A COMPREHENSIVE NUMERICAL STUDY OF THE ETHANOL BLENDED FUEL EFFECT ON THE PERFORMANCE AND POLLUTANT EMISSIONS IN SPARK-IGNITION ENGINE

by

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In the present work, the performance and pollutant emissions in a spark-ignition engine has been numerically investigated. For this purpose, the coupled KIVA code with CHEMKIN is used to predict the thermodynamic state of the cylinder charge during each cycle. Computations were carried out for a four cylinder, four strokes, multi point injection system (XU7 engine). Numerical cases have been performed up to 30 vol.% of ethanol. Engine simulations are carried out at 2000, 2500, and 3000 rpm and full load condition. The numerical results showed that pollutant emissions reduce with increase in ethanol content. Based on engine performance, the most suitable fraction of ethanol in the blend was found to be nearly 15% for the XU7 engine.

Key words: *ethanol, MPFI engine, KIVA-4, CHEMKIN*

Introduction

Alcohols, which can be made from renewable resources such as locally grown crops and waste products, have been suggested as engine fuel almost since automobile was invented [1]. Among various alcohols, ethanol is likely alternative fuel that its properties allow its use in modern engines with minor modifications [2]. Balki *et al.* [3] investigated the effect of alcohol (ethanol and methanol) use on the performance, pollutant emissions and combustion characteristics of SI engine. According to the obtained results, the use of alcohol increase engine torque, brake specific consumption and decrease the CO, HC, and NO_x emissions in comparison with gasoline fuel.

In 2004, Wu *et al.* [4] used an open-loop operation in a fuel injection spark-ignition (SI) engine. They investigated the effects of air-fuel ratio and ethanol addition to the ethanol-gasoline blended fuel on engine performance and pollutant emissions. The experimental results showed that torque output increased slightly with adding ethanol at small throttle opening. It was also shown that CO, CO_2, and HC emissions were reduced with the increase in ethanol content in the blended fuel.

Yucesu *et al.* [5], used unleaded gasoline and unleaded gasoline-ethanol blends in a single cylinder, four-stroke, SI engine with variable compression ratio. It was found that blending unleaded gasoline with ethanol slightly increased the brake torque and decreased CO and HC emissions.

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Ceviz and Yuksel [6] studied the effect of ethanol addition on cyclic variability and pollutant emission in a SI engine. According to their results, using ethanol-unleaded gasoline blends decreased the coefficient of variation in indicated mean effective pressure. In this study, 10 vol.% ethanol was introduced as the optimum percentage of ethanol.

Al-Hasan [7] blended ethanol with gasoline up to 25% and investigated the effect of ethanol-unleaded gasoline blends on performance and pollutant emission. It was shown that brake power, torque and brake thermal efficiency is increased with ethanol blending. The best percentage of ethanol volume fraction was found to be 20 vol.%

He *et al.* [8] found that in most cases, ethanol-blended fuels can reduce CO, THC (Total HC), and NO_x emissions.

Stojiljković *et al.* [9] studied the effect of bioethanol-gasoline blends on performance and pollutant emission. It was observed that the maximum values of engine power, torque, and specific fuel consumption are approximately identical with pure gasoline. Pollutant emission tests revealed no significant influence of bioethanol addition on exhaust gases CO content for all tested mixtures. Altun *et al.* [10] investigated experimentally the effect of 5 and 10% ethanol and methanol blending in unleaded gasoline on engine performance and pollutant emission. Compared to unleaded gasoline, M10 and E10 blended fuels produced the best results in exhaust pollutant emissions. The HC emission of M10 and E10 are reduced about 13% and 15%, respectively, and the CO emission by about 10.6% and 9.8%, respectively. On the other hand, increased CO_2 emissions were observed for M10 and E10 compared with unleaded gasoline. The addition of ethanol or methanol to unleaded gasoline caused an increase in the brake specific fuel consumption and a decrease brake thermal efficiency in comparison to unleaded gasoline.

Bayraktar [1, 11] investigated the effects of ethanol addition to gasoline on an SI engine performance and exhaust pollutant emissions and flame propagation. The most suitable volume fraction of ethanol in the blend for SI engines was determined about 7.5% experimentally and 16.5% theoretically from the engine performance and CO emissions points of view. It was shown that CO emission was reduced while NO emission was found to increase due to the rising temperature of cylinder content.

