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Developing of a 1-D combustion model using laminar burning velocity correlations for gasohol and natural gas spark-ignition engines

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Abstract

This study is aimed to develop the 1-D combustion model of Spark-Ignition (SI) engines for predicting the effect of various fuel types and compositions on engine performances and fuel consumption on various engine operating conditions without engine modifications. Laminar burning velocity correlations of each alternative fuel: gasohol and natural gas (CH_4 + H_2 + CO_2 + O_2), were used to calculate the combustion duration in Wiebe function. The model was implemented into the well-calibrated 4-cylinder gasoline engine model. Results showed that for gasohol, when increasing ethanol blends, combustion duration was decreased with higher fuel consumption. At lean mixture condition, adding more ethanol blends made torque lower and the maximum torque was shifted to higher equivalent ratio at rich mixture condition. For natural gas, when increasing H_2 or decreasing CO_2 amounts in fuel composition, combustion duration and fuel consumption were decreased with higher torque. In addition, when increasing O_2 amounts, combustion duration was also decreased with higher fuel consumption and torque was increased especially at rich mixture condition.

***Keywords**:* Laminar burning velocity, Gasohol, Natural gas, Spark-Ignition engine

1. Introduction

Alternative fuels are widely used nowadays since they are derived from resources other than petroleum. The benefit of these fuels is because they produces less air pollutants compared to gasoline and most of them are more economical and renewable. The most common alternative fuels are natural gas, propane, ethanol, methanol and hydrogen. A lot of works have been done on engine operating with these fuels individually but few publications have compared some of these fuels together in the same engine [1–4]. Methane, the main content of natural gas, is the most common alternative fuel and is one of the cleanest burning fuels. It can be used in the form of compressed natural gas (CNG) or liquefied natural gas (LNG) for vehicles [4,5]. In Thailand, it is quite problem because CNG contains diluents such as carbon dioxide (CO_2). Ethanol is alcohol-based fuels made by fermenting and distilling starch crops. Its energy density is roughly two-thirds compared to gasoline but it has higher octane number that can improve knock tolerance and has less emission than gasoline [2,6,7]. Hydrogen (H_2) is also an attractive fuel that is being widely used in fuel cells to power electric motors or burn in internal combustion engines (ICEs) with no air pollutants and good control of emission of NO_x and unburned HC [4,8].

Engine simulation is becoming an increasingly important engineering tool for time and cost efficiency in the development of ICEs. Many phenomena in engines are 3-D but it requires high levels of knowledge and large computation time. Thus simplified 1-D simulation is often used. In 1-D simulation, equations for conservation of mass, momentum, and energy are solved in time and in one dimension along the main flow direction in the engine pipes. Additional models, correlations, or measurements are needed in 1-D for capture 3-D phenomena such as flow over valves and combustion [9,10].

Thus the present paper is aiming to develop the 1-D combustion model of Spark-Ignition (SI) engines for predicting the effect of various fuel types and compositions on engine performances on various engine operating conditions without engine modifications. For this purpose, simulation of calibrated gasoline engine model was used as base operating condition and the laminar burning velocity correlations of each alternative fuels were implemented for calculating the changed combustion duration. The engine performances: torque and specific fuel consumption were compared and discussed.

2. Simulation Setup

The 1-D engine simulation program, AVL BOOST, has been employed to study the influences of various fuels by adding the correlation in the FORTRAN user-defined module.

The engine model used in this simulation was performed on a four-stroke, four-cylinder spark-ignition engine. This gasoline model was calibrated by AVL and its layout is shown in Fig. 1 with engine specifications shown in Table. 1.

