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Full Length Article

Numerical analysis of the effects of reformer gas on supercharged *n*-heptane HCCI combustion

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HIGHLIGHTS

- A multi zone model is applied to investigate the effect of RG on *n*-heptane combustion.
- RG addition retards start of combustion of *n*-heptane.
- Chemical effect of RG is greater than its dilution and thermodynamic effects.
- H_2 has more chemical effects in comparison to CO.
- Dilution effect of H_2 is close to dilution effect of CO.

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ABSTRACT

Main purpose of this paper is investigating on the effect of reformer gas addition on combustion, performance and emission characteristics of a *n*-heptane fueled HCCI supercharged engine. A validated multi zone model, which is accurate for modeling of HCCI engine, is used. Heat and mass transfer between zones and convective heat transfer between in-cylinder charge and combustion chamber walls are considered in the multi zone model. A semi detailed chemical kinetics mechanism, containing 57 species and 290 reactions, is used for simulating the combustion process of *n*-heptane. Four different values of reformer gas are added to the main fuel and its effects on engine performance and chemical reactions are studied. The results show that addition of reformer gas retards the start of combustion and causes to lower in-cylinder peak pressure and temperature. Chemical, dilution and thermodynamic effects of RG are studied and the results show that the chemical effect of reformer gas is more significant than its dilution and thermal effects. Hydrogen in comparison to carbon monoxide has more chemical effects. Chemical analyses show that RG affects the chemical reactions and intermediate species concentration.

1. Introduction

Homogeneous Charge Compression Ignition (HCCI) engines are one of the new developed types of internal combustion engines. HCCI engines have two main advantages including improved fuel economy and low NOx and PM emissions [1–4]. However they have three important disadvantages; the lack of a direct way for combustion timing control, high unburned hydrocarbons (UHC) and carbon monoxides (CO) and the limited operating range [4,5].

Different strategies are developed to overcome the HCCI engines disadvantages. Using different fuels and blending of additives and the main fuel are the methods that can be used to reduce the limitations [6–8]. One of the additives, which have been used in recent years for HCCI combustion control, is hydrogen (H_2). H_2 is a clean fuel and doesn't produce carbon dioxide (CO_2) during combustion [9]. Pure H_2 is expensive and for this reason reformer gas is used as an additive in different studies [9]. Reformer gas is a mixture of light gases such as H_2 and CO and inert gases such as nitrogen (N_2) and water (H_2O) [10]. Reformer gas can be produced by reaction between hydrocarbons and steam or oxygen [11].

Shudo et al. [12,13] first examined the effect of RG addition on HCCI combustion of di methyl ether (DME). They showed that RG retards start of combustion of DME. In their next study, two types of DME reformed gases were added to DME. One type of reformer gas was produced by partial oxidation and the other one was produced by steam reforming. Both reformed gases contained H_2 and CO but their concentrations were different. The results showed that RG composition has the same effect on combustion timing of DME [14]. Eng et al. [15] blended H_2 to *n*-Heptane and iso-

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Nomenclature

A_R	effective flow area (m^2)
Cr	connecting rod length (m)
c_v	specific heat constant at constant volume (J/kg K)
C_D	discharge coefficient
D	cylinder diameter (m)
k	thermal conductivity (Jm/s K)
m	mass (kg)
Mw	molecular weight
n_s	number of species
P	pressure (Pa)
Q	heat (J)
Rc	compression ratio
rpm	engine speed (revolution per minutes)
R_u	universal ideal gas constant (J/mol K)
T	temperature (K)
t	time (s)
U	internal energy (J)
u	specific internal energy (J/kg)
V	volume (m^3)
W	work (J)
Y	mass fraction

Greek symbols

θ	crank angle position (Degree)
ρ	density (kg/m^3)
$\dot{\omega}$	molar rate of production ($mole/m^3$ s)

Subscripts

Conv	convection
Cond	conduction
d	downstream
i	ith zone
in	inlet
j	jth species
out	outlet
u	upstream

octane and they showed that H_2 affects *n*-heptane HCCI combustion when external EGR is used.

