yet be measured. Other studies have used model results in this way. For example, Gordon et al. [37,38] simulated lifted laboratory flames using the TPDF method and investigated the flame stabilisation mechanism for different coflow temperatures. Ameen and Abraham [39] studied an n-heptane gas jet using flamelet progress variable (FPV) model and examined the fundamental physics affecting the lift-off length. Irannejad et al. [40] modelled an n-heptane spray and studied the ignition behaviour for different ambient conditions using TPDF method. Jangi et al. [19] simulated Spray A and also investigated the flame stabilisation behaviour using transport budgets analysis.

The goal of this paper is therefore to examine results from simulations of Spray A using a relatively complete model of turbulent combustion, the TPDF method, and infer some important characteristics of the flame structure associated with the two-stage ignition process and stabilisation mechanism. Specifically the objectives are to understand the effects of turbulence, mixing, and chemistry on the process of ignition, the transition to a stabilised flame, the mechanism of flame stabilisation, and the structure of the stabilised flame in terms of the combustion mode (premixed, non-premixed, etc.), turbulence parameters, forms of scalar PDFs, and the dimensionality of the thermochemical state-space.

Table 1
Experimental boundary conditions.

Fuel	*n*-dodecane
Fuel density (kg/m^3)	698
Fuel temperature (K)	363
Nominal nozzle-hole diameter (mm)	0.09
Common-rail pressure (MPa)	150
Injection velocity (m/s)	595 [a]
Ambient density (kg/m^3)	22.8
Ambient mixture composition (%)[b]	O_2 (15) N_2 (75.15) CO_2 (6.22) H_2O (3.62)

[a] Not measured. Computed using nozzle discharge coefficient.
[b] Mole fraction.

Table 2
Investigated cases.

$T_{amb}(K)$	O_2 (%)	P_{amb} (MPa)
800	15	5.25
900	15	5.94
1100	15	7.30

The paper is organised as follows. The experimental and simulation details are briefly described in Section 2, which also includes a brief summary of earlier validation of the modelling results against experimental data. 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 [8]. In the present work, modelling results are validated against data from a constant volume preburn combustion vessel operated at Sandia National Laboratories [9,10]. The experiments considered fuel injection into a high pressure and high temperature ambient environment. This environment is achieved through igniting a pre-filled diluted mixture, then cooling for a relatively long period (seconds) to reach the target ambient conditions. 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. Key experimental details are listed in Table. 1.

Three cases that having different initial temperatures are considered in this study for numerical investigations, as shown in Table 2.

2.2. Model and numerical parameters

The modelling methods used are outlined extensively in previous work [26,27,41,42], so only a brief account is repeated here.

TPDF model. The composition TPDF model is implemented in the commercial code Fluent [43] using a Lagrangian Monte Carlo approach. The conventional hybrid Eulerian-Lagrangian method is adopted, where the flow is modelled with a Reynolds-Averaged Navier–Stokes (RANS) based $k-\epsilon$ turbulence model. The unclosed turbulent flux term is modelled using the assumption of gradient diffusion, which is implemented by incrementing particle positions using a Wiener process. The Euclidean Minimum Spanning Tree (EMST)

Please cite this article as: Y. Pei et al., An analysis of the structure of an n-dodecane spray flame using TPDF modelling, Combustion and Flame (2016), http://dx.doi.org/10.1016/j.combustflame.2015.11.034