SI Engine Simulation Using Residual Gas and Neural Network Modeling to Virtually Estimate the Fuel Composition

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Abstract— **Research in electronic controlled internal combustion engines mainly focuses on improving performance and lowering the emissions. Combustion performance depends on the geometry of cylinders and on the design of all mechanical parts, which are based on the laboratory experimental research. Due to the limitations of the materials used in the engine and the continuous high operating temperature, engines function in either spark ignition or charge ignition processes. Recent research on computer controlled engines uses sensors and electronic actuators which allows switching the engine operational mode between spark ignition and charge ignition. Thus, this makes possible to mix intake fuel compositions in order to give more choices to consumers.**

This study employs a neural network which is capable of estimating fuel composition using the parameters of residual gas. The simulation is based on a thermodynamic engine model implemented in Matlab Simulink. The main advantages are the capabilities of the model to 1) calculate the gas exchange as a function of time in transient mode, and 2) to generate data for the design control algorithms without the need of the engine bed test environment to test various fuel compositions.

***Index terms*—Matlab, neural-network, SI-engine, simulation**

I. Introduction

Most of modern vehicle engine productions are used with engine control unit (E.C.U.) to control engines performance[1][2].Various sensors have been used to monitor the engine combustion process, where emissions are decisive to meet the emission limitation by law while producing the best efficiency. Those collected data are sent to the E.C.U in which the actuators make adjustments according to the given best performance parameters tested in laboratories. The in-house laboratory test uses known named fuel with standard composition, either gasoline or diesel, which are designed for spark ignition or charge ignition engines [3][4]respectively. While consumers obtain such fuels from fuel suppliers, the correct chemical composition varies from fuel standards, e.g. gasoline consists of 4 to 12 hydrocarbon atoms per molecule, or chemically named octane, ethanol etc. Therefore settings stored in E.C.U. are generally based on diesel or gasoline engine process instead of in the actual composition.

Engine research is mainly focus on emission or fuel consumption control network in diesel engine [5]-[8][16]. In this study, we use computer engine simulations tools to investigate the use of the estimated fuel composition as a control parameter without engine bed test. The simulation mapped the engine for spark ignition (SI) process. Several composition obtained from various books [10][12][13] are used as initial composition of fuel. By considering the combustion process, the residual gas generates different chemical products [3]. Compared to real engine available sensors and actuators [5], the simulation uses obtainable parameters to estimate the initial composition. This idea will also give the flexibility of using more choice of fuel composition in the real engine. The engine is capable to accept an unknown composition, i.e. fuel mixture, and control the engine performance. This study implements such idea to computer simulation, which is able to perform a four-stroke engine process based on thermodynamic modelling [9][10]. The neural network is trained with the results of oxygen level (O) and carbon dioxide (CO2) level in the residual gas with the exhaust gas temperature which in reality can be obtained from lambda (oxygen) sensor, CO2 sensor and exhaust gas temperature sensor respectively. The training set in generated with three varying parameters, namely the known or mixed fuel composition, air to fuel ratio (Φ) [11] and ignition timing. This paper is organized as follows. The engine model description and the neural network model are described in Section II. Behaviour of exhaust gas composition for different parameters is discussed in Section III. Simulation results are analysed and shown in Section IV. Finally, conclusions are drawn in Section V.

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II. METHODOLOGY

The model consists of two parts as shown in Figure 1. The engine model built for engine control research based on thermodynamic equations, since various useful parameters can be calculated. The second part is the neural network, where the training inputs and targets are taken from the engine model. Once the neural network is trained, the network is connected to the engine so the number of atoms in a molecule of carbon (C), hydrogen (H) and oxygen (O) are estimated.

A. Engine Model

The estimation of the engine in software can be divided into four strokes of spark ignition engine. Pressure is calculated in a single zone. Temperature estimation is divided into two zones, burned and unburned zone. The unburned zone is used prior to combustion without any heat generated during combustion. Temperature is calculated from the volume changes, with heat transfer and gas exchange estimation. The burned zone calculates the temperature with heat release estimation. The work done is calculated by volume from crankslider model [10]. The burning process and heat transfer are calculated using sub-models shown in Figure 1.

