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Relationship between the variations of hydrogen in HCNG fuel and the oxygen in exhausted gas

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Abstract

The variation of the mixing ratio between hydrogen and compressed natural gas (CNG) in hydrogen enriched compressed natural gas fuel (HCNG) gives different results in terms of engine performances, fuel consumption, and emission characteristics. Therefore, the engine performance using HCNG as fuel can be optimized if the mixing ratio between the two fuels in HCNG can be adjusted in real time while the engine is being operated. In this research, the relationship between the amount of oxygen in the exhausted gas and the mixing composition between the hydrogen and CNG in HCNG is investigated based on the equilibrium equation of combustion. It is found that the main factors affecting the amount of oxygen in exhausted gas when using HCNG as fuel include the error from the air-fuel-ratio (AFR) control, the error from the HCNG composition control, and the intended change of the HCNG composition. Theoretically, the amount of the oxygen in the exhaust should increase by 0.78% for every 5% addition of H_2 at stoichiometric condition. This value can be higher or lower for lean and rich engine operation, respectively. The experimental results found that at the equivalent ratio around 0.8 the amount of O_2 in the exhaust gas increases about 1.23% for every 5% H_2 addition, which inclines with the proposed calculations.

Keywords : Hydrogen, Compressed natural gas, Oxygen sensor, Fuel mixing ratio**,** HCNG

1. Introduction

The use of hydrogen (H_2) mixed with compressed nature gas (CNG) as an alternative fuel, so called HCNG, is currently being implemented in many countries [1-2]. The majority of the earlier studies focused on the pollution reduction related to the mixing ratio of HCNG. There are also studies those not only discuss the emission, but also explore the performance of the engine using HCNG [3-8]. It is commonly found that different mixing ratio, which is dictated by the variation of the volume of H_2 in the total volume of fuel, i.e. 20% HCNG contains 20% H_2 by volume and 80% CNG by volume, affects the performance of the engine. For optimum engine performance, the required mixing ratio can be different depending on the operating condition of interest. The required mixing ratio can also be different from engine to engine. Therefore, it is believed that if the mixing ratio of the HCNG can be adjusted on-demand while the engine is being operated, the benefits of HCNG fuel can be maximized [9-10].

To be able to adjust the HCNG mixing ratio, a mean to monitor the mixing ratio must be developed. An oxygen sensor or a lambda sensor is normally used to monitor amount of oxygen left over from combustion, which is directly related to the Air-Fuel Ratio (AFR) of the air-fuel mixture entering the engine's combustion chamber. The data from the oxygen sensor is used to monitor AFR such that AFR can be controlled at the desired values throughout the operation of the engine. Since addition of the hydrogen to the combustion of any commercial fuel affects the actual AFR [1, 4, 6], the oxygen sensor should then be used to detect this additional amount of H_2, hence the HCNG mixing ratio. Therefore, the main objective of this research is to investigate the potential of using the oxygen sensor to monitor the HCNG mixing ratio by studying the relationship between the amount of oxygen in exhaust gas and the variation of H_2 in HCNG.

The contents of this paper are arranged as the following. Section 2 presents the derivation of the theoretical relationship between the amount of oxygen in exhaust gas and the variation of H_2 in HCNG. Section 3 describes the experimentation setup which includes the test vehicle, method of controlling H_2 in HCNG, and the mean to measure the exhausted oxygen. Section 4 presents the calculations and experimentation results. Section 5 and 6 give some discussion and conclusion respectively.

2. Prediction of O_2 using equilibrium equation

Premakumara et al., 2012 [11] developed a combustion model for SI engine to simulate the use of HCNG fuel. Based on their model, for the combustion of a fuel having the chemical formula represents by $C_pH_qO_rN_s$ mixed with hydrogen in the form of H_2, the equilibrium equation for the combustion can be described by equation (1).

