

ISSN: 2395-3470

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Simulating Combustion of Gasoline and HHO in an Internal **Combustion Engine**

Toledo V., M.*1, Hareter, M. 2, Toledo G., M.1, López B., R.1

*Author for correspondence ¹Instituto Politécnico Nacional.

Escuela Superior de Ingeniería Mecánica y Eléctrica. Sección de Estudios de Posgrado e Investigación. Laboratorio de Ingeniería Térmica e Hidráulica Aplicada. Edificio 5 3er. piso. Av. IPN s/n, Colonia Lindavista, 07738, México D.F. Tel. 57296000 ext. 54754 E-mail mtv49@yahoo.com

ABSTRACT

The problems associated with the natural resource of crude oil prompts engineers to improve combustion engines or to search for viable alternatives or to significantly improve the existing technology. One of such improvements is to supply hydrogen to a gasoline or Diesel fuel engine of a vehicle. Significant fuel savings can be achieved with low additional cost.

In this article, we deal with a vehicle equipped with an onboard hydrogen generator. We developed a computer program in order to estimate the required dimensions of such a hydrogen generator for a particular vehicle. The program consists of three modules, where the first of which simulates the Otto cycle of a four-stroke spark ignition gasoline engine. The second module calculates the important characteristics of a hydrogen generator that uses stainless steel plates as electrodes.

KEYWORDS

Energy and environmental systems, hydrogen energy, combustion

INTRODUCTION

In the wake of environmental problems associated with fossil fuels, engineers and scientists are seeking viable alternatives, that are both, economically and environmentally viable.

The manufacturers of automobiles in the industrial nations are working on alternatives to ICE vehicles, like electrical cars or fuel cell cars, while in countries like Mexico, the engineers are seeking to improve the combustion process to save fuel. One such fuel is hydrogen, because of its CO2-free combustion and high energy content. The drawback of hydrogen is, that its very low density makes it difficult to store. Numerous attempts were maid to generate hydrogen on the fly by use of hydrogen dry cells, that perform electrolysis of water to provide the hydrogen for immediate use.

Experimental studies have shown a reduction of gasoline consumption of up to 35 % in different climate conditions (see e.g. [2], [3]). These experiments used an onboard hydrogen generator that feeds into the intake manifold of a gasoline

Such an approach is promising yet not economically viable, due to various unsolved issues, which concern the safety, ease of use and long-term reliability of the hydrogen generators. Furthermore, there is a lack of long-term studies on the effects of the use of hydrogen on gasoline or Diesel engines.

The aim of this work is to provide a computer program, that can be adapted easily to a specific engine and a specific design of a hydrogen generator dry cell, in order to estimate the saving of fuel when HHO gas is supplied to the air intake of the engine. The program serves as a tool, how to construct the hydrogen generator cell to achieve the goals before physically building and experimenting with a specific hydrogen generator. This saves cost in the design process.

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COMBUSTION PROPERTIES

An ideal gas is assumed as working fluid, which is pure octane in our case. The combustion properties of gasoline are well studied, and we use the equations of [4] to compute the basic quantities (see also [5])

The equation of state (EOS) of the combustion process can be described as follows (see [2]):

$$PV_{u} = m_{u}R_{u}T\tag{1}$$

$$u_{u} = Cv_{u}T + hf_{u} \tag{2}$$

For the unburnt fuel-air mixture, whether P is the pressure, V_u is the volume of the unburnt fuel-air mixture, m_u is the mass of the unburnt fuel-air mixture, R_u is the gas constant and T the temperature, hf_u is the zero-degree-enthalpy for the unburnt gas mixture.