Table I Sub-models use in engine simulation modelling

Process	Sub-models
Heat release in combustion	Wiebe function [10]
Heat transfer	Woschni correlation [15]

B. Neural Network

Computer simulation on engine is able to provide most of the engine operating parameters and the gas products based on equations. In order to design a neural network to estimate the fuel composition, one needs to take into consideration that a real engine can only record data from limited parameters due to the limited choice or functionality of sensors. In this study, we use simulated parameters that could be obtained to monitor the condition of the exhaust gas with the following sensors in the real engine: lambda sensor, CO2 sensor and exhaust temperature sensor.

The fuel composition data being tested are extracted from Ferguson [10], Raine [13] and Heywood [12] and are shown in Table II. Those data include a number of atoms per molecule of carbon (C), hydrogen (H) and oxygen (O), respectively, as well as polynomial approximations of enthalpy, entropy and specific heat capacity at constant volume and constant pressure. The gas exchange model calculates specific heat, internal energy and combustion product.

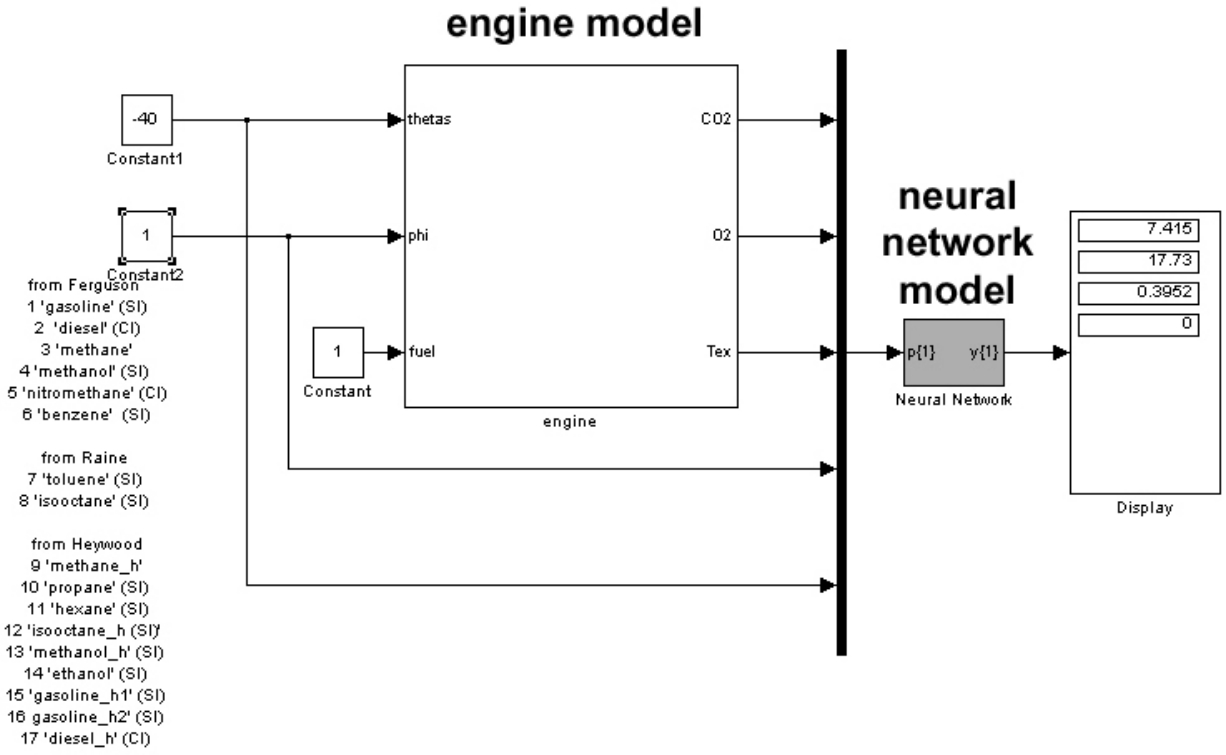

Figure 1 Engine model with neural network used in Matlab Simulink

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Table II Fuel compositions being tested according to Ferguson [10], Raine [13] and Heywood [12]