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$$\begin{aligned}&\phi\times \text{Sto}\times\{(1\text{-x})\text{C}_{\text{p}}H_qO_rN_s+xH_2\}+0.210O_2\\&+0.79N_2 \quad\rightarrow\quad n_1CO_2+n_2H_2O+n_3N_2+\\&n_4O_2+n_5CO+n_6H_2+n_7O+n_8H+n_9OH\\&+n_{10}NO\end{aligned} \tag{1}$$

$$\phi=\frac{Act}{Sto} \tag{2}$$

where,
ϕ = Equivalent Ratio
x = Percentage of H_2 (by volume)
$n_{i,i=1-10}$ = Mole Fraction of Exhaust Components
Sto = Stoichiometry Fuel-Air Ratio
Act = Actual Fuel-Air Ratio

It is noting that equation (1) can be used only when the equivalent ratio does not exceed 3. Moreover, the Stoichiometry Fuel-Air Ratio (Sto), for the case of completed combustion can be described by equation (3) [1].

$$Sto=\frac{0.21}{((1\text{-x})(\text{p}+0.25\text{q}-0.5\text{r})+0.5\text{x})} \tag{3}$$

Solving equation (1) to find n_i relies on balancing the mole fraction of each element between the left and the right sides of equation (1). To support this balancing step, other information must also be used to help identify many multiply factors. These include the dissociation of substances under combustion which can be assumed from JANAF experimentation results, along with equation solving algorithm such as Newton Ralphson Method or the algorithm developed by Olikara and Borman, 1975 [12].

In case of this study, the results from equation solving reported by Premakumara et al., 2012 [11] is used directly. Though, our main focus is the amount of exhausted oxygen as indicated by the factor n_4 in equation (1). It is found that when ϕ > 1 or rich mixture, n_4 = 0 or O_2 is all used up in the combustion. On the other hands, when ϕ < 1 or lean mixture, the amount of the oxygen in the exhaust gas can be estimated by equation (4).

$$\text{n}_4=0.21\times(1-\phi) \tag{4}$$

Equation (4) states that the amount of oxygen left in exhaust gas is proportional to the lean percentage as compared to the stoichiometric value (the term $(1-\phi)\times 100$ tells the lean percentage). Since the value of n_4 is the mole fraction of O_2, n_4 must be multiplied by the mole number of the actual air, and the molecular weight of O_2, in order to find the amount of oxygen. For the case of this study, the main fuel is CNG which is assumed to be Methane (CH_4). Therefore, equation (1) and (2) can be written as,

$$\begin{aligned}&\phi\times \text{Sto}\times\{(1\text{-x})\text{C}H_4+xH_2\}+0.210O_2\\&+0.79N_2 \quad\rightarrow\quad n_1CO_2+n_2H_2O+n_3N_2+\\&n_4O_2+n_5CO+n_6H_2+n_7O+n_8H+n_9OH\\&+n_{10}NO\end{aligned} \tag{5}$$

The Stoichiometry Fuel-Air Ratio for this case can be derived from equation (3) as,

$$Sto=\frac{0.105}{1-0.75x} \tag{6}$$

The relationship in equation (6) shows the change of the stoichiometric value as the H_2 or the mixing ratio of HCNG changes. It is noted that when equation (1) is set to represent the combustion of HCNG and the results is shown in equation (5), the value of O_2 from the combustion shown by equation (4) is not changed. This dues to the fact that changing of r and s (the composition of oxygen and nitrogen) do not affect the amount of oxygen from combustion described by equation (4). However, the amount of oxygen in exhaust gas can be changed if the ϕ is changed. Though, considering equation (2) and (6), it is also found that ϕ can be changed by altering the amount of the H_2 in the mixed fuel. Therefore, we investigate the variation of the oxygen from the following 3 cases.

2.1 Relationship between O_2 and ϕ

The change of O_2 when ϕ changes can be considered from equation (4). Applying the Taylor's Series expansion and ignoring the higher order terms, we have,

$$\Delta\text{n}_4=-0.21\Delta\phi \tag{7}$$

Equation (7) states that the amount of oxygen in exhaust gas varies 0.21 times inversely proportional to the change of ϕ, e.g. for every 0.1 reduction ϕ (10% leaner than the stoichiometric, $\Delta\phi=-0.1$), $\Delta n_4=0.021$ or the amount of oxygen increases by 2.1%. Based on this investigation, if the amount of fuel and the mixing ratio of the HCNG can be precisely controlled, the relationship shown by equation (7) can be used, which the amount of oxygen tells the equivalent ratio of the burned fuel.