For the burnt fuel-air mixture the same equations apply, but now the quantities correspond to the burnt gas, which leads to the following equations.

$$PV_b = m_b R_b T (3)$$

$$u_b = Cv_bT + hf_b \tag{4}$$

Adding the equations for the gas before and after the combustion leads to the following equations, where the mass ratio x of the burnt (mb) to the total mass of the fuel (m) was introduced:

$$x = \frac{mb}{m} \tag{4}$$

$$PV = m(xR_b + (1-x)R_u)T = mRT$$
 (5)

$$U = mu = m(xCv_b + (1-x)Cv_u)T + xhf_b + (1-x)hf_u$$
(6)

U denotes the internal energy, lower case u denotes the specific internal energy, the subscripts u and b refer to the quantities for the unburnt and burnt gas, respectively.

MATHEMATICAL MODEL OF THE ENGINE

The engine is a four stroke Otto-Motor, where the crank wheel completes two full cycles (4π) . The first cycle is called the power cycle $(0 - 2 \pi \text{ crank angle})$, where the first stroke is the compression stroke. The valves are closed, and the fuel-air mixture is compressed $(0 - \pi)$. Then the fuel-air mixture is ignited, and the expansion stroke follows $(\pi - 2 \pi)$.

The second cycle (strokes 3 and 4) are called the gas exchange cycles, where the valves open, the burned gas is exhausted $(2 \pi - 3 \pi)$ and fresh air-fuel mixture is brought to the combustion chamber $(3 \pi - 4 \pi)$.

Since a constant angular velocity is assumed, the time can be expressed in terms of the crank angle. The volume of the combustion chamber can be described by the following equation (see [4]):



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$$v(\theta) = V_m \left(\frac{1}{r_c} + \frac{1}{2} \left(1 - \frac{1}{r_c} \right) \right)$$

$$\left(1 + \cos(\theta) + R_c - \sqrt{\left(R_c - \sin(\theta) \right)} \right)$$
(7)

 $v(\theta)$ is the volume at crank angle θ , R_c is the ratio of the connecting rod length to the stroke length, and r_c is the compression ratio.

The stokes can be described using two fundamental laws: 1. The law of mass conservation:

$$\frac{dm}{dt} = m'_{i} - m'_{e},\tag{8}$$

where m is the total mass of the working fluid, m'_{i} is the mass flow into the cylinder and m'_{e} is the mass flow out of the cylinder.

and 2. the conservation of energy:

$$\frac{dU}{dt} = Q' - W' + H'_{i} - H'_{e} \tag{9}$$

where dU/dt is the change of the internal energy over time, Q' is the heat rate, W' is the work rate, H'_i denotes the enthalpy flow rate into the cylinder and H'_e denotes the enthalpy flow rate out of the cylinder. For a more detailed mathematical description the reader is referred to [4],[5])

Fig. 1 and 2 show characteristic diagrams for Otto-engines. Fig. 1 shows the Otto cycle calculated with the characteristic quantities of the Nissan QR25 engine. Fig. 2 shows the pressure as a function of the crank angle θ for a complete four stroke cycle. Both diagrams are calculated at an engine speed of 2000 rpm.

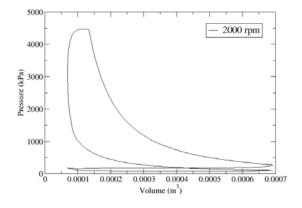


Fig. 1 Pressure Volume Diagram for the Nissan QR25 engine at 2000 rpm



HHO GENERATOR

To safe fuel a vehicle may be equipped with an HHO generator. Various designs have been proposed and are patented. For this study we use a generator of the type of dry cell. The design principle is outlined in Fig 1.), see also [6]

The generator implements the electrolysis of water, where various substances can be added to enhance the hydrogen production. A detailed study of such generators and electrolytes is beyond the scope of this study. The generator assumed for this study is a dry cell, where the electrodes are not submerged in the electrolyte but rather the electrolyte flows through holes in the electrolytic plates. The plates are sealed to prevent loss of the liquid.

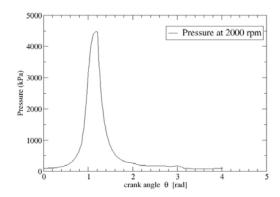


Fig. 2 Pressure versus crank angle diagram for the Nissan QR25 engine at 2000 rpm

The produced gas is fed to a bubbler, where the gas and the liquid separate. This serves also as a security feature to prevent backfire into the hydrogen generator itself, which may cause an explosion and damage the generator.