Fuel	# of atoms of C	#of atoms of H	# of atoms of O	Chemical composition
gasoline_f (Ferguson[10])	7	17	0	C7-H17
gasoline_h1 (Heywood[12])	8.26	15.5	0	C8.26-H15.5
gasoline_h2 (Heywood[12])	7.76	13.1	0	C7.76-H13.1
isooctane_r (Raine[13])	8	18	0	C8-H18
isooctane_h (Heywood[12])	8	18	0	C8-H18
methanol_f (Ferguson[10])	1	4	1	C1-H4-O1
methanol_h (Heywood[12])	1	4	1	C1-H4-O1
ethanol_h (Heywood[12])	2	6	1	C2-H6-O1

The following three parameters are modified in the model to generate training and generalisation data sets: ignition timing, air to fuel ratio and fuel type. The parameters ranging between -20° to -60° TDC for the ignition timing, and ranging between 0.8 to 1.2 of stoichiometric mixture and between air to fuel ratio. The training algorithm used is Levenberg-Marquardt backpropagation. The neural network produces then three outputs as follows: number of atoms per molecule of C, H and O, respectively. Number of epochs is 500. Engine speed is set to 1000 rpm to reduce the simulation parameters.

III. Exhaust Gas Composition Analysis

The simulation estimates gas products based on chemical equilibrium theory. The results have been validated with complete equilibrium calculations using NASA equilibrium program TRANS72 [12], which gives similar results. Figure 2 shows the behavior at different ignition timing ranging from -20° to -60° TDC of combustion stroke, in the step of 2°, and different air to fuel ratio ranging from 0.8 to 1.2 with the step of 0.2. Figure 2 shows the molecule fractions of CO2, O2 and exhaust gas temperature against two input parameters.

A. Exhaust Gas Composition vs. Time

To simplify the simulation, two parameters, speed (1000 rpm) and load are kept constant. In order to train the neural network, a test run is needed to see how long the engine reaches the saturated state from idle start. Fuel 'gasoline_f' is being tested. The mole fraction of CO2 (Figure 3a)and O2 (Figure 3b), and exhaust gas temperature (Figure 3c) settle after 5 cycles, which corresponds to 0.6 seconds at 1000 rpm, and 0.3 seconds at 2000 rpm etc. Other tests have been performed for other fuels. It has been found that the engine settling time is not affected by different fuel compositions, and always settles at around the fifth cycle. Therefore, data of exhaust gas composition will be collected on the fifth cycle.

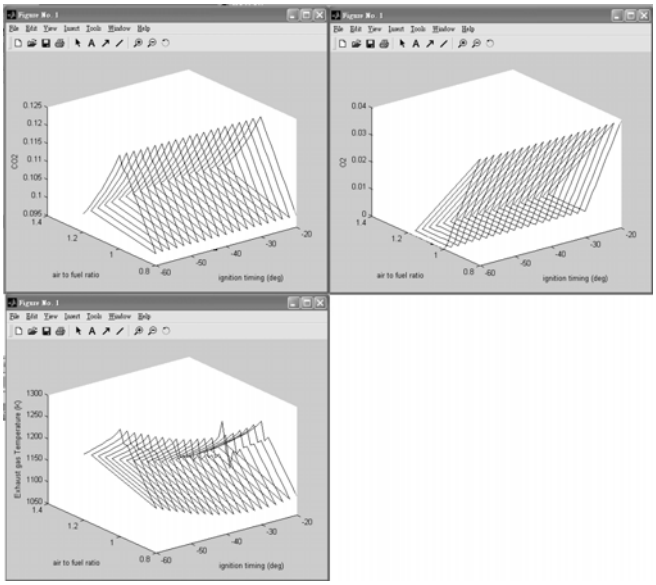

Figure 2 Exhaust gas products, a) CO2 level (top), b) O level (middle), and c) exhaust gas temperature (bottom), of gasoline_f against air to fuel ratio and ignition timing

