Applied Energy 136 (2014) 373–381

Contents lists available at ScienceDirect

Applied Energy

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

Large eddy simulation of *n*-Dodecane spray combustion in a high pressure combustion vessel

Cheng Gong *, Mehdi Jangi, Xue-Song Bai

Division of Fluid Mechanics, Dep. of Energy Sciences, Lund University, Box 118, SE 22100 Lund, Sweden

HIGHLIGHTS

- Improved understanding of the ignition process in spray combustion under diesel engine conditions.
- Detailed reaction zone structures captured under different ambient temperatures.
- Two different mechanisms proposed to explain the flame stabilization.

ARTICLE INFO

Article history:
Received 6 May 2014
Received in revised form 30 August 2014
Accepted 10 September 2014

Keywords:
Diesel combustion
Autoignition
Flame stabilization
Large eddy simulation

ABSTRACT

Autoignition and stabilization of *n*-Dodecane spray combustion under diesel engine like conditions are investigated using large eddy simulation and detailed chemical kinetics. The Spray A cases of Engine Combustion Network (ECN) with ambient temperatures of 900 K and 1000 K are considered. Two-stage ignition behavior is predicted in the studied conditions. It is found that the first-stage ignition occurs on the fuel-lean mixture, whereas the second-stage ignition starts on the fuel-rich mixture. The first stage ignition in the fuel-lean mixture promotes the first and the second stage ignition in the fuel-rich mixture owing to rapid turbulent mixing. Two mechanisms, autoignition and flame propagation coupling with the low temperature ignition, are used to explain the lift-off position and stabilization of the combustion process. They compete with each other, and their relative importance depends on the ambient temperature. The ambient temperature is shown to affect the soot emission in the flame through its influences on the lift-off length and the reaction zone structure. Higher ambient temperature results in a shorter lift-off length, which gives rise to higher soot emission due to the lower air entrainment to the fuel-rich zone in front of the flame. In the lower temperature case, the flame is stabilized by an autoignition induced flame front where a considerable amount of fuel is oxidized to CO at the leading front of the flame. Consequently, it reduces the soot formation in the flame.

1. Introduction

Reduction of pollution emissions is one of the most challenging tasks in the development of diesel engines. Emission control can be achieved using after-treatment and in-cylinder solutions. The latter reduces pollutant formation in the engine cylinder through the use of improved combustion technologies, such as high-pressure injection strategies, low compression ratio bowls, and exhaust gas recirculation (EGR). The latter is used to generate a low temperature combustion condition as a means of reducing NOx emissions [1]. To develop advanced combustion control strategies, comprehensive understanding of the combustion characteristics is necessary, e.g., the onset of ignition, and the mechanism of flame lift-off and stabilization.

Lifted turbulent jet flames have been widely investigated under atmospheric conditions. Various theories have been proposed to explain the stabilization mechanism of the lifted flames [2,3], e.g., reaction front propagation at the flame base [4], local extinction due to high scalar dissipation rate [5], and vortex/flame interaction [6]. Autoignition plays an important role in the lift-off and stabilization of combustion when the ambient temperature and pressure are higher than the atmospheric conditions, e.g., jet flames under diesel engine conditions. Recent review on the experimental studies of the lift-off of diesel flames can be found in Ref. [7]. Several experimental studies demonstrated the importance of the autoignition process on the lift-off process under diesel combustion conditions, e.g., the cool flame (first-stage ignition) upstream of the lift-off [8–10], shorter lift-off lengths for fuels with

* Corresponding author. Fax: +46 462224717.
E-mail address: cheng.gong@energy.lth.se (C. Gong).

http://dx.doi.org/10.1016/j.apenergy.2014.09.030
0306-2619/

Nomenclature

Variables

$\widetilde{T}$	temperature
J_H	mass fraction of H-atom
α	a modified scalar dissipation rate
$\varepsilon_{\widetilde{Y}_k}$	error of the kth species due to the mapping
p	thermodynamic pressure
Z_{st}	stoichiometric mixture fraction
τ_{ign}	ignition delay time
τ_l	first-stage (low temperature) ignition delay time
τ_h	second-stage (high temperature) ignition delay time

Abbreviations

ASI	after the start of injection
AIIF	auto-ignition induced flame-front
CCM	chemistry coordinate mapping
CMC	conditional moment closure
DISI	direct injection spark ignition engine
DNS	direct numerical simulation
ECN	engine combustion network
EGR	exhaust-gas recirculation
HRR	heat-release rate
LES	large eddy simulation
LTI	low temperature ignition site
NTC	negative-temperature-coefficient
WSR	well stirred reactor

shorter ignition delay and the appearance of isolated ignition kernels upstream of the lift-off [8,9]. Moreover, lift-off heights and reaction zone structures depend on the ambient conditions and the injections, e.g., two different structures of flame base were found for different fuels based on the OH measurements [9]. Swirl motion inside the cylinder can also affect the lift-off and stabilization of flames in diesel engines [11].

