Fuel 221 (2018) 61–71

Contents lists available at ScienceDirect

Fuel

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

Full Length Article

Modeling study of hydrogen or syngas addition on combustion and emission characteristics of HCCI engine operating on iso-octane

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ARTICLE INFO

Keywords:
HCCI engine
Iso-octane
Hydrogen
Synthetic gas
Combustion
Emission
Numerical simulation

ABSTRACT

Numerical study of energetic and emission characteristics of HCCI engine operating on iso-octane based fuel blends comprising hydrogen or syngas as additives is conducted on the basis of 2D CFD simulation for two values of fuel-to-air equivalence ratio $\phi = 0.4$ and 0.2. The features of combustion are analyzed for the case when the maximal mass-average temperature $(T_{ev})_{max}$ during the combustion of different fuels is realized at an identical crank angle, which can be implemented at adequate intake temperature for every fuel blend. It is shown that the addition of H_2 or syngas retards the ignition and decreases the combustion duration. This effect is more pronounced for leaner mixture with $\phi = 0.2$. The admixture of H_2 to iso-octane leads to the increase of the specific indicated work both for $\phi = 0.2$ and $\phi = 0.4$. The opposite tendency is detected when syngas $H_2/CO = 2/1$ is added to iso-octane. The total emission index $EINO_x + EICO$ is determined mostly by the emission of NO_x at $\phi = 0.4$ and by the emission of CO at $\phi = 0.2$. At $\phi = 0.4$, the replacement of iso-octane by iso-octane/hydrogen (syngas) blend increases the NO_x emission index (by 86% for iso-$C_8H_{18}/H_2 = 20/80$ blend), which occurs due to the growth of maximal temperature in the cylinder. At $\phi = 0.2$, the addition of H_2 or syngas decreases the emission indices of CO, unburned hydrocarbons, and organics. The higher is the H_2 amount in the blend, the more significant is the effect. The emission indices of NO_2 and N_2O, in this case, are essentially higher than that of NO. As N_2O is a very harmful gas, its emission should be taken into consideration when evaluating the total emission of the engine at low load regimes.

1. Introduction

Nowadays, the dual fuels, consisting of traditional hydrocarbons and hydrogen, attract a special attention. Such fuels have advantageous combustion properties: the higher laminar and turbulent burning velocities, broader flammability limit range and improved flame stability, as compared with pure hydrocarbons. A lot of works are devoted to the study of the influence of H_2 addition on the combustion of gasoline, diesel or primary reference fuels (PFR) in the internal combustion (IC) engines [1–12]. It has been shown that addition of H_2 improves the performance of diesel or spark ignition IC engines: increases the burning rate, reduces the cycle-to-cycle variations, extends the lean burning limit, and raises the engine lean burning ability [2,4,5,9,10,12]. The addition of hydrogen to hydrocarbons can improve engine thermal efficiency due to essentially higher (almost in three times) energy density of hydrogen as compared with the commonly used fuels for IC engines [8,9,12]. Moreover, the emission of CO, CO_2, C_xH_y, and soot decreases during burning of hydrogen-enriched fuels due to the smaller carbon content [1,2,4–12]. The emission of NO_x depends on the engine operating regime and can be less [7,8,11,12] or higher than that with the pure hydrocarbon fuel operation [1,6,8–10]. The recent review [13] provides a detailed overview of hydrogen either as a primary fuel or as an additive for diesel engines.

Synthetic gas (or syngas) consisting mostly of H_2 and CO is also an attractive additive to hydrocarbons. The advantage of syngas upon pure hydrogen in technical applications is that syngas can be produced onboard by reforming the part of the primary fuel and there is no necessity of two tanks for different fuels. In the case of high hydrogen content, syngas possesses the higher mass heating power than hydrocarbons. The studies of the combustion of syngas/hydrocarbon blends in IC engines have been carried out in [14–18]. It has been shown experimentally [14,15] that the injection of syngas to gasoline engine at the lean and stoichiometric conditions raises the indicated thermal efficiency, shortens the combustion duration, reduces the HC and NO_x emissions, and increases CO emission. At the same time, the slight increase in NO_x emissions was indicated in [16]. The numerical studies [18] have supported this finding and have shown that the reformer gas addition can enhance the combustion efficiency and decrease CO

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https://doi.org/10.1016/j.fuel.2018.02.062
Received 18 October 2017; Received in revised form 29 December 2017; Accepted 8 February 2018

Nomenclature

E	indicated work (J)
EI	emission index (g/kgFuel)
k	turbulent kinetic energy (m^2/s^2)
m_f	mass of the fuel in the charge (kg)
P	pressure (Pa)
P_{ev}	volume-average static gas pressure (Pa)
T	gas temperature (K)
T_{ev}	mass-average static gas temperature (K)
$(T_{ev})_{\max}$	maximal mass-average temperature (K)
T_w	wall temperature (K)
V	volume
W	specific work (J/kgFuel)
β	crank angle position (degree)
ε	energy dissipation rate (m^2/s^3)
ϕ	fuel-to-air equivalence ratio
μ	molar mass (g/mole)
τ_{in}	ignition delay (s)

Subscripts

IVC	intake valve closing (β = −160° BTDC)
EVO	exhaust valve opening (β = 120° ATDC)
0	start of simulation (β = −90° BTDC)
max	maximal

emission in a natural gas/diesel engine.