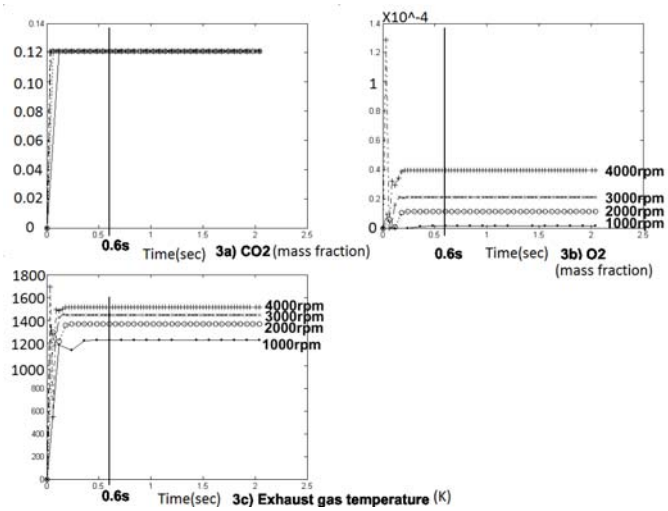

Figure 3 a) CO2 (top left), b) O2 (top right) and c) exhaust gas tempeture (bottom left) of fuel gasoline_f against time. Different speed is run. Point is 1000rpm, circle is 2000rpm, x-mark is 3000rpm, plus is 4000rpm.

The network is generated using a fixed speed engine simulation, which is 1000rpm. Engine simulation is run for different speed. Result showed that higher speed produced hotter exhaust gas and move residual oxygen remaining unburned, but also settles after fifth cycle. It can be concluded that more training with an additional input for engine speed is required for different set speed.

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B. Exhaust Gas Composition vs. Air to Fuel Ratio

The air and fuel ratio is defined as:-

$$AFR(\phi) = \frac{mass_{air}}{mass_{fuel}},$$

where *massair* is mass of air and *massfuel* is mass of fuel

When the air to fuel ratio is larger than 1, the mass of fuel is lower than the mass of air. This is defined as a lean mixture. Vice versa, less air than fuel is defined as a rich mixture. Engine is simulated with fixed ignition timing (-40°) for 5 cycles. The result of simulation is shown in Figure 4. CO2 lies at around 9-12% mole fraction. When Φ equals to 1, engine performs a perfect combustion, therefore at his point the simulation shows the highest CO2 level, as shown in Figure 4a. When Φ is less than 1, the product in the engine combustion of rich mixture contains significant amount of O unburned due to incomplete combustion, as shown in Figure 4b. Lean mixture burns more oxygen, but the torque produced is lower [5]. Exhaust gas temperature is the highest at stoichiometric or slightly lean mixture, as shown in Figure 4c. This can be explained by the enthalpy which is the lowest when the air to fuel ratio is stoichiometric, it produces higher energy combustion and hence the temperature is higher.

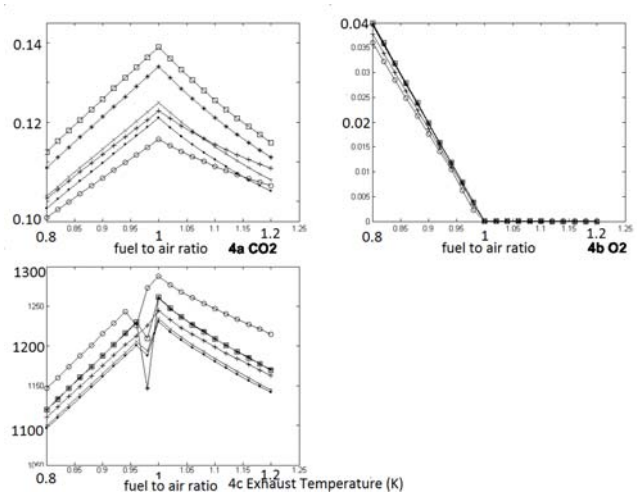

Figure 4 a) CO2 (top left), b) O2 (top right) and c) exhaust gas tempeture (bottom left) of different fuel against air to fuel ratio with fixed ignition timing (-40 deg). Point is gasoline_f, circle is methanol_f, x-mark is isooctane_r, plus is ethanol_h, star is gasoline_h1, square is gasoline_h2

C. Exhaust Gas Composition vs. Ignition Timing

The same engine simulation is produced for different ignition timing with fixed Φ (equals 1) for 5 cycles. Ignition timing does not have effect on CO2 since Φ is to 1, as shown in Figure 5. The result shows a trend on O2 level and exhausts gas temperature, as shown in Figure 5b and 5c.

This trend can be explained by the factors which affect the residual oxygen in exhaust depending on combustion performance due to the engine dimensions, material of combustion chamber and factors such as blowby or type of fuel. It can be concluded that there is no direct relationship between residual gas and igniting timing.