The studies on the combustion of ethanol-gasoline blends have shown that the optimum percentage of ethanol-gasoline blends depends on the type of engine. An overview of the studies which include the optimum percentage is given in tab. 1.

Table 1. Overview of studies on optimum percentage of ethanol blending with gasoline

	Author	Type of study	Type of engine	Optimum percentage	Reference
1	Abdel-Rahman	Experimental	VARICOMP	10%	1997, [12]
2	Al-Hasan	Experimental	Toyota, Tercel	20%	2003, [7]
3	M. A. Ceviz	Experimental	FIAT	10%	2005, [6]
4	H. Bayraktar	Experimental Numerical	single-cylinder, variable compression	25%	2007, [11]
5	M. B. Celik	Experimental	Single cylinder, Lombardini LM 250	25%	2008, [13]
6	W. Y. Lin	Experimental	Single cylinder, Honda GX160	6% (pollutant emission), 9% (performance)	2010, [14]

The use of computational tools in engine design is increasing rapidly. This is due to recent rapid advances in computer power, as well as the reduced cost of simulations in comparison with engine experiments [11].

Computer simulations of internal combustion engine cycles are desirable because of the aid they provide in design studies, predicting trends, serving as diagnostic tools, giving more data than are normally obtainable from experiments, and in helping one to understand the complex processes that occur in the combustion chamber [3].

Experimental studies on the combustion of ethanol-gasoline blends have shown that the optimum percentage of ethanol-gasoline blends on the type of engine. Therefore the aim of this study is to simulate of SI engine fueled with various blend of ethanol and unleaded gasoline, with coupling KIVA-4 code with CHEMKIN II, to determine the optimum percentage of ethanol-gasoline blends.

Engine and operating conditions

In this paper the experimental results were obtained from the XU7 engine located at the Irankhodro Powertrain Cooperation. These experimental results are used to validate numerical results. This engine is a 4-cylinder multi point fuel injection engine which fuel is injected into the intake ports just upstream of each cylinder's intake valve. In this study, the engine is operated at 2000, 2500, and 3000 rpm engine speed and full load condition and the fuel consumption for the blended fuel is considered equal with pure gasoline case in each speed.

The engine specifications and operating condition are listed in tab. 2.

Table 2. Engine Specifications and operating conditions

Engine type	XU7JP/L3, MPFI		
Cylinder bore [mm]	83		
Stroke [mm]	81.4		
Displacement [cm^3]	1761		
Compression ratio	9.3		
IVC	29.3 aBDC		
IVO	8.5 bTDC		
EVO	43.3 bBDC		
EVC	5.5 aTDC		
Engine speed [rpm]	2000	2500	3000
Fuel injected [g]	0.03373	0.03786	0.037008
Start of injection [deg.]	–84 bTDC	–116 bTDC	–199 bTDC
Injection duration [deg.]	78	115	243
Spark timing [deg.]	15 bTDC	11 bTDC	12.5 bTDC

Numerical approach

The numerical simulations are performed using KIVA-4 code developed by U. S. Department of Energy [15]. The Taylor Analogy (TAB) model is used for describing spray droplet aerodynamic break-up. The O'Rouke drop collision model are activated [16, 17]. KIVA-4 also features a multicomponent fuel evaporation algorithm in spray simulation [18, 19]. The RNG k-ε turbulence model is used for convection and diffusion transport between different computational cells.

The CHEMKIN chemistry solver is integrated into the KIVA-4 code for solving the detailed chemistry during multidimensional engine simulations. Firstly, a binary linking file that contains all the reaction and species information is executed as an input to KIVA-4. The interpreter of CHEMKIN is first executed to generate a binary linking file that contains all the reaction and species information as an input to KIVA. An interface program was developed such that CHEMKIN is used as the chemistry subroutine in KIVA. Basically the reaction mechanism is solved for every computational cell at each time step.

The KIVA code provides the species and thermodynamic data of the computational cells for CHEMKIN, and the CHEMKIN code returns the new species information and energy release after solving the chemistry.

