Available online at www.sciencedirect.com

ScienceDirect

Proceedings of the Combustion Institute 35 (2015) 2975–2982

Proceedings of the Combustion Institute

www.elsevier.com/locate/proci

Direct numerical simulation of PRF70/air partially premixed combustion under IC engine conditions

F. Zhang, R. Yu, X.S. Bai *

Division of Fluid Mechanics, Lund University, Lund, Sweden

Available online 1 October 2014

Abstract

A three-dimensional direct numerical simulation (DNS) is performed to study the ignition and the combustion process of a primary reference fuel (PRF) under conditions relevant to partially premixed combustion (PPC) engines. Detailed transport properties together with a skeletal PRF chemical kinetic mechanism are employed in the simulations. The initial partially premixed charge is prescribed according to a two-injection of fuel strategy with a 50% exhaust gas recirculation (EGR). The motion of the piston, hence, the effect of compression of the charge due to the piston motion is considered. The simulations are performed with a fine mesh with a spatial resolution of 1.2 micrometers in a cubic domain of 614 micrometers on each side. The results show that there are three distinctive combustion regions in a domain under PPC conditions, a lean homogeneous mixture region, a fuel-rich region, and in between a region with stoichiometric mixture. Auto-ignition occurs first in the lean and stoichiometric mixture regions, followed by a partially premixed flame in the fuel-rich region and at last a CO oxidation phase in the fuel-rich region. In the lean mixture region, the fuel and the combustion intermediates such as CO are consumed almost completely due to the relatively fast combustion and the abundant oxygen. The CO formed in the regions with the stoichiometric and the fuel-rich mixture is consumed in a mixing controlled mode, which requires a high-level turbulence mixing or a sufficiently long residence time. NO is formed mainly due to the premixed combustion in the region with the stoichiometric mixture.

Keywords: Direct numerical simulation; Partially premixed combustion; PRF fuel; IC engines

1. Introduction

Partially premixed combustion (PPC) engine can be considered as a hybrid of the classical diesel engine and the homogeneous charge compression ignition (HCCI) engine. The diesel engine suffers from high soot and NOx and the HCCI engine is challenged by the high pressure-rise-rate and the high engine noise level at high load. With PPC, a compromise of diesel and HCCI engines can be achieved. For certain temperature and charge stratification, the ignition in PPC engines can be initiated at different time in different spatial locations of the charge, and as such a longer

* Corresponding author at: Division of Fluid Mechanics, Lund University, S 221 00 Lund, Sweden. Fax: +46 462224717.

E-mail address: Xue-Song.Bai@energy.lth.se (X.S. Bai).

http://dx.doi.org/10.1016/j.proci.2014.09.004
1540-7489/

combustion duration and hence a low noise level can be achieved while maintaining high engine efficiency [1,2].

The fuel reactivity and the split of fuel injection affect the behavior of PPC engines. Kalghatgi et al. [3] showed that PPC engines with highly reactive fuels required a large amount of exhaust gas recirculation (EGR) or low compression ratio to separate the end of the fuel injection and the start of combustion, and thus high octane number fuel was suggested. Manente et al. [4] examined the performance of a PPC engine with gasoline fuel and a rather high pressure-rise-rate with reduced engine efficiency was noticed. A way to ensure a desirable mixture for PPC is to inject the fuel at different times. Hanson et al. [5] investigated a heavy duty PPC engine with two injections of gasoline. They examined the effect of the fuel split between the first and the second injections and found that there was a tradeoff between emissions of NOx and soot, i.e., the reduction of NOx was accompanied by the increase of soot emission. In the experiments of an ethanol fueled PPC engine Manente et al. [6] reported that the optimum pilot-main fuel mass ratio was about 1. The optimal mass-ratio is however known to change when the fuel, the operating condition, or the configuration of the PPC engine are changed.

Extensive experiments have been conducted to examine the potential to run PPC engines with low emissions and high efficiency; however, detailed information about the multi-scale physical and chemical process is not available, due to the limitations in engine experiments, e.g. the lack of spatial and temporal resolutions, and frequently, the limitation to pointwise or two-dimensional data. Direct numerical simulation (DNS) aiming to provide insights into the PPC process has emerged as a viable approach, but it is rarely carried out due to the high demand on computers and computational methods. Several authors have performed DNS of HCCI combustion with certain charge stratification [7,8]. One of the main conclusions is that the charge stratification has a lower impact on the combustion process than that of the temperature stratification. In PPC engines the charge stratification is significantly larger than that in HCCI engines; due to the split of fuel injection, in particular the second injection near TDC, there are fuel-rich zones in the charge. The combustion characteristics in PPC engines are thus different from those in HCCI engines. Detailed reaction zone structures and their relation to the split of the fuel injection require further studies. In our previous 2D DNS study of syngas combustion under PPC engine conditions with two injections [9] it was found that the reaction zone structures in PPC were very complex: there were fairly different types of reaction zones in the flow field, including premixed charge ignition sites and thin flame zones. Turbulence was shown to play a more important role in PPC engines than it did in HCCI engines. Owing to this it is desirable to use three-dimensional (3D) DNS to study PPC. This has motivated the present study in which we carry out 3D DNS of PPC with a primary reference fuel – PRF70 (70% isooctane and 30% *n*-heptane on volume basis). PRF has been used in engine experiments as a gasoline surrogate. The aim is to gain deeper understanding on the PPC reaction zone structures of gasoline-like fuels with the Octane number about 70 and on the emission of pollutants such as NOx, unburned hydrocarbons and CO.

2. Governing equations and numerical methods

Turbulent reacting flows in PPC engines are governed by the Navier–Stokes equations, the continuity equation, and the transport equations for energy and species mass fractions. Since the flow velocity is relatively low, we have adopted the low Mach number assumption. The body force, the Soret/Dufour effects and the radiation heat transfer are neglected. The mixture is assumed to be a perfect gas and the mass diffusion of species is assumed to obey the Fickian law. All thermal and transport coefficients for both the individual species and the mixture-averaged form are calculated based on the Chemkin database [10]. An inhouse DNS code is used. The DNS solver is based on a symmetrical 2nd order Strang splitting scheme. The chemical reaction rate is integrated with a high accuracy stiff ordinary differential equation (ODE) solver. All spatial derivatives in the governing equations, except the convective terms in the transport equations for species and energy, are discretized using a 6th order central difference scheme; the convection terms in the species and energy equations are discretized using a 5th order WENO scheme. A detailed description of the DNS solver is given in Ref. [11]. The DNS solver has been applied to study various combustion processes [7,12].

The pressure and temperature in a realistic IC engine vary with the movement of piston. This physical compression/expansion process is modeled through source terms to the respective mass, momentum and energy equations. Assuming that the compression/expansion process is locally isentropic one can show that the source term is $S_\rho = -\gamma\rho_0(V_0/V^2)(\mathrm{dV/dt})$ for the continuity equation, where V is the volume of the engine cylinder, which is a function of the engine configuration and speed. Subscript 0 denotes a reference state, e.g. the initial field. γ is the ratio of specific heats. For the momentum equations, the source term is $S = S_\rho u_i$, where u_i is the velocity component. For the transport equations of scalar Y, the source term is $S = S_\rho Y$. It can be shown that