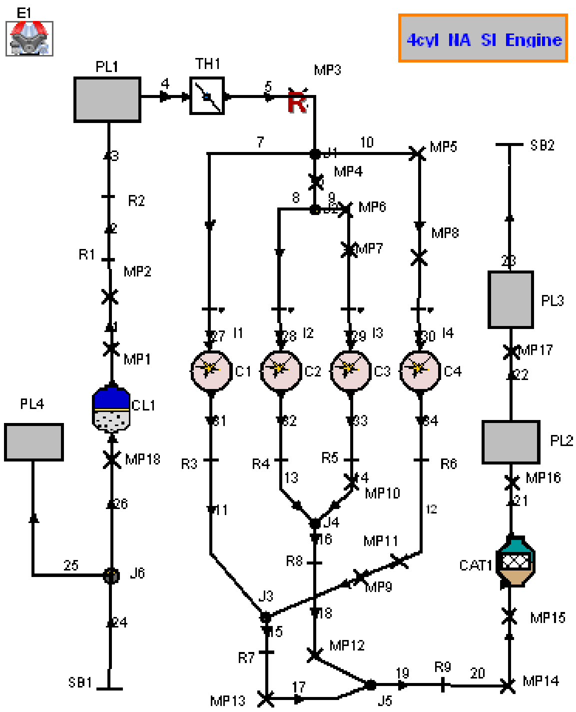

Fig. 1 Layout of gasoline engine model

Table. 1 Engine specifications

Bore [mm]	86
Stroke [mm]	86
Compression ratio	10.5
Con-rod length [mm]	143.6
Engine displacement [cc]	2000
IVO [deg]	20 bTDC
IVC [deg]	70 aBDC
EVO [deg]	50 bBDC
EVC [deg]	30 aTDC

For simulating the combustion process, a single-zone model that is a thermodynamic model assumed that the properties of substance in combustion chamber are averaged was used [11,12].Heat transfer model was employed according to Woschini's equation (1978) [13].

2.1 Wiebe Function

For specifying the combustion rate in the single-zone combustion model, the Wiebe function was used and its functional form:

$$x_b = 1 - exp\left[-b\left(\frac{\theta-\theta_0}{\Delta\theta}\right)^{m+1}\right] \quad \text{Eq. (1)}$$

x_b is used to describe the fraction of fuel burnt. θ is the crank angle, θ_0 is the start of combustion, $\Delta\theta$ is the total combustion duration and m and b are called the Wiebe parameters. At first step, m and b were chosen as 2 and 5 along to the values for gasoline [11].

For total combustion duration, Lindström et al. [9] gave the linear correlation of burn durations that was influent of operating conditions as shown in Eq. (2) – (3). The spark timing and engine speed were adjusted same as the base operating condition in this paper.

$$\Delta\theta = \Delta\theta_0 \cdot \frac{G_{S_l}}{G_{S_{l0}}} \cdot \frac{G_{spk}}{G_{spk_0}} \cdot \frac{G_N}{G_{N_0}} \quad \text{Eq. (2)}$$

$$G_{S_l} = \frac{1}{S_l} \quad \text{Eq. (3)}$$

2.2 Laminar Burning Velocity

Laminar burning velocity is an important intrinsic property defined as velocity relative to and normal to flame front that depends strongly on fuel types and compositions. Laminar flame speed is quite necessary because it is used to calculate turbulent flame speed but Lindström et al. shown that effects of turbulence could be distributed to engine speed and spark timing in correlation of combustion duration.

From previous literatures, various methods for measuring and fitting laminar burning velocity have been presented up to now for different fuels and compositions [7,14-16]. The correlations of laminar burning velocity used in this work were as follows:

2.2.1 Gasoline and gasoline–ethanol blends.

Flame speed of gasoline–ethanol/air mixture was calculated according to Bayraktar's research [7]. The empirical correlation of burning velocities was used in Eq. (4):

$$S_l(\emptyset, T, P) = S_{l0}(\emptyset)\left[\frac{T_u}{T_0}\right]^{\alpha}\left[\frac{P}{P_0}\right]^{\beta}(1-2.5\psi) \quad \text{Eq. (4)}$$

where P is the pressure, T_u is the unburned temperature, $\emptyset$ is the equivalence ratio and ψ is the residual gas content. α and β are pressure and temperature exponents and other coefficients are shown in Table. 2.

