Combustion and Flame xxx (2014) xxx–xxx

Contents lists available at ScienceDirect

Combustion and Flame

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

Direct numerical simulations of the ignition of a lean biodiesel/air mixture with temperature and composition inhomogeneities at high pressure and intermediate temperature

Minh Bau Luong [a], Tianfeng Lu [b], Suk Ho Chung [c], Chun Sang Yoo [a,*]

[a] School of Mechanical and Nuclear Engineering, Ulsan National Institute of Science and Technology, Ulsan 689-798, Republic of Korea
[b] Department of Mechanical Engineering, University of Connecticut, Storrs, CT 06269, USA
[c] Clean Combustion Research Center, King Abdullah University of Science and Technology, Thuwal, Saudi Arabia

ARTICLE INFO

Article history:
Received 20 January 2014
Received in revised form 21 April 2014
Accepted 6 May 2014
Available online xxxx

Keywords:
DNS
Homogeneous charge compression ignition (HCCI)
Stratified charge compression ignition (SCCI)
Biodiesel
Chemical explosive mode analysis (CEMA)

ABSTRACT

The effects of the stratifications of temperature, T, and equivalence ratio, ϕ, on the ignition characteristics of a lean homogeneous biodiesel/air mixture at high pressure and intermediate temperature are investigated using direct numerical simulations (DNSs). 2-D DNSs are performed at a constant volume with the variance of temperature and equivalence ratio (T'' and ϕ'') together with a 2-D isotropic velocity spectrum superimposed on the initial scalar fields. In addition, three different $T-\phi$ correlations are investigated: (1) baseline cases with T'' only or ϕ'' only, (2) uncorrelated $T-\phi$ distribution, and (3) negatively-correlated $T-\phi$ distribution. It is found that the overall combustion is more advanced and the mean heat release rate is more distributed over time with increasing T'' and/or ϕ'' for the baseline and uncorrelated $T-\phi$ cases. However, the temporal advancement and distribution of the overall combustion caused by T'' or ϕ'' only are nearly annihilated by the negatively-correlated $T-\phi$ fields. The chemical explosive mode and Damköhler number analyses verify that for the baseline and uncorrelated $T-\phi$ cases, the deflagration mode is predominant at the reaction fronts for large T'' and/or ϕ''. On the contrary, the spontaneous ignition mode prevails for cases with small T'' or ϕ'', especially for cases with negative $T-\phi$ correlations, and hence, simultaneous auto-ignition occurs throughout the entire domain, resulting in an excessive rate of heat release. It is also found that turbulence with large intensity, u', and a short time scale can effectively smooth out initial thermal and compositional fluctuations such that the overall combustion is induced primarily by spontaneous ignition. Based on the present DNS results, the generalization of the effects of T'', ϕ'', and u' on the HCCI combustion is made to clarify each effect. These results suggest that temperature and composition stratifications together with a well-designed $T-\phi$ correlation can alleviate an excessive rate of pressure rise and control the ignition-timing in homogeneous charge compression-ignition (HCCI) combustion.

1. Introduction

Over the past decade, several advanced combustion concepts for the next-generation internal combustion (IC) engines have emerged with the aim of achieving high-thermal efficiency and meeting stringent pollutant emission regulations. In general, the new concepts rely primarily on the principle of fuel-lean, dilute, premixed or partially premixed, compression ignition at high pressure and low temperature, thereby providing high diesel-like efficiency with ultra-low NO_x and soot emissions [1–4].

Among the novel combustion concepts, homogeneous charge compression-ignition (HCCI) combustion has been investigated extensively by the engine community and is now believed to be one of the most probable alternatives in the near future to the conventional IC engines. However, a few challenges remain in the development of real HCCI engines, the two most pertinent to HCCI combustion being the precise control of the ignition timing of combustion and prevention of an excessive pressure-rise rate (PRR) under high-load conditions.

A strategy of controlling mixture inhomogeneities has been proposed as a promising means of controlling the ignition timing and PRR. Thermal stratification can be introduced to a fuel/air mixture by high levels of exhaust gas recirculation (EGR), intake charge heating, and wall heat transfer controls. It has been demonstrated

* Corresponding author. Fax: +82 52 217 2308.
E-mail address: csyoo@unist.ac.kr (C.S. Yoo).

http://dx.doi.org/10.1016/j.combustflame.2014.05.004
0010-2180/

experimentally and numerically that thermal stratification can tailor PRR by prolonging combustion duration, thereby enabling HCCI combustion under conditions of higher load [5–16].

However, the manipulation and exploitation of the thermal stratification of in-cylinder charge is not easy and remains a challenge [1,17,18]. For this reason, stratified-charge compression ignition (SCCI) combustion has been investigated as an alternative solution for enlarging the operating range of HCCI combustion [11,17,19]. With the help of fuel stratification, a sequential ignition event can be achieved as a locally-richer mixture tends to ignite initially and then ignition propagates towards a nearby leaner mixture. As a result, SCCI combustion enables a smooth combustion sequence, preventing any rapid release of energy and reducing the peak rate of pressure rise. In practice, fuel stratification can be achieved by multiple high-pressure injectors with flexible injection timing [11,3,4]. In two-stage injection, for instance, a major fraction of the fuel is initially supplied by port fuel injection to generate a relatively-homogeneous mixture [11]. The remainder of the fuel (up to 20% of total fuel volume) is then directly injected during the late compression stroke or close to the top dead center (TDC) to introduce a certain amount of equivalence ratio (ϕ) fluctuations [4].