Once the CHEMKIN is called, it updates species densities and heat release based on the following equations:

$$\frac{\mathrm{d}Y_\mathrm{k}}{\mathrm{d}t}=\frac{\dot{\omega}_\mathrm{k}W_\mathrm{k}}{\rho} \tag{1}$$

$$\dot{\rho}_\mathrm{k}^\mathrm{chem}=\rho\frac{\mathrm{d}Y_\mathrm{k}}{\mathrm{d}t} \tag{2}$$

$$\dot{Q}^\mathrm{chem}=-\sum_{k=1}^{K}\frac{\mathrm{d}Y_\mathrm{k}}{\mathrm{d}t}\frac{\Delta h_{\mathrm{f}_\mathrm{k}}^0}{W_\mathrm{k}} \tag{3}$$

The vapor mass is updated due to density variation. By adding amount of energy releases from chemical reactions, cell enthalpy and internal energy are updated. Although the change of temperature is calculated within CHEMKIN code, Instead of it, KIVA-4 calculates the change in temperature throughout the CFD simulation cycle using the updated species densities and mass fractions. Figure 1 shows the calculation flow diagram of linking KIVA-4 and CHEMKIN.

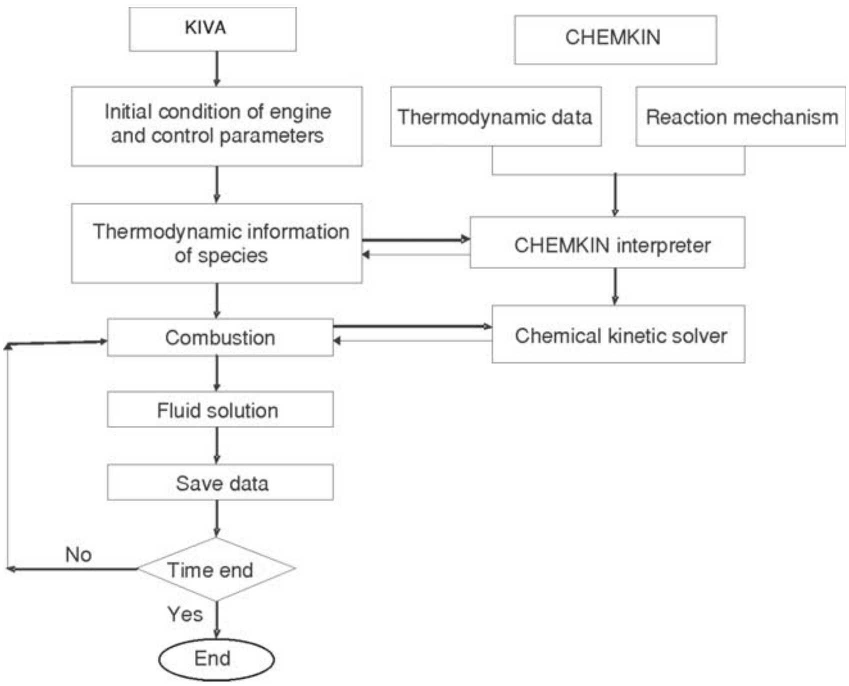

Figure 1. The combine of KIVA-4 code and CHEMKIN solvers

In addition, to consider the effects of turbulent mixing on the reaction, we used the turbulent mixing effect formulation which more information are available in [20].

A multi component reaction mechanism consisting of 113 species and 487 reactions are used to simulate the gasoline chemistry. In this mechanism, iso-octane is considered as representative of gasoline. The thermo physical properties of isooctane and ethanol are available in KIVA-4 fuel library.

The mechanism has been validated by comparing the ignition delay times at constant volume for various initial temperature and equivalence ratios with those obtained using a comprehensive mechanism [21]. The frictional process in an internal combustion engine includes mechanical friction, the pumping work and the accessory work. In this study, it just considered the pumping work and so it is neglected the mechanical friction and the accessory work [22].

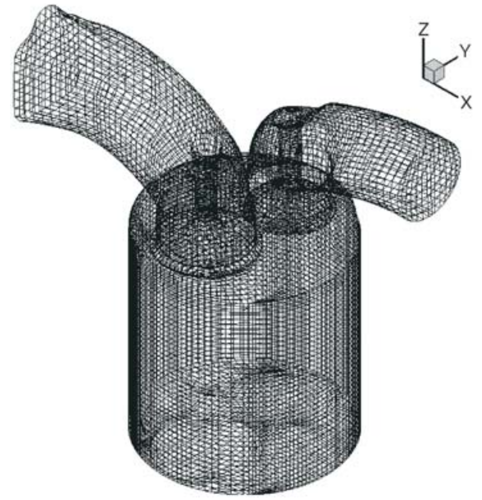

Figure 2. Computational grid

The full cycle is used to simulate engine. The 360° computational grid used in the modeling is presented in fig. 2. This engine mesh constructed with the help of the ANSYS ICEM CFD12.1 software. The full cycle is used to simulate engine.