The laminar flame speed at the reference conditions (T_0 = 300 K and P_0 = 1 atm) was determined as:

$$S_{l0}(\emptyset) = ZW\phi^{\eta}\exp[-\xi(\phi-1.075)^2] \quad \text{Eq. (5)}$$

2.2.2 Natural Gas

Laminar burning velocity of natural gas depended on its composition. For CH_4 + H_2 + O_2 + N_2, works of Hermanns et al. [14] and Liao [15]

Table. 2 Coefficients and exponents for the laminar burning velocity equations

	Gasoline	Gasohol	CH_4 + H_2 + O_2	CH_4 + CO_2
Z	1	$1+\gamma X_e^{\tau}$	$1+\gamma R_{H2}^{\tau}$	–
γ	–	0.007	0.0034	–
τ	–	0.35	1.3580	–
W	0.4658	0.4658	0.4881	–
η	-0.326	-0.326	-2.1870	–
ξ	4.48	4.48	6.7619	–
α	1.56	$1.56+0.23X_e^{0.46}$	$9.1105-14.8013\emptyset+7.2796\emptyset^2-0.0028R_{H2}$	$1.42-1.98(\emptyset-1)$
β	-0.22	$\phi\le 1:\ \beta_g X_g-\frac{0.17}{\sqrt{\phi}}X_e$ $\phi>1:\ \beta_g X_g-0.17\sqrt{\phi}X_e$	$-0.925\emptyset^2+2\emptyset-1.473$	$-0.314+0.608(\emptyset-1)$
σ	–	–	1.2103	–
ω	–	–	0.0002	–

were used. Laminar burning velocity is calculated by the following formula:

$$S_l(\emptyset,R_{H2},R_{O2},T_u,P)=S_{l0}(\emptyset,R_{H2})(1-\mathcal{A}\mathcal{D})\left[\frac{T_u}{T_0}\right]^{\alpha}\left[\frac{P}{P_0}\right]^{\beta} \qquad \text{Eq. (6)}$$

$$\mathcal{A}=10.7787-15.2661\emptyset+6.9656\emptyset^2 \qquad \text{Eq. (7)}$$

where T_0 = 298 K, P_0 = 1 atm and $\mathcal{D}$ is the diluent fraction and defined as:

$$\mathcal{D}=1-\frac{R_{O_2}}{20.95} \qquad \text{Eq. (8)}$$

and R_{H_2} is the hydrogen content and defined as:

$$R_{H_2}=\frac{x_{H_2}}{x_{H_2}+x_{CH_4}}\cdot 100\% \qquad \text{Eq. (9)}$$

whereas the oxygen content is defined as:

$$R_{O_2}=\frac{x_{O_2}}{x_{O_2}+x_{N_2}}\cdot 100\% \qquad \text{Eq. (10)}$$

The laminar burning velocity of methane–air mixtures and constants are shown as:

$$S_l(\emptyset,R_{H2})=ZW\phi^{\eta}e^{-\xi(\phi-\sigma-\omega R_{H2})^2} \qquad \text{Eq. (11)}$$

Table. 3 Fuel properties

Fuel type	LHV [kJ/kg]	Stoichiometric air/fuel ratio
Gasoline	43500	14.5
Ethanol	26800	9
Pure Methane	50000	17.2

Moreover, laminar burning velocity of CH_4 + CO_2 + air is used from Stone et al.'s paper [16]. Their correlation is defined as followings with T_0 = 298 K, P_0 = 1 atm.

$$S_l(\emptyset,T_u,P)=S_{l0}\left[\frac{T_u}{T_0}\right]^{\alpha}\left[\frac{P}{P_0}\right]^{\beta}\left[1-1.242\psi^{(1.23-0.487(\emptyset-1))}\right] \qquad \text{Eq. (12)}$$

$$S_{l0}=0.376+0.151(\emptyset-1)-2.21(\emptyset-1)^2-0.458(\emptyset-1)^3+3.58(\emptyset-1)^4 \qquad \text{Eq. (13)}$$

Although the combustion model in this work was the single-zone model that had no unburned zone which was a mainly important for calculation of NO_x formation but unburned temperature and unburned pressure could be assumed to be constant (450 K and 5 atm) because of quite small difference between single-zone and two-zone combustion models on engine performance [13,14]. Fuel properties employed in the current study are shown in Table. 3. All values are default values in AVL-BOOST and the other engine parameters are shown in Table. 4.

Table. 4 Tested Engine Operating Conditions

Engine parameter	
∅	0.8-1.2
EGR [%]	0
Engine speed [rpm]	2500
θ_0 [deg]	-10 bTDC
$\Delta\theta_0$ [deg]	45
Fuel Composition	
Ethanol blends [%]	0, 20, 50, 85
H_2 in CH_4 [%]	0-20
CO_2 in CH_4 [%]	0-30
O_2 in CH_4 [%]	0-20

All above correlation equations were added into the user-defined module and then they were compiled and built to be executable file by FORTRAN compiler. Finally this file was implemented into the computing program for calculating the results.