2.2 Relationship between O_2 and H_2 in HCNG

If the stoichiometric fuel-air ratio is represented by equation (6), the actual fuel-air ratio can then be written as,

$$Act=k\,\frac{0.105}{1-0.75x'} \tag{8}$$

where,
k = the changing value of AFR from Stoi
x' = actual ratio of H_2

Assuming that the engine is running by 100% CNG and is able to operate precisely at stoichiometric, we now are trying to investigate the variation of the amount of oxygen in the exhaust gas if the fuel is changed from 100% CNG to HCNG at any level of H_2 fraction. To see this, substitute equations (2) and (8) into equation (4), we have the equation (9) below.

$$n_4=0.21\times\left(1-k\,\frac{1-0.75x}{1-0.75x'}\right) \tag{9}$$

The variation of the amount of oxygen as k, x, x' are varied (around $k = 1, x = x' = 0$) can be written as the following.

$$\Delta n_4 = -0.21\Delta k + 0.1575\Delta x - 0.1575\Delta x' \quad (10)$$

The first term on the right hand side shows similar results to the case in section 2.1. The second term shows the change of the amount of oxygen if the assumed fuel (the based fuel) is having different H_2 composition than 0%. This affects the assumed stoichiometric value (as described by equation (6)). And if this is the case, there would be some amount of oxygen appears in the exhaust gas, e.g., based on equation (10), for every 5% addition of H_2 (x = 0.05), the amount of the oxygen in the exhaust is increased by 0.1575 × 0.05 = 0.0078 or 0.78%.

The third term on the right hand side gives similar results as the second term. Though, the different between the second and the third terms is that the former represents the error from the assumed fuel composition, and the latter represents the effect of the intended variations of the HCNG mixing composition.

Figure 1 shows the calculation results based on equation (10) assuming that the engine is operated at stoichiometric (ϕ = 1). The x-axis represents the %HCNG at stoichiometric. The y-axis represents the mole fraction of the oxygen in exhaust gas. It can be seen that if stoichiometric is known the amount of the oxygen shown in the exhaust gas can be used to identify the fraction of H_2 in the fuel. The known stoichiometric means that the reference fuel and its composition must be known, hence the stoichiometric can then be calculated, and the reference point on the x-axis is then fixed. From the reference point on the x-axis, the found amount of oxygen in the exhaust gas gives the reference point on y-axis, therefore the amount of H_2 in the fuel can be found. Again, regardless of the stoichiometric setting, for every 5% addition of H_2 the amount of the oxygen in the exhaust is increased by 0.1575 × 0.05 = 0.0078 or 0.78%.

Figure 2 shows again the calculation results plots based-on equation (10), here ϕ = 0.8 in this case. This represents the case when attempting to operate the engine under lean combustion, which is one of the main benefits from using HCNG as fuel. Figure 2 shows similar tendency for the variation of H_2 versus the amount of oxygen in the exhaust as compared to Figure 1. Though, noticing that the value of the oxygen shown on the y-axis for each case are higher than what shown in Figure 1. This suggested that if the initial fuel composition is known (x-axis can be marked), and if the controlled fuel-air ratio is known (ϕ is fixed), the amount of oxygen shows obviously the amount of hydrogen composition in the burned fuel.

2.3 The amount of O_2 when H_2 and CNG are not at their predefined ratio

Considering now the case when the mixing composition between H_2 and CNG is not at the predefined mixing ratio, in this case, the summation of the fraction of each gas by volume can be higher or lower than 100% as compared to the predefined or desired composition. This case can be expected or should be aware, especially for the control of a practical HCNG fueling system. The amount of the injected fuel can be inaccurate especially for the hydrogen injection part which normally requires very short injection timing [2].

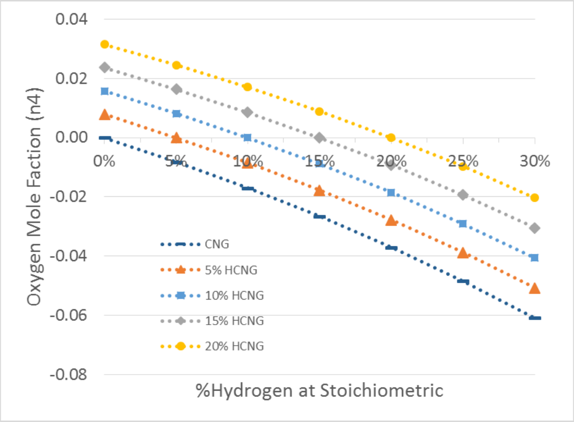

Figure 1 Effect of changing of H_2 to the exhausted O_2 (ϕ = 1)