Table 3. Measured and predicted pollutant emission data for pure gasoline fuel (N = 2500 rpm, T = 153 Nm)

Pollutant emission	Measured	Predicted
CO [%]	2.48	2.28
NO_x [ppm]	1416.63	1434
UHC [ppm]	2312.7	2128

Numerical validation

To valid the numerical method, the pure gasoline is used and the various parameters including pollutant emissions such as HC, NO_x and CO as well as performance parameter such as in-cylinder pressure at full load are investigated.

Table 3 shows the predicted and measured pollutant emissions which are in good agreement. The in-cylinder pressure for the engine speed of 2500 rpm at full load is shown in fig. 3 which confirms that the numerical results are in good propinquity with the experimental results.

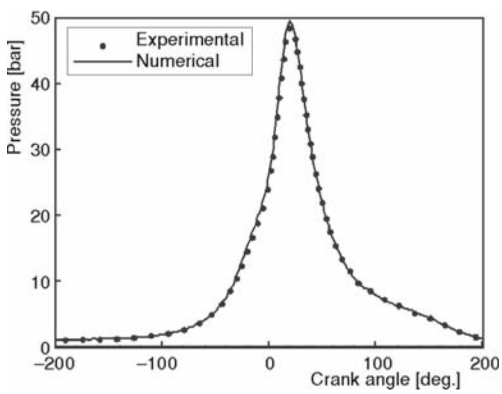

Figure 3. Confirmation of numerical simulation (pressure-crank angle diagram for full load condition at 2500 rpm)

Results and discussion

Predicted SI engine performance and exhaust emissions are presented for different ethanol addition percentage at 2000, 2500, and 3000 rpm engine speed for full load condition.

The blended fuel equivalence ratio is calculated as [7]:

$$(\mathrm{AFR})_{\mathrm{act}} = \frac{m_{\mathrm{a}}}{m_{\mathrm{f}}} \tag{4}$$

$$(\mathrm{AFR})_{\mathrm{st,\,b}} = \Sigma(\mathrm{AFR})_{\mathrm{st,i}}\, v_{\mathrm{i}} \tag{5}$$

$$\phi = \frac{(\mathrm{AFR})_{\mathrm{st,\,b}}}{(\mathrm{AFR})_{\mathrm{act}}} \tag{6}$$

The equation is used to calculate the volumetric efficiency is:

$$\eta_{\mathrm{v}} = \frac{m_{\mathrm{a}}}{\rho_{\mathrm{a,i}} V_{\mathrm{d}}} \tag{7}$$

where m_{a} is the mass of air inducted into the cylinder per cycle and $\rho_{\mathrm{a,i}}$ is the inlet air density taken based on the inlet manifold condition.

Ethanol is an oxygenated fuel; therefore, it has higher stoichiometric fuel/air ratio than gasoline stoichiometric fuel/air ratio [4]. For this reason, ethanol addition to gasoline leads to leaner operation.

Figure 4 indicates the variation of equivalence ratio with the ethanol concentration in blend. As shown, with increasing the percentage of ethanol in blended fuel, the equivalence ratio decreases.

Figure 5 shows an increase in the volumetric efficiency as the percentage of ethanol in the fuel blends increases. The heat of evaporation is higher than that of gasoline. High heat of evaporation can provide fuel-air charge to cool in the end of induction process and density to increase. Therefore with the increase of the percentage of ethanol in blended fuel, the amount of inlet air increases and volumetric efficiency is increased.