3. Simulation results

3.1 Combustion duration

The total combustion duration is based on the laminar burning velocity. For gasoline (E00), the combustion duration was shortest at the stoichiometric mixture condition and it was longer at more and less equivalence ratios as shown in Fig. 2a. When increasing ethanol blends by volume to be 20% (E20), E50 and E85, combustion duration would be average decreased by 9.3%, 14.2% and 18.6% comparing to E00, respectively.

For natural gas, the results are shown in Fig.2b (lower). When increasing H_2 amounts for 10% and 20% in fuel composition, combustion durations compared to pure methane would be decreased by 5.6% and 13.7% and they would be reduced by 10.5% and 22% when O_2 were 10% and 20%. But they would be higher by 7.9% and 21% when CO_2 of fuel composition were 10% and 20% with lowest combustion duration at the equivalence ratio about 1.0 – 1.5.

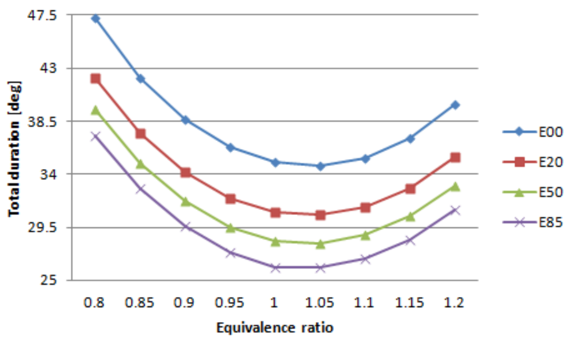

Fig. 2a Total durations of gasohol

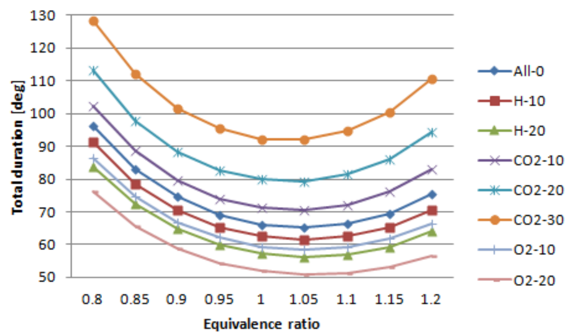

Fig. 2b Total durations of natural gas

3.2 Engine performance

The engine performance characteristics are directly affected by the type and composition of fuel. These characteristics studied in this work include: torque and indicated specific fuel consumption (ISFC).

Fig.3 presents a comparison of torques from different fuels. For gasoline (Fig.3a), the torque would be highest at equivalence ratio ≈ 1. When increasing ethanol, the maximum torque would shift to equivalence ratio ≈ 1.2 (rich mixture condition). Its reason was the added ethanol that had Oxygen atoms would produce the leaning effect and made the burning closer to be stoichiometric [17,18]. For natural gas, when increasing H_2 amounts for 10% and 20%, torque would be average increased by 2.5% and 6%. When increasing O_2 in fuel compositions, torque would be higher with maximum torque shifting to higher equivalence ratio. This was because increasing O_2 could make combustion completely. For increasing amounts of CO_2, torque would be changed very little with small CO_2 (less than 10%) and it would be decreased by 2% and 6.5% averagely when CO_2 were 20% and 30%.