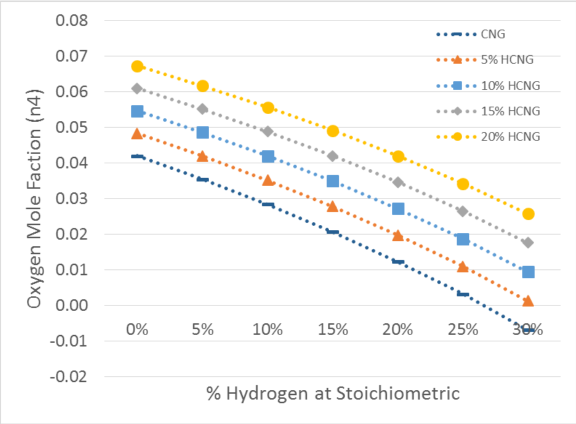

Figure 2 Effect of changing of H_2 to the exhausted O_2 (ϕ = 0.8)

In this case, for any error in the composition of HCNG as compared to the desired value, the new HCNG composition is formed. Therefore, the results presented in section 2.2 can be adopted directly. To be specific, the desired value of the HCNG fuel composition marks the reference point on the x-axis in the Figure 1 and 2 depending on the equivalent ratio. The detected amount of oxygen is then marks the reference point on the y-axis. Therefore, the true composition of the burnt fuel can then be found. Noting that, in this case, the cause of the error cannot be told, i.e. the gas which is injected inaccurately and causes the composition of the HCNG to be different than desired. Adjusting the injection timing of each gas should change the indicated fuel composition. This can be done by trial and error. Though, the following can be used as a guideline to adjust the fuel.

Consider equation (3), assuming that the fraction (% by volume) of CNG and H_2 in HCNG represented by a and b, respectively, equation (3) becomes,

$$Sto = \frac{0.105}{a + 0.25b} \quad (11)$$

Therefore, the actual fuel-air ratio can be written as,

$$Act = k\frac{0.105}{a' + 0.25b'} \quad (12)$$

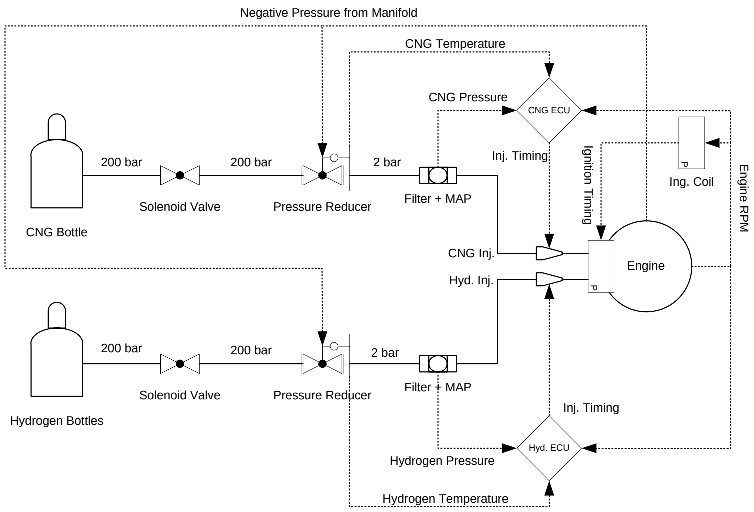

Figure 3 Schematic diagram of the HCNG Fueling System

where,

k = the changing value of AFR from Sto

a' = actual ratio of CNG

b' = actual ratio of H_2

Assuming also that the engine is operate at Sto, which implies that the initial HCNG composition is known, the amount of the oxygen in the exhaust gas can then be described by,

$$n_4 = 0.21 \times \left(1 - k\,\frac{a + 0.25b}{a' + 0.25b'}\right) \quad (13)$$

The variation of the amount of oxygen as k, a, a', b, b' are varied (around $k = 1, a = a' = 1, b = b' = 0$) can be written as the following.

$$\Delta n_4 = -0.21\Delta k + 0.21\Delta a' + 0.0525\Delta b' \quad (14)$$

The second term on right hand side shows the effect of oxygen variation from the change of CNG fraction in HCNG. Here, every 5% by volume increase of CNG, or $\Delta a' = 0.05$ the value of O_2 in the exhaust gas increases approximately 1.05%. The third term on right hand side shows that for every 5% increase of hydrogen by volume, or $\Delta b' = 0.05$ the amount of O_2 in the exhaust gas increases approximate 0.26%. Therefore, adjusting the amount of CNG has greater effect in terms of changing the mixing composition of HCNG and the amount of oxygen shown in the exhaust gas.