Hosseini et al. [16] showed that RG addition expands the operating range of lean mixtures of compressed natural gas (CNG) and air. Other studies were done by Hosseini et al. to investigate the effects of RG addition on the HCCI combustion of primary reference fuels (PRFs). They found that RG addition allows a wider operating range of HCCI engines and it retards the start of combustion using the low octane PRFs [17,18].

Guo and Neil [9] used a multi zone for HCCI combustion model and showed that H_2 addition retards the combustion timing of *n*-heptane. They divided RG effects into two groups including chemical and dilution effects. They showed that the dilution effects of RG are more significant than its chemical effects. The effects of RG addition on a natural gas fueled HCCI combustion was studied by Voshtani et al. [19]. In this study, the RG effects were categorized into three types; chemical, dilution and thermodynamics. They found the chemical effects of RG are greater than its dilution and thermodynamic effects. Kozlov et al. [20] investigated the effect of H_2 addition on HCCI combustion of methane by using a CFD model. The results showed that H_2 causes NOx and CO to be lowered at engine exhaust.

Notwithstanding the numerous amount of researches focused on the effects of RG addition on HCCI combustion of different hydrocarbons, little is known on the different effects of RG on HCCI combustion. Meanwhile, the chemical effects of RG on different reactions and species of a reaction mechanism are not focused yet. Therefore, the main contribution of present study is to investigate the different effects of reformer gas addition on *n*-heptane HCCI combustion. In addition, more attention is paid to the chemical effects of RG on chemical reactions and species.

2. Methodology

2.1. Model configuration

A multi zone model is used for the HCCI engine closed loop simulation. The gas exchange process is simulated by a single zone model, which is coupled to the multi zone model. Pressure is assumed to be uniform throughout the cylinder at each time step. Temperature and composition are assumed to be uniform in each zone at each time step, too. There are four types of zones containing the crevice zone, boundary layer zone, outer zones and core zone. The volume of crevice zone is constant and equal to 3 percent of clearance volume. The boundary layer zone is the nearest zone to the wall. Heat and mass transfer are considered between the zones and there are heat transfer between in-cylinder charges and combustion chamber walls. For each zone, the first law of thermodynamics equation and the chemical kinetics equations are solved, simultaneously. Eqs. (1)–(8) are the governed equations. The model is explained in detail in the published papers in the literature [21,22].

$$\frac{dU_i}{dt} = -\frac{dW_i}{dt} + \frac{dQ_i}{dt} \tag{1}$$

$$\frac{dU_i}{dt} = c_v^i m_i \frac{dT_i}{dt} + m_i \sum_{j=1}^{n_s} u_j \frac{dY_j}{dt} + \sum_{j=1}^{n_s} u_j Y_j \frac{dm_i}{dt} \tag{2}$$

$$\frac{dW_i}{dt} = P\frac{dV_i}{dt} \tag{3}$$

$$\frac{dQ_i}{dt} = \frac{dQ_{i,cond}}{dt} + \frac{dQ_{i,conv}}{dt} + \frac{dQ_{i,mtran}}{dt} \tag{4}$$

$$\frac{dQ_{i,cond}}{dt} = -kA_i\frac{\partial T}{\partial z} \tag{5}$$

$$\frac{dQ_{BL,conv}}{dt} = h(T_{wall} - T_{BL})A_{wall} \tag{6}$$

$$\frac{dQ_{i,mtran}}{dt} = \frac{dm_{in,i}}{dt}H_{in} - \frac{dm_{out,i}}{dt}H_{out} \tag{7}$$

$$\frac{dY_{k,i}}{dt} = \frac{\dot{\omega}_{k,i}Mw_k}{\rho_i} \tag{8}$$

The in-cylinder pressure is calculated using Eq. (9) at each time step.

$$P = \frac{R_u \sum_{i=1}^{n_z} \frac{m_i}{Mw_i}}{\sum_{i=1}^{n_z} \frac{V_i}{T_i}} \tag{9}$$