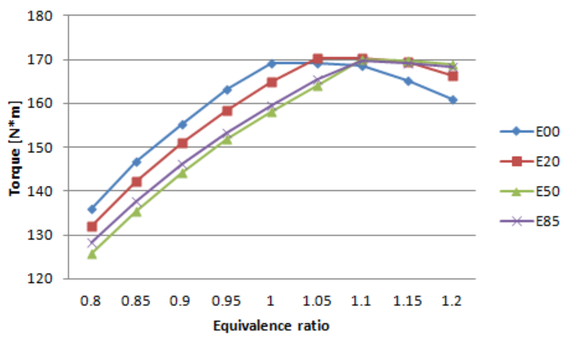

Fig. 3a Torque of gasohol

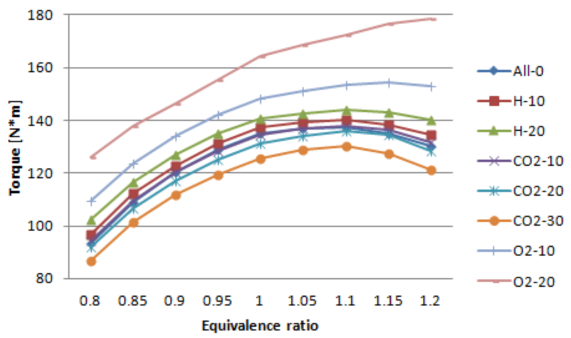

Fig. 3b Torque of natural gas

ISFC for different fuels are compared in Fig. 4. The results showed that when ethanol was increased in small amounts (20%), there were little differences especially at equivalence ratio about 1.15-1.2. When adding more ethanol blends, ISFC would be higher by 15% and 35% for E50 and E85. Then increasing H_2 for natural gas, ISFC were deceased as shown in Fig. 4b. They were about 4% and 9% for H_2 of 10% and 20%. When increasing CO_2 amounts to 10% and 20%, ISFC would be increased quite a lot: 28.6% and 66.9%, respectively. For increasing O_2, ISFC were same trends as CO_2 but they were smaller (14.1% and 32.9%), for 10% and 20% of O_2 amounts.

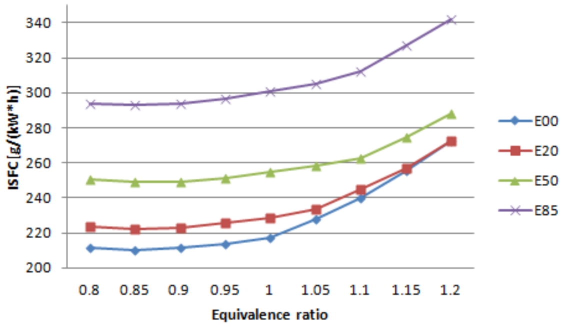

Fig. 4a ISFC of gasohol

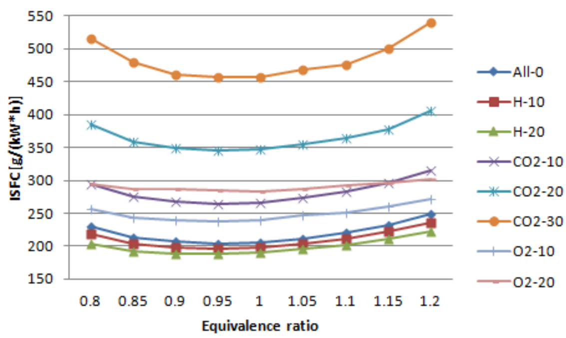

Fig. 4b ISFC of natural gas

4. Conclusions

A computer code was developed in the user-defined module of AVL BOOST, a 1-D engine simulation program, to simulate a calibrated gasoline four-stroke, four-cylinder, spark-ignition engine model fueled by gasoline, gasohol and natural gas (CH_4 + H_2 + CO_2 + O_2) without engine modifications.

The correlations of laminar burning velocity and combustion duration from previous literatures were implemented into the software package via a user defined function. Finally combustion durations of various fuels and compositions were predicted and engine performance characteristics were calculated.

For gasohol, when increasing ethanol blends, combustion duration was decreased with higher fuel consumption. At lean mixture condition, torque was lower when adding more ethanol blends and the maximum torque was shifted to higher equivalent ratio when combusted in rich mixture condition because Oxygen atoms in ethanol made the burning closer to the be stoichiometric condition.

For natural gas, when increasing H_2 or decreasing CO_2 amounts in fuel composition, combustion duration and fuel consumption were decreased with higher torque. In addition, when increasing O_2 amounts, combustion duration was also decreased with higher fuel consumption and torque was increased especially at rich mixture condition because O_2 made combustion perfectly.

For the future work, the developed model will be implemented into a Gas Engine model and calibrated with experimental results with various spark timings and engine speeds. Tunings of Wiebe parameters are required and effects of gas compositions on engine performance and fuel consumption will be further analyzed.

5. Acknowledgement

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6. References

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