3. Fueling system design and installation

The type of fueling system to supply the HCNG in this study is an on-boarded separately stored and controlled HCNG fuelling system. To be specific, each individual gas is separately stored in each individual tank, while the amount of gas being fed to the engine is separately controlled. The main reason of choosing this system configuration is that it offers flexibility to control the mixing ratio between H_2 and CNG [10]. Watechagit et al., 2014 proposed that the commercially available CNG fueling system could be adopted for H_2 fueling system. According to their design, the only modification is the fitting required to attach the H_2 tank to the system. Once installed, the engine would look like having two regular CNG fueling systems on board, except that one of them is attached to the H_2 storage tank. Each engine's cylinder then accepts fuel from 2 injectors. There are also 2 injection control units, one is for CNG and the other is for H_2. Figure 3 shows a simplified schematic diagram represents the HCNG fueling system used in this research and how each component are interconnected.

4. Results

Section 2 presented the derivation and analysis in attempting to detect the HCNG composition using oxygen measurement. Due to some limitations of the current pilot vehicle, especially the lacking of an independent AFR control and monitoring capability, the testing and study here follows what described in section 2.3, namely the detection of the amount of oxygen when H_2 and CNG are not at predefined ratio. The amount of oxygen in the exhaust gas can be measured using oxygen sensor. The readout in this case though, instead of reading through the engine ECU, a combustion analyzer is used to output the amount of oxygen in terms of percentage (%) of the exhaust gas. To investigate the H2 and exhausted oxygen relationship throughout the engine operating conditions, the steady-state testing is used where the level of oxygen is measured as the engine is steadily controlled at the engine speed ranged from 2,000 to 5,000 rpm. The results are shown in Table 1 and Figure 4 for different variation of HCNG mixing composition.

Here, according to the electronics control unit, the initial fuel is CNG 100% and the engine is assumed running at stoichiometric condition, i.e. the stoichiometric is calculated from CNG 100%. The value of O_2 in the exhaust gas increases approximately 2.44% for 5% reduction of CNG by volume (see the results of CNG 95% as compared to CNG 100%). For the effects of using HCNG with the variation of H_2, results are a bit different between the engine speeds lower and higher than 3,000 rpm. For cases when engine speeds are lower than 3,000 rpm, it is found that the amount of O_2 in the exhaust gas increases approximate 1.50% for every 5% increase of hydrogen by volume. For cases when engine speeds are lower than 3,000 rpm, it is found that the amount of O_2 in the exhaust gas increases approximate 1.13% for every 5% increase of hydrogen by volume. And on average, the amount of O_2 in the exhaust gas increases approximate 1.23% for every 5% increase of hydrogen by volume.

Table 1 Testing results measuring O_2 in exhaust gas for different HCNG compositions

Engine Speed RPM	% O_2					
	CNG	CNG	HCNG			
	95%	100%	5%	10%	15%	20%
2000	6.84	4.43	6.54	7.75	8.67	10.32
2500	6.89	4.45	6.69	7.21	8.52	10.25
3000	7.12	4.78	7.03	7.26	8.36	9.23
3500	7.23	4.96	7.23	7.52	8.65	9.32
4000	7.01	3.97	6.96	6.90	8.5	9.16
4500	6.87	4.53	6.54	7.03	7.93	9.01
5000	6.88	4.61	6.62	7.25	7.90	8.89

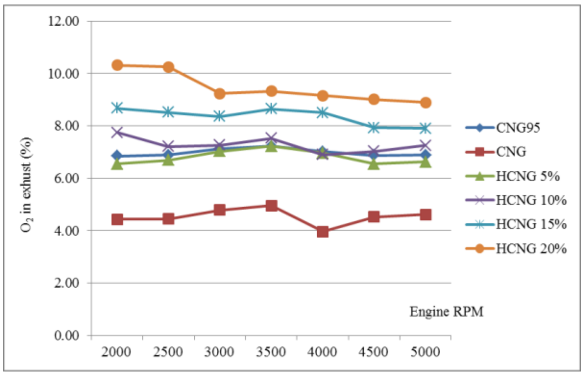

Figure 4 Amount of O_2 in exhaust gas for different HCNG compositions

5. Discussions

From the results, the amount of oxygen in exhaust gas increases when the mixing ratio of HCNG increases. The theoretical estimation from section 3 indicated that every 5% reduction of CNG, O_2 in the exhaust gas increases approximately 1.05%. And every 5% increase of hydrogen by volume, O_2 in the exhaust gas increases approximate 0.26%. However, the testing results showed higher value of O_2. This higher values of O_2 is the results from the change of the equivalent ratio as the actual CNG is reduced or H_2 is increased. Table 2 shows the calculation demonstrating the change of the equivalent ratio as the fuel composition changes. This change of equivalent ratio is not known by the engine ECU. Therefore, as the fuel composition changed, the engine runs with lean condition automatically.