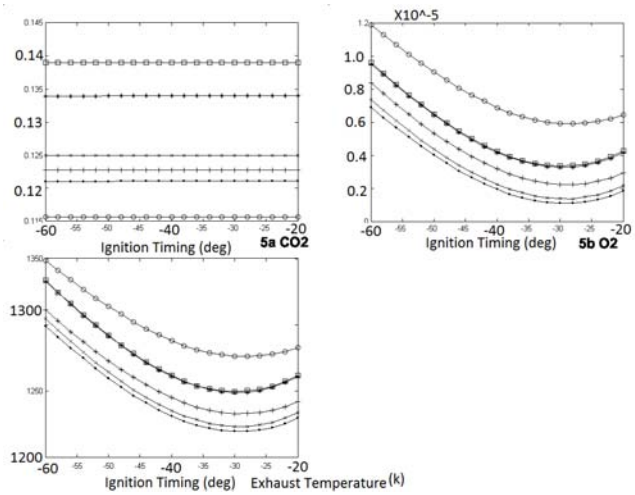

Figure 5 a) CO2 (top left), b) O2 (top right) and c) exhaust gas tempeture (bottom left) of different fuel against ignition timing with fixed air to fuel ratio (1). Point is gasoline_f, circle is methanol_f, x-mark is isooctane_r, plus is ethanol_h, star is gasoline_h1, square is gasoline_h2

IV. Results

A. Settling time

As described previously, the exhaust gas composition needed time to settle from idle start. The data are collected at the fifth cycle and used to train the neural network. Therefore, the correct estimation is targeted after 5 cycles. The results of engine simulation ran for 2 seconds with fixed air to fuel ratio and ignition timing which are shown in Figure6. Results show that the estimations are unstable for the first 5 cycles as expected. After 5 cycles the simulations generate relatively stable estimation.

B. Air to Fuel ratio

The simulation runs on a fixed value of ignition timing (-40°). The results of fuel composition estimation against different fuel composition and Φ are shown in Figure7. The neural network generates good estimations with the most of the results having less than one mole difference in C, H and O molecule for all different gasoline compositions (Figure 7a, 7b, and 7c),. The results allow distinguishing between isooctane (C8H18), methanol (C1H4O1), and (C2H6O1).

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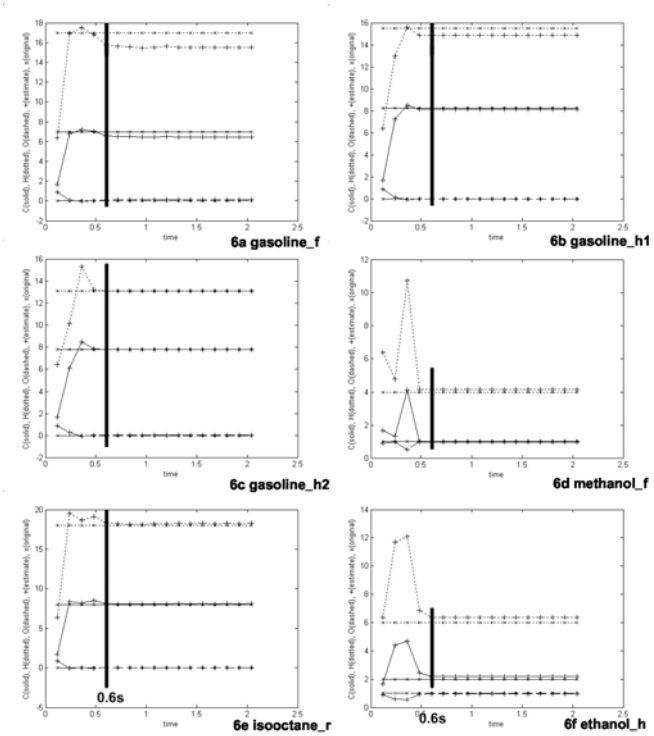

Figure6 Fuel composition estimation for 2 seconds. a) gasoline_f (top left), b) gasoline_h1 (top right), c) gasoline_h2 (middle left), d) methanol_f (middle right), e) isooctane_r (bottom left) and f) ethanol_h (bottom right)