The production rate of HHO of the generator depends on the surface area of its electrolytic plates that is covered by liquid, and the electric current that is applied. The power supply for the generator comes from the vehicle itself, no external source of electric energy like batteries are required.

We adopt the design of [2] for calculating the hydrogen production rate and the volumetric and mass ratio of gasoline to hydrogen that is being injected in the combustion chamber of the motor.

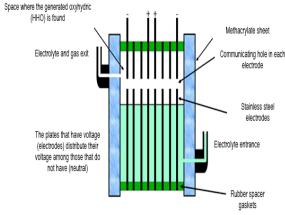


Fig. 3 Schematic view of the hydrogen generator dry cell. Source: http://hidrogenocomosolucion.wordpress.com/el-generador/)



STOICHIOMETRIC AIR FUEL RATIO

To guarantee a complete combustion an optimal fuel to air ratio is required. The supply of hydrogenoxygen gas mixture is limited by the design of the hydrogen generator. Optimal gasoline savings could only be achieved, if pure hydrogen is injected, but this requires large amounts of electric power for the electrolysis. Thus, a viable compromise must be provided.

Air contains 78% nitrogen, which is inert to the reaction in the ideal case. Experiments with both, pure gasoline, and dual fuel (gasoline + HHO), however have shown that Nitrogen-Oxygen compounds form, where more NO_x form when HHO is injected. The reduction of this pollutant is a challenge for the design of hydrogen combustion engines.

In our study we assume a chemical composition of the air as 21% Oxygen (O_2) and 79% (N_2) . We neglect other constituents, like Argon (Ar) or CO_2 .

Therefore, for a mixture of gasoline and air, the following stoichiometric equation holds:

$$C_x H_y + a(O_2 + 3.76N_2) \rightarrow bCO_2 + cH_2O + dN_2$$
(10)

The factor 3.76 is simply the ratio of N_2/O_2 of air (= 79 / 21), where a = x + y/4, b = x, c = y/2, d = 3.76*a. If the fuel is octane, then x = 8 and y = 18, a = 12.5, which reflects the ratio air / fuel, b = 8, c = 9, d = 47.

The equation then reads for optimal combustion as

$$C_8H_{18} + 12.5(O_2 + 3.76N_2) \rightarrow 8CO_2 + 9H_2O$$

+47 N_2 (11)

If *e* moles of hydrogen are added to the gasoline fuel, the equation becomes:

$$C_x H_y + a(O_2 + 3.76N_2) + eH_2 \rightarrow bCO_2 + cH_2O + dN_2$$
 (12)

where a = air/fuel ratio, e hydrogen/fuel ratio. We assume the same amount of air per mol of octane fuel is introduced into the combustion chamber, i.e., a = 12.5, and e = 0.125 mol of HHO from the generator is added to that mixture. Then, b = 8, c = 9.125, d = 47, and c = 8, c = 9.125, divided above. The equation then reads as:

$$C_8H_{18} + 12.5(O_2 + 3.76N_2) + 0.125N_2 \rightarrow (13)$$

 $8CO_2 + 9.125H_2O + 47N_2$

We assume that the combustion is ideal and all of the introduced HHO gas is burned to H_2O .

PROGRAM

The programming language GDL (GNU data language, [7]) was used, which is a free clone of the Interactive Data Language (IDL) [8]. Its syntax is based on FORTRAN and it offers convenient



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handling of arrays and convenient plotting routines. The program is composed of three modules, flowcharts of each module are shown in Fig. 4 - 6. Each module can operate independently.

First, we want to calculate basic quantities of the engine itself. Therefore, we used the program developed in [1] and adapted to the Nissan QR25 engine as a starting point.