The IC engines with the compression ignition of the premixed homogeneous fuel-air charge (HCCI) are considered now as the most promising ones [19–21]. The ignition of the fuel in such engines occurs in the whole working volume of the cylinder, without arising of the flame front, and is controlled mostly by chemical kinetics. Operating at fuel-lean conditions, HCCI engines emit smaller amounts of NO, CO, unburned hydrocarbons, and soot as compared with spark ignition IC engines [20]. However, the HCCI engines work stably in a rather narrow operating range. Several strategies for the control of the combustion phasing in HCCI engine, which are summarized in [22], have been suggested. One of them is the dual-fuel control strategy.

The usage of hydrogen or syngas for controlling the ignition and combustion timing in HCCI engine was studied intensively [23–30]. It has been shown that the addition of hydrogen or reformed gas (RG) (RG is a mixture of mainly H_2, CO and some diluents CO_2, H_2O, and HC that form during hydrocarbon reforming) retards combustion phasing of the fuels with low octane number (for example, *n*-heptane) and, depending on the intake temperature and fuel structure, delays or accelerates the ignition of the fuels with high octane number (for example, iso-octane). The experimental studies [27] of the combustion and emission characteristics of a diesel HCCI engine, operating on *n*-heptane and two distillates with cetane numbers of 46.6 and 36.6, have shown that the addition of hydrogen retards the combustion phasing, reduces the combustion duration, improves the combustion stability, increases the power output and fuel conversion efficiency. At the same time, the hydrogen enrichment may narrow the operational compression ratio range and increase the knocking tendency. Emission index of CO is reduced, and emission index of C_xH_y does not significantly change, although overall amount of unburned hydrocarbons decreases. Emission index of NO_x decreases or does not significantly change with hydrogen enrichment. The modeling of combustion processes in the HCCI engine carried out in [28] with the use of eight zones model captures the most experimental observations and explains them. Park et al. [31] also have concluded that the control of combustion phasing in diesel HCCI engine can be improved by using hydrogen enrichment due to the retarded combustion phasing with a higher hydrogen ratio, and the hydrocarbon and carbon monoxide emissions can be significantly reduced with a similar NO_x emissions level.

The effect of RG addition on combustion, performance and emission characteristics of the HCCI engine operating on PRF has been studied in [23–26,32,33]. Experimental studies [25,26] have shown that RG blending to *n*-heptane and iso-octane retards combustion timing for both RG compositions, and the retardation is less for RG with the low H_2 fraction (H_2/CO = 1/1) than that with the high H_2 fraction (H_2/CO = 3/1). The results of the study support the possibility of the usage of RG addition for the HCCI timing control. The numerical studies [33], carried out with the use of multi-zone model and a semi-detailed chemical kinetics mechanism, have also shown that the addition of RG retards the start of *n*-heptane combustion in HCCI engine and leads to lower in-cylinder peaks of pressure and temperature. The chemical effect of RG is more significant than its dilution and thermal effects, although the influence of RG is smaller than that of hydrogen.

The goal of the present paper is the 2D CFD numerical study of energetic and emission characteristics of HCCI engine operating on iso-C_8H_{18}/H_2(syngas) fuel blends. The analysis is performed for the case when the maximal mass-average temperature $(T_{ev})_{max}$ during the combustion of different fuels is realized at an identical crank angle, which can be implemented at adequate intake temperature of the charge for every fuel blend. In this case, the effect of additives is determined mostly by physical and chemical properties of the fuel, but not the change of operating mode. The effect of hydrogen or syngas addition is compared for a different amount of additives and two values of fuel-to-air equivalence ratio ϕ = 0.2 and 0.4. The careful analysis of observed effects is carried out.

2. Kinetic model

The auto-ignition and combustion phasing in HCCI engines is mainly driven by chemical kinetics. In order to describe with a rather high accuracy the ignition and combustion of the considered fuels in HCCI engine, the detailed reaction mechanism is required. However, the detailed mechanisms of iso-octane oxidation are rather cumbersome [34–37]. They include hundreds of species and are not applicable for two- or tree-dimensional CFD calculations. In recent years several reduced and skeletal mechanisms of iso-octane oxidation have been constructed for the usage in CFD modeling [38–43]. Machrafi et al. [38] constructed a semi-reduced (70 species, 210 reactions) and a skeletal (27 species, 29 reactions) chemical reaction mechanisms for iso-octane oxidation. The validation of these mechanisms was conducted with regard to the ignition delay for several parameters typical for HCCI conditions: inlet temperature (303–363 K), equivalence ratio (0.2–0.7) and compression ratio (10–16). Mechanism [39], including 38 species and 69 gas phase reactions, was optimized against iso-octane ignition delay under engine relevant conditions. In [40], a reduced chemical

Table 1
Parameters of the HCCI engine.

Engine speed, rpm	1200
Cylinder bore diameter, mm	102
Cylinder clearance volume, cm^3	78.48
Crank radius, mm	60
Connecting rod length, mm	192
Compression ratio	13.5
Intake valve closing (IVC), degree	−160° BTDC
Exhaust valve opening (EVO), degree	120° ATDC
Swirl ratio	0.9
Start of simulation, degree	−90° BTDC
End of simulation, degree	120° ATDC
Equivalence ratio, ϕ	0.2; 0.4
P_0, Pa	250000