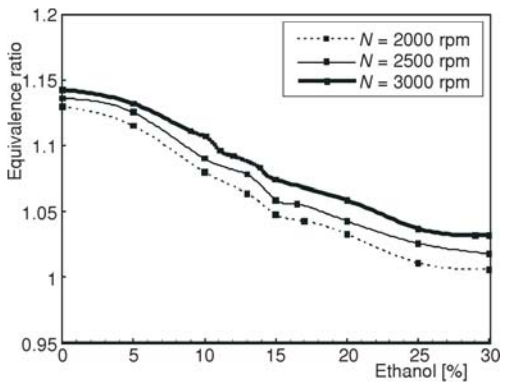

Figure 4. The effect of ethanol addition on equivalence ratio

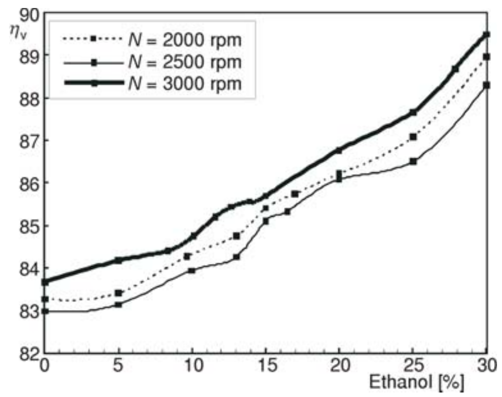

Figure 5. The effect of ethanol addition on volumetric efficiency

As shown in fig. 6, the maximum in-cylinder temperature is reduced with increase in ethanol blending with gasoline. As described the heat of vaporization of ethanol is more than gasoline, therefore the mixture's temperature at the end of intake stroke decrease which can causes the reduction in combustion temperature and it's maximum. Since in-cylinder temperature cannot be measured experimentally, the effect of ethanol blending on cylinder temperature is just reported based on numerical data.

As it was said, the heat of ethanol evaporation is higher than that of gasoline and ethanol addition causes decreasing fuel-air temperature charge and increase in density. In addition to this matter, adding ethanol to blended fuel causes the equivalence ratio of blended fuel approaches to stoichiometric condition which can lead to a better combustion. On the other hand, the ethanol heating value is lower than gasoline and it can be neutralize the previous positive effects. Therefore, with increasing ethanol in blended fuel, the engine power decreases to some extent, and after that, due to predomination of the negative effect of ethanol heating value, the engine power decreases. Figure 7 describes the variation of engine power with ethanol content in blended fuel.

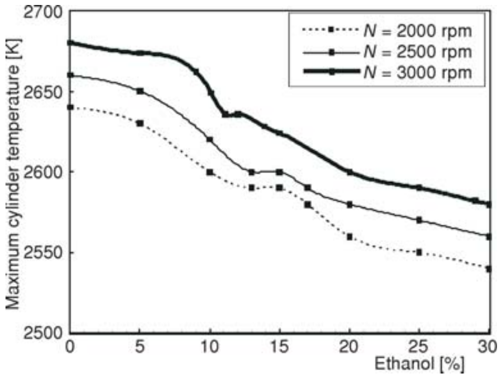

Figure 6. The effect of ethanol addition on maximum in-cylinder temperature

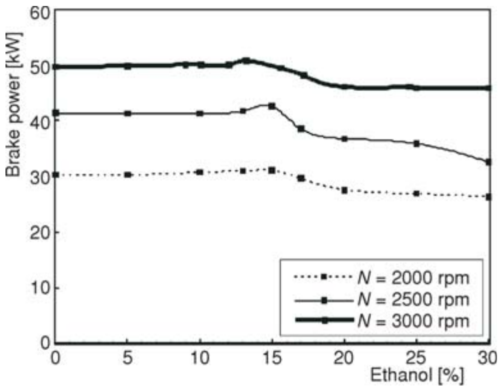

Figure 7. The effect of ethanol addition on brake power

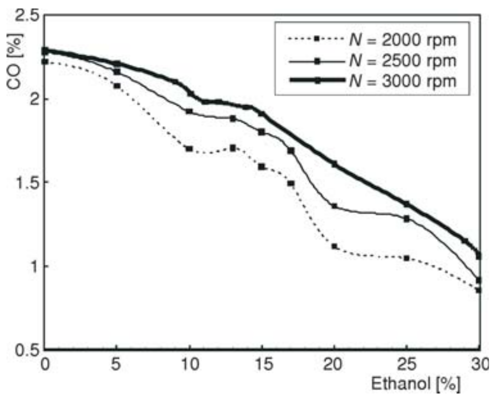

Figure 8. The effect of ethanol addition on CO emission

Figure 8 shows the effect of ethanol addition to blended fuel on CO emission. Since carbon content of blended fuel is decreased with increasing ethanol percentage (one mole ethanol has 2 mole carbons but each mole gasoline adds 8 mole carbons to blended fuel), with increasing ethanol content, the amount of oxygen is more for combustion process. Also this agrees with behavior shown in fig. 4. With equivalence ratio approaching unity, CO emission is reduced due to oxygen enrichment coming from ethanol. As a result, CO concentration decreases with increasing ethanol percentage in blended fuel.