The engine is a four-stroke spark ignition (SI) machine, based on the Otto principle. Basic parameters of the motor are taken from [1] and listed in Table 1, and the results for the Nissan QR25 engine are listed in Table 2.

The second module calculates the HHO production for a specific design, as well as an estimate of the power consumption by the intended design of the generator. The generator should provide sufficient HHO gas and should not consume to much power, so that the desired fuel savings can be achieved.

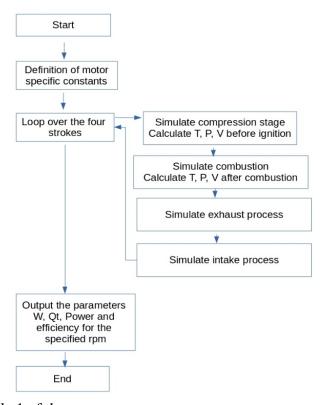


Fig. 4 Flowchart of Module 1 of the program

The input parameters for the second module are listed in Table 3. Here plate sizes and numbers of electrolytic cells can be varied to find a suitable production rate of hydrogen. An efficiency of the electrolysis is assumed as 60%, which is taken from [2]. The real efficiency depends on the solution, which is used and on various other parameters. Thus, a measurement of the efficiency on a real hydrogen generator is advised. The results are given in Table 4.

The third module calculates the stoichiometric reaction for the ideal case of combustion. The input parameters are, apart from the cylinder volume of the motor, moles of octane and moles of hydrogen. It calculates the mass ratio and volumetric ratio of hydrogen to gasoline and evaluates the stoichiometric equations. An eventual rest of atoms, that are not burnt ideally are calculated.

For our test case, we use one mole of octane and 0.125 moles of HHO as input. Different combinations can be tried to adjust for the production rate of the hydrogen generator.

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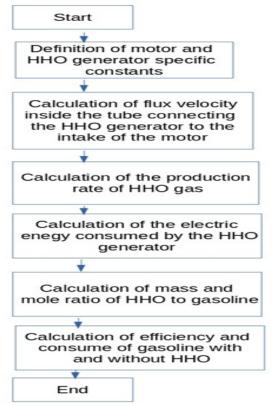


Fig. 5 Flowchart of module 3 of the program

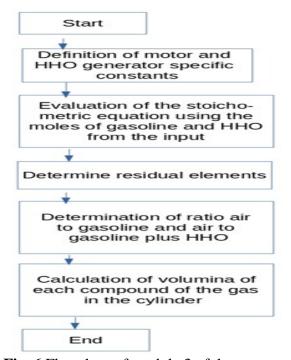


Fig. 6 Flowchart of module 3 of the program



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Table 1: Input parameters of the Nissan QR25 gasoline engine for the simulation program

Parameter	Value	Unit
Compression Ratio	10	
Stroke	100	mm
Displacement Volume	2488	cm ³
Bore	89	mm
Valves per Cylinder	4	-
Cylinders	4	-
Engine speed	2000	rpm

Table 2: Output of the simulation module

RPM	Power [kW]	Efficiency [%]	Work [KJ]
1000	6.11	0.43	0.73
2000	12.33	0.48	0.74
3000	17.48	0.55	0.70
4000	19.37	0.66	0.58
5000	18.07	0.72	0.43

Table 3: Input for the hydrogen generator type dry cell

Input quantity	Value	Unit
Length of charged Plate	6	cm
Width of one plate	14	cm
Strength of plate	0.1	cm
Width of neutral Plate	12	cm
Width of a cell	0.2	cm
Number of cells	15	-
Total of charged plates	6	-
Total of neutral plates	10	-

Table 4: Results of the second module

Parameter	One plate / cell	Total
Area of a charged plate	84 cm ²	504 cm ²
Area of a neutral plate	72 cm ²	720 cm ²