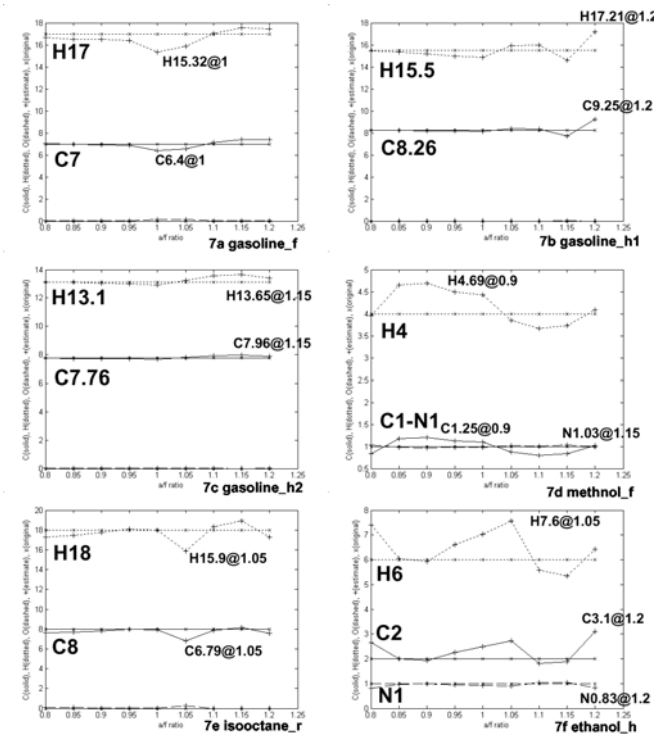

Figure7 Fuel composition estimation against different air to fuel ratio with fixed ignition timing. a) gasoline_f (top left), b) gasoline_h1 (top right), c) gasoline_h2 (middle left), d) methanol_f (middle right), e) isooctane_r (bottom left) and f) ethanol_h (bottom right)

C.Ignition Timing

The simulation runs with a fixed value of air to fuel ratio equals to 1. The results of fuel composition estimation against different ignition timing are shown in Figure8. For fuel gasoline (Figure8a, Figure8b, and Figure8c), methanol (Figure8d) and isooctane (Figure8e), simulation generates accurate estimation between -25° to -50°. The results also show that the neural network estimate fewer C and H atoms, but more O atom at ignition timing above -25° and below -50°.

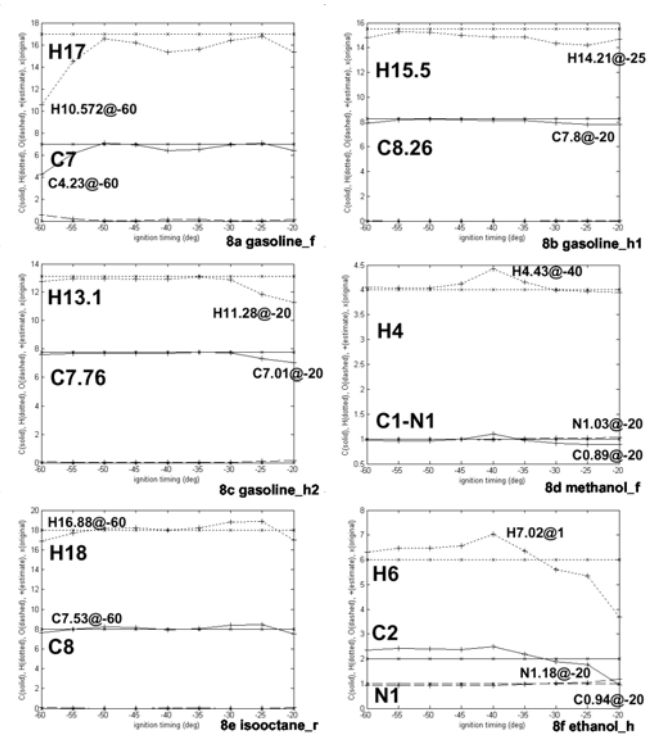

Figure8 Fuel composition estimation against ignition timing, with fixed air to fuel ratio equals to 1, a) gasoline_f (top left), b) gasoline_h1 (top right), c) gasoline_h2 (middle left), d) methanol_f (middle right), e) isooctane_r (bottom left) and f) ethanol_h (bottom right)

D.Fuel mixture

As discussed in Section I, correct chemical composition of gasoline varies because gasoline suppliers provide gasoline composition mixed with substances such as methanol and ethanol. In section *IV A*, *IV B* and *VI C*, fuel composition estimation was performed and discussed. Here, we intend to genate the same neural network to estimate the mixed fuel composition. We assumed that the fuels were prefect mixed. Two case studies, namely isooctane-methanol and isooctane-ethanol mixtures have been used, with methanol and ethanol of 5%, 10%, 15%, and 20% into isooctane.