The effect of ethanol-gasoline blends on HC emission for different speeds is shown in fig. 9.

It shows that adding ethanol, the HC concentration decreases. The reason for the decrease of HC concentration is similar to that of CO concentration described.

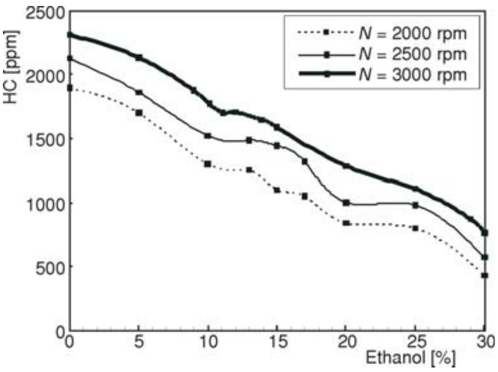

Figure 9. The effect of ethanol addition on HC emission

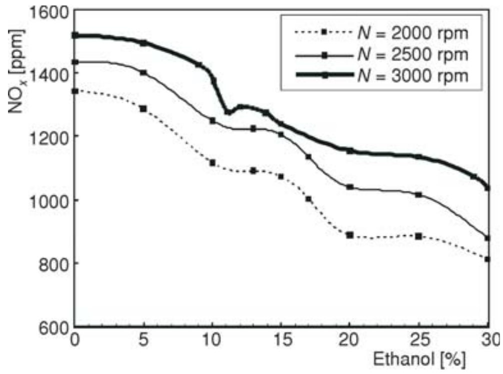

Figure 10. The effect of ethanol addition on NO_x emission

NO_x concentration decreases as the percentage of ethanol addition increases (fig. 10). This is a result of the higher heat of vaporization of ethanol in comparison with gasoline. Due to higher heat of ethanol evaporation, the temperature charge and the peak of temperature inside the cylinder are decreased (fig. 6) and therefore NO_x production reduces. It has been reported that the NO_x emissions can be related to fuel property, the *H/C* ratio [23, 24]. Fuel with higher *H/C* ratio indicates lower NO_x emissions. For the present data, this principle applies.

Conclusions

In this paper, the KIVA-CHEMKIN code is used to numerically simulate the effect of ethanol addition on the SI engines key parameters. The engine speeds of 2000, 2500, and 3000 rpm at full load condition are simulated and the performance parameters such as in-cylinder pressure and engine power as well as the pollutant emissions due to CO, HC and NO_x are investigated in details.

The numerical results show that in case of using up to 15 vol.% ethanol-gasoline blends, the engine power is increased. However, increasing the value of ethanol addition for more than 15 vol.%, the engine power decreases due to the decrement of the heating value of the blended fuel. Anyway, using the ethanol addition leads to the reduction of the CO, HC, and NO_x emissions.

In general, it can be concluded that the most suitable ethanol addition for XU7 engines is nearly about 15 vol.% ethanol-gasoline blends.

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Nomenclature

$\dot{m}$ – mass flow rate, [kgh^{-1}]
N – engine speed, [rpm]
V_d – displacement volume, [m^3]
v – volume fraction, [%]
$\dot{Q}^{chem}$ – heat release rate from all chemical reactions, [kJs^{-1}]
W_k – molecular weight for species k
Y_k – mass fractin for species k

Greek symbols

ϕ – equivalence ratio
h_v – volumetric efficiency
ρ – density, [kgm^{-3}]

Subscripts

a – air
act – actual
f – fuel

Acronyms

ABDC – after bottom dead center
$(AFR)_{act}$ – actual air-fuel ratio of fuel blend
$(AFR)_{st,b}$ – stoichiometric air-fuel ratio of fuel blend
$(AFR)_{st,i}$ – molar stoichiometric air-fuel ratio of fuel blend
aTDC – after top dead center
bBDC – before bottom dead center
EVC – exhaust valve closure
EVO – exhaust valve open
IVC – inlet valve closure
IVO – inlet valve open

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