The large hydrocarbon fuels used in diesel engines usually have strong low temperature behavior [12]. Oxidization of this type of fuels undergoes a complex chemical process, e.g., two-stage ignition. This can further affect the ignition and stabilization of diesel spray combustion. Due to the lack of detailed temporal and spatial distribution of temperature and species in most experiments, it is often not possible to determine whether the lift-off and flame stabilization are controlled by the flame propagation or by the autoignition in the diesel flame; for instance, although cool flames were found upstream of the lift-off, their role is not fully understood. They may enhance flame propagation, or they may also lead directly to second-stage ignition without flame propagation [8]. Motived by this, large eddy simulations (LES) of the ignition and lift-off stabilization processes are carried out in this work under conditions relevant to diesel engine combustion. Numerical simulation can offer more detailed data about the reaction layer structures to improve the understanding of the combustion process [13]. LES is proven to be able of capturing intrinsically time and space dependent phenomena. LES coupled with Lagrangian particle tracking methods are widely employed in simulations of the combustion process in internal combustion engines, e.g., Solsjö et al. carried out LES of spray combustion process in diesel engines [11,14]; Goryntsev et al. investigated the combustion process in direct injection spark ignition (DISI) engines [15–17].

The Spray A cases of Engine Combustion Engine Network (ECN) [18] with the fuel of *n*-Dodecane are considered here, since *n*-Dodecane features more similar characteristics to the diesel fuel than the usual surrogate, *n*-heptane [19] and also the ECN cases offers systematically varied flame conditions [20–23]. The objectives of this study are to improve the understanding of the ignition process and the lift-off stabilization mechanisms, and to delineate the effect of ambient temperature on the reaction zone structure and soot emission.

2. LES spray combustion model and case setup

Eulerian–Lagrangian approach is used within the LES framework for spray modeling. The gas phase is described using spatially filtered transport equations, where sub-grid turbulence is modeled using a one-equation eddy model [24]. The liquid phase is considered as a discrete phase consisting of a large number of evaporating droplets, which are tracked in the Lagrangian framework. Huh–Gosman [25] model and WAVE model [26] are used for the primary break-up and secondary break-up processes, respectively. Gas and liquid phases are coupled through the mass, momentum, and energy exchange source terms in the corresponding transport equations. Details of the numerical approach can be found in Ref. [27]. OpenFOAM [28], an open source 3-D CFD code, is used to numerically solve the governing equations. Second order finite-volume schemes are used for the spatial discretion (filtered linear scheme) and temporal integration (backward Euler scheme).

The well stirred reactor (WSR) combustion model, based on a moderately detailed chemical kinetic mechanism [19] for *n*-Dodecane, is chosen to simulate the Spray A cases. The chemical mechanism consists of 103 species and 370 reactions. This mechanism is derived from a detailed mechanism for *n*-Dodecane [29], consisting of 2115 species and 8157 reactions. To integrate the source terms due to elementary reactions in the species transport and energy equations, a recently developed acceleration method, the so-called chemistry coordinate mapping (CCM) method [30–33], is employed. The phenomenological Nagle-Strickland soot model [34] is used for numerical simulations of soot formation and oxidization. The model has been shown to provide reasonable prediction of soot behavior in engines [34].

The basic idea of the CCM method is to map the thermo-chemistry identical cells in the physical space to a multidimensional phase space made up of temperature, $\widetilde{T}$, mass fraction of H-atom, J_H, and a modified scalar dissipation rate, $\alpha = \log_{10}(\nabla J_H \cdot \nabla J_H + 1)$. The mass fraction of H-atom is defined as

$$J_H = \sum_{k=1}^{Ns} \frac{W_H}{W_k} \beta_{H,k} \widetilde{Y}_k, \tag{1}$$

where W_H and W_k are the atomic and molecular weights of H-atom and the kth species, respectively. $\beta_{H,k}$ is the number of H-atom in the kth species. Ns is the total number of species in the mixture. The phase space $(J_H, \widetilde{T}, \alpha)$ is discredited into N_J, N_T and N_α zones in the J_H, $\widetilde{T}$ and α coordinate, respectively. The (i, j, k) cell in the physical domain is mapped to the (l, m, q) zone in the $(J_H, \widetilde{T}, \alpha)$ space.

The mean values of the variables in each phase space zone are determined and used as the initial conditions for integrating the reaction rates, i.e.,

$$\widehat{Y}_k(l, m, q, t_n) = \frac{1}{N_c} \sum_{(i,j,k)\to(l,m,q)} \widetilde{Y}_k(i, j, k, t_n) \tag{2}$$