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Area of plates in contact with solution	-	969 cm ²
Volume	11 cm ³	165 cm ³
H production (ideal case)	78.284 cm ³ /min	1174.263 cm ³ / min
O production (ideal case)	39.142 cm ³ /min	587.131 cm ³ / min
H production 60% efficiency	-	704.558 cm ³ / min
O production 60 % efficiency	-	352.279 cm ³ / min
Electrical energy consumption	-	78.68 Wh
Consumption of gasoline without HHO		86.692 g/Kwh
Consumption of gasoline with HHO		67.875 g/KWh

RESULTS

We compare the gasoline consumption of our vehicle when using a HHO generator to the same vehicle without such a device. The module of our program provides us with the basic characteristics of the engine in question. Table 2 lists the output power, the efficiency and the work delivered by the engine without the use of HHO gas. These values are calculated for five engine speeds, that representative for the usual working range of this engine. The maximum power of the engine is achieved at rpm between 4000 and 5000 rpm.

The the second module of our program provides us with the HHO gas yield of the envisioned HHO generator. Based on this rate of HHO gas production we estimate the fuel savings. Table 4 lists the effective area in contact with the solution (in this case water). The resulting production rates of HH and O are listed for the ideal case and for a more realistic assumption of 60% efficiency of the electrolysis. The cost in terms of consumption of electric power. For a yield of approx. 1060 cm³ / min of HHO gas we expect a consumption of 78.68 Wh electrical energy.

The consumption of gasoline, where 1060 cm³ / min of HHO gas is injected to the air intake of the engine leads to a decrease in the fuel consumption from 86.7 g/KWh to 67.9 g/KWh, which corresponds to a saving of fuel of 21.7%.

The third module is intended to help adjust the molar ratio of HHO gas to gasoline, in order to optimize the combustion. It indicates residual compounds if the combustion is not optimal.

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CONCLUSIONS

In this study, we assume a vehicle, a Nissan NP300 equipped with a gasoline engine (QR25), with the aim to save gasoline fuel by adding Hydrogen to the air intake. The engine is a four-stroke spark ignition Otto engine. The Hydrogen to be supplied to the combustion chamber is produced onboard by a dry cell hydrogen generator, that produces the hydrogen just in time. This approach avoids the difficulties associated with hydrogen tanks. In our example, we expect a fuel saving of 21.7%.

We describe a computer program, written in the language GDL intended to estimate expected fuel saving of an additional HHO generator. The focus is put on the implementation of the basic equations of the combustion in an internal combustion engine, type four stroke Otto-Motor. The expected rate of hydrogen production and the stoichiometric equations are computed by the program. This allows designers to find an optimal design that yields sufficient hydrogen to meet the intended goal of gasoline savings, while the electric power consumption of the hydrogen generator being acceptable.

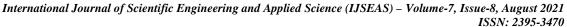
The program described in this work can be easily adapted for other four stroke Otto-motors by supplying the characteristic quantities as input. Additionally, the intended design of the hydrogen generator can be evaluated and adjusted to optimal yield before it is assembled physically.

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Miguel Toledo-Velázquez. Received his M.S degree

in Mechanical Engineering from the National Polytechnic Institute of Mexico (IPN) and his Ph.D. degree in Mechanical Engineering from the Hannover University. Founder and chief of the LABINTHAP (Thermal Engineering and Hydraulics Applied Laboratory) at IPN (1990-1996). Director of the School of Mechanical and Electrical Engineering Unit Culhuacan (1998-2001) and director of the AMIME-ASME Mexico (2004-2006). Since 1974, he has been research professor at the





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National Polytechnic Institute of Mexico. He is member of the National Researchers System of Mexico (SNI). His research interests are in the areas of energy, turbomachinery, gas turbines, steam turbines, axial compressors, thermal fluids and wind energy.

Markus Hareter received his M.S. and his Ph.D. in Astronomy at the University of Vienna. From 2013 to 2014 he was post-Doc researcher at the Konkoly Observatory of the Hungarian Academy of Sciences, Budapest. Currently, he holds a post-Doc position at the Universidad Autonoma Metropolitana (UAM) Campus Azcapotzalco, Mexico City.