SCCI combustion under HCCI condition has been studied extensively [20,11,21,22,1,23–30,18,17,31,19,32–35]. Recently, Bansal and Im [27] investigated the ignition characteristics of a hydrogen/air mixture with both temperature and composition inhomogeneities using two-dimensional (2-D) DNSs. It was found that composition inhomogeneities together with temperature fluctuations spread out the heat release rate (HRR) more than temperature fluctuations alone. However, it is not clear that the results will be directly applicable to hydrocarbon/air mixtures exhibiting two-stage ignition.

The objective of the present study is, therefore, to provide a fundamental understanding of the ignition characteristics of a hydrocarbon/air mixture with temperature and composition stratifications under high pressure and intermediate temperature using 2-D DNSs. The DNSs are conducted by systematically changing three key parameters: (1) initial temperature fluctuation, (2) initial equivalence ratio fluctuation, and (3) turbulence time scale. In the present study, biodiesel is adopted as a fuel exhibiting two-stage ignition similar to *n*-heptane [14] such that the results of its ignition under HCCI condition may be readily extended to other hydrocarbon fuels with similar two-stage ignition behavior. Biodiesel is a renewable fuel that can contribute toward reducing the demand of fossil fuels. In practice, biodiesel can be blended with petrodiesel to improve the overall combustion performance in terms of efficiency and emissions. For the present study, however, neat biodiesel is utilized to provide a more in-depth understanding of its ignition characteristics under HCCI conditions by using DNSs [36–40].

2. Numerical method and initial conditions

The compressible Navier–Stokes, species continuity, and total energy equations for a reacting gas mixture are solved numerically using the Sandia DNS code, S3D [41,42]. A fourth-order explicit Runge–Kutta method for time integration [43] and an eighth-order central differencing scheme for spatial discretization [44] are used with a tenth-order filter. CHEMKIN software libraries [45,46] are linked with S3D to evaluate reaction rates, thermodynamic and mixture-averaged transport properties. For details of the numerical methods, readers are referred to [41,42].

As mentioned above, we adopted biodiesel as a hydrocarbon fuel, which is a mixture of mono-alkyl esters of long-chained fatty acids produced from vegetable oils or animal fats by transesterification in the presence of a catalyst. The chemical kinetics of biodiesel oxidation is extremely complex due to its large molecular structure, especially at low temperatures. For the present DNSs, a 73-species reduced mechanism was developed from a previous skeletal mechanism for a tri-component biodiesel surrogate that consists of 25% methyl decanoate (MD), 25% methyl 9-decenoate (MD9D), and 50% *n*-heptane by volume [47,48]. The skeletal mechanism was developed from a detailed mechanism of LLNL [49] for the numerical studies of compression ignition engine applications with a reasonable computational time and cost. Linearized quasi steady state approximations (QSSA) are applied to the skeletal mechanism to further reduce the number of transported species [50].

The skeletal and reduced mechanisms were originally validated based on reaction states sampled from auto-ignition and perfectly stirred reactors (PSR) covering the parameter range of pressures from 1 to 100 atm, equivalence ratios from 0.5 to 2.0, and initial temperature from 700 to 1800 K for auto-ignition [47,48]. Extended validation of the reduced mechanism relevant to the present DNSs is shown in Fig. 1 for biodiesel/air at equivalence ratio of 0.3 and pressure of 40–100 atm. The accuracy of the reduced mechanism is mostly identical to that of the skeletal mechanism over the entire parameter range of the reduction. Although it is significantly reduced from the original detailed chemistry, the reduced mechanism shows a good agreement with the detailed mechanism and experimental results in terms of ignition delays, flame propagation speeds, and extinction residence times. Details of the skeletal and reduced mechanisms of biodiesel oxidation can be found in [47,48]. In addition, the method of dynamic stiffness removal [14–16,51] is employed to eliminate chemical time scales shorter than 10 ns such that explicit time integration could be applied in DNSs.

For all DNSs in the present study, the initial mean temperature, T_0, mean equivalence ratio, ϕ_0, and the initial uniform pressure, p_0, are 850 K, 0.45, and 40 atm, respectively. The initial conditions are chosen to employ the low temperature heat release of two-stage ignition of biodiesel/air mixture relevant to high-load naturally aspired HCCI engines such that the initial pressure of 40 atm is relatively low compared to that in modern boosted engines at the TDC. Twelve different DNSs are performed by changing two key parameters: temperature fluctuations, T', of 15 K and 60 K, and equivalence ratio fluctuations, ϕ', of 0.05 and 0.10. Three additional DNSs are carried out to elucidate the effect of turbulence on HCCI combustion by varying turbulence intensity, u', from 1.0 to 5.0 m/s.

Note that ϕ_0 and ϕ' are carefully selected such that local ϕ is maintained precisely below unity, thereby preventing locally-high temperature that may cause excessive NO_x formation [4]. Furthermore, the initial conditions are representative of the TDC under high-load conditions in air-diluted HCCI combustion [5,52]. From 0-D simulations, the homogeneous ignition delay of a

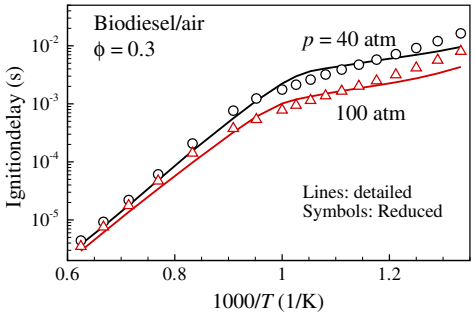

Fig. 1. Ignition delay of biodiesel/air as a function of the initial temperature for constant pressure auto-ignition at equivalence ratio of 0.3 and different pressures, calculated with the detailed and reduced mechanisms, respectively.