Case 1 isooctane- methanol mixture

The simulation is run for 5 cycles, with Fuel 1 used isooctane (C8H18) and Fuel 2(C1H4O1) used methanol. The original composition estimation is shown in Table III, and percentage error is shown in

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Table IV. The error is higher as the percentage of methanol increases. The mixture includes a small amount of oxygen atom from calculation. It is too tiny and hence the error is significant. To improve the results, laboratory experiments may be needed to find the specific heat capacity, enthalpy and entropy for the new mixed compositions.

Table III Number of C, H and O estimation with isooctane-methanol mixture

Fuel 1 %	Fuel 2 %	C (# of atom)	H (# of atom)	O (# of atom)	Calculated composition
95%	5%	7.874	17.8	0.044	C7.65H17.3 O0.05
90%	10%	7.662	17.4	0.079	C7.3H16.6 O0.1
85%	15%	7.428	16.9	0.117	C6.95H15.9 O0.15
80%	20%	7.176	16.4	0.158	C6.6H15.2 O0.2

Table IV Number of C, H and O estimation with isooctane-methanol mixture

Fuel 1 %	Fuel2 %	C % error	H % error	O % error	Calculated composition
95%	5%	3.0	3.0	20	C7.65H17.3 O0.05
90%	10%	5.0	4.8	21	C7.3H16.6 O0.1
85%	15%	6.9	6.4	22	C6.95H15.9 O0.15
80%	20%	7.5	9.2	25	C6.6H15.2 O0.2

Case 2 isooctane- ethanol mixture

Same experiment is run after substituting Fuel 2 into ethanol, which has different composition (C2H6O1). The original composition estimation is shown in Table V, and percentage error is shown in Table VI. The error same trend, therefore we can draw the same conclusion as in Case 1.

Table V Number of C, H and O estimation with isooctane-ethanol mixture

Fuel 1 %	Fuel 2 %	C (# of atom)	H (# of atom)	O (# of atom)	Calculated composition
95%	5%	7.929	18.03	0.029	C7.7H17.4 O0.05
90%	10%	7.868	17.81	0.045	C7.4H16.8 O0.1
85%	15%	7.752	17.57	0.064	C7.1H16.2 O0.15
80%	20%	7.633	17.33	0.084	C6.8H15.6 O0.2

Table VI Number of C, H and O estimation with isooctane-ethanol mixture

Fuel 1 %	Fuel 2 %	C % error	H % error	O % error	Calculated composition
95%	5%	3.0	3.6	43.1	C7.7H17.4 O0.05
90%	10%	6.3	6.0	54.6	C7.4H16.8 O0.1
85%	15%	9.2	8.5	57.2	C7.1H16.2 O0.15
80%	20%	12.3	11.1	58.1	C6.8H15.6 O0.2

V. Conclusion

This paper present a neural network model capable to estimate the fuel composition based on the thermodynamic calculation of exhaust gas product. To match the possible parameters which can be obtained from a real engine, the network input parameters used are carbon dioxide (CO2), oxygen (O), and exhaust gas temperature. The simulation produces result using different air to fuel ratio and ignition timing, which aimed for control parameters. The result returns the estimated composition number of atom of carbon (C), hydrogen (H), and oxygen (O) in a molecule. The effect of residual gas against speed, time, air to fuel ratio and ignition timing has been discussed.

By considering a stable estimation, a neural network is built by using the exhaust gas composition at the fifth engine. It can be concluded that engine needed some cycles to settle; therefore different approach is needed for early fuel estimation. With analysis using different engine speed, more training set is needed and engine speed can be added as an additional parameter as control input. The network produced good estimations of original fuel composition input before gas exchange. The error, in terms of number of atom in a molecule, agreed less than one atom difference in most of cases, with air and fuel ratio is near stoichiometric; and ignition timing between -25° to -50°. Further, the neural network is tested with two different fuel mixtures with different percentages. The error increased with respect to the pure composition. Future work will consider training the neural network also with mixed compositions to try to solve this problem.

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