The data from the testing results is also used to validate the proposed theoretical estimation of O2. Here, the appearance of O_2 for the case of running the engine with CNG indicated that the engine ran with the equivalent ratio around 0.8. And by knowing the amount of injected fuel in each case, we can then estimate the amount of O_2 in the exhaust gas for different fuel composition and engine speed as shown in Table 3. The testing results shown in Table 1 are compared to the calculation results shown in Table 3 by plotting the averaged amount of O_2 from different engine speed as shown in Figure 5. It can be seen that the changing trends of the amount of O_2 in the exhaust gas shown by the testing results are in similar fashion as the calculations. The higher the mixing ratio of HCNG, the more amount of O_2 in the exhaust gas, and the lesser equivalent ratio. Though the amount of O_2 in the exhaust gas increases about 1.23% from the test results, while it is about 1.71% from the calculation. This difference should come from the error from the equivalent ratio assumption which is usually not a constant value throughout the engine operation. The addition of an individual AFR control should improve the estimation accuracy.

Table 2 Equivalent ratio and O_2 increase in the exhaust gas

Fuel	Sto-AFR (by mass)	Equivalen t ratio	Increased O_2 (%)
CNG 100%	17.2 : 1	1.00	-
CNG 95%	18.1 : 1	0.95	1.05
HCNG 5%	18.0 : 1	0.96	0.92
HCNG 10%	18.8 : 1	0.91	1.84
HCNG 15%	19.8 : 1	0.87	2.76
HCNG 20%	20.8 : 1	0.83	3.67

Table 3 Calculation results of O_2 in exhaust gas for different HCNG compositions

Engine Speed RPM	% O_2					
	CNG	CNG	HCNG			
	95%	100%	5%	10%	15%	20%
2000	6.53	4.43	6.14	7.85	9.56	11.26
2500	6.55	4.45	6.16	7.87	9.58	11.28
3000	6.88	4.78	6.49	8.20	9.91	11.61
3500	7.06	4.96	6.67	8.38	10.1	11.79
4000	6.07	3.97	5.68	7.39	9.10	10.80
4500	6.63	4.53	6.24	7.95	9.66	11.36
5000	6.71	4.61	6.32	8.03	9.74	11.44

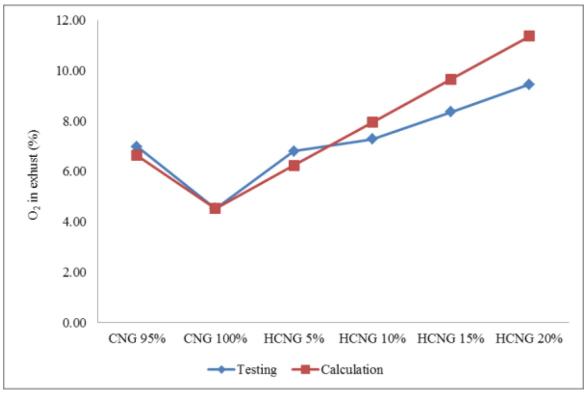

Figure 5 Comparison of O_2 in the exhaust gas

6. Conclusions

It is found that the mixing ratio of HCNG affects the amount of O_2 in exhaust gas. As the mixing ratio of HCNG increases, the amount of O_2 in exhaust gas increases accordingly. Therefore, knowing amount of O_2 in exhaust gas can help controlling the mixing ratio of HCNG to be more precise. It is also found also that there are many factors affecting the amount oxygen in exhaust. One of the main factors is the equivalent ratio variations. For every 0.1 reduction of the equivalent ratio the amount of oxygen increases by 2.1%. If the equivalent ratio can be precisely controlled, the amount oxygen in exhaust can indicate the mixing ratio of HCNG. The theoretical estimation shows that the amount of the oxygen in the exhaust increases by 0.23% for every 5% addition of H_2 at stoichiometric condition. This value can be increased or decreased for lean and rich conditions respectively. The experimental results found that at the equivalent ratio around 0.8 the amount of O_2 in the exhaust gas increases about 1.23% for every 5% change of HCNG mixing ratio. This result agrees well with the proposed calculation.

7. Acknowledgements

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