

# Analyzing Performance and Emissions of Diesel and Hydrogen Fuels in a Combustion Nozzle - Using Computer Numerical Techniques

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**Abstract** – Analyzing the performance and emissions of Diesel and Hydrogen Gas in a combustion nozzle has become an area of interest for researchers and manufactures. Aiming for a sustainable development, where economic and environmental issues are of high importance. This paper discusses the partial rather than complete introduction of Hydrogen fuel, in combination with Diesel fuel.

**Methodology**; This paper uses numerical software tools in analyzing various Hydrogen gas percentages added to Diesel in a combustion process.

Results were obtained for; energy output and temperature of exhaust gas. Emissions such as; Carbon Dioxide, Carbon Monoxide, and Nitrogen Oxides, were also recorded and analyzed. Equations were derived relating the mentioned quantities, avoiding length stoichiometric calculations. Accuracy of equations was assessed on statistical basis.

Conclusion shows how numerical combustion software tools can be used to produce simple equations to calculate the output of a combustion process, avoiding lengthy traditional stoichiometric calculations. The benefits of gradual rather than complete introduction of Hydrogen fuel were discussed.

**Keywords** – Combustion Computer Numerical Analysis, Sustainable Energy, Environment, Hydrogen, Diesel.

## I. INTRODUCTION

The addition of Hydrogen to Diesel in a combustion process has become an area of interest for researchers and manufacturers. Investigating in how to improve power output and environmental impact. With the known facts of non-existing Hydrogen combustion by-product pollutants. Manufacturers and end users are ever becoming more interested in this technology. However, limiting factors imposed by the non-existing Hydrogen fuel infrastructure, remain as obstacles in the way of Hydrogen fuel development.

Combustor nozzles of different characteristics are used in gas turbines, and water heating boilers, naming two examples. Optimizing performance and reducing emissions in such combustion processes can impact in a positive way the two mentioned industrial examples.

This research utilizes established numerical combustion software tools. The aim is to demonstrate the effect of Hydrogen dosage on energy output, temperature and exhaust output pollutants. Graphical contour pictures and graph plots were generated to provide a visual assessment of the combustion process at different percentages of injected Hydrogen.

Graphically displayed results in pictures and graphs were used in discussions. Curve fitting techniques were employed to mathematically describe the relationship between Hydrogen and Diesel fuel in a non-premixed

combustion process. The developed equations cover the following in relation to Hydrogen dosage; Total Energy output, Total Temperature output, Carbon monoxide, Carbon dioxide, and Nitrogen Oxides. Integrity of equations developed by using curve fitting techniques was statically assessed for integrity.

## II. EFFECTS OF ADDING HYDROGEN TO DIESEL IN A COMBUSTION NOZZLE

In this section background discussion on the usage of Hydrogen fuel, are conducted first, and then the effects of gradual introduction of Hydrogen as an alternative fuel are discussed. This paper focuses on gradual introduction with Diesel fuel, rather than just Hydrogen fuel as an alternative fuel, for the reasons discussed below.

## III. DISCUSSION ON HYDROGEN AS AN ALTERNATIVE FUEL

Using Hydrogen as a combustion fuel has its advantages, with no polluting by products. However, a number of restrictions have and continue in preventing the progress of Hydrogen as an alternative fuel. Examples of restrictions: -

a. Though Hydrogen is the most common element in the universe, on earth Hydrogen atoms are mainly bound with other elements. Energy is required to separate Hydrogen atoms from the bound-to-elements, and then use Hydrogen as a fuel. An example of this is splitting water into its common parts; Hydrogen and Oxygen.

b. Cost is a hurdle in using hydrogen widely as a fuel, according to Michael Hordeski [1]. Changes in the energy infrastructure are needed to use hydrogen. Electricity is required for many hydrogen production methods. The cost of this electricity tends to make hydrogen more expensive than the fuels it would replace.

c. Hydrogen's flammability is a major safety risk. Hydrogen can ignite in low concentrations and can leak through seals. Leaks in transport and storage equipment can be hazardous to the public safety. These are the practical considerations that need to be addressed before wide-scale use of hydrogen becomes a reality. Researchers are developing new technologies that can use hydrogen that is stored or produced, as needed, onboard vehicles and transport systems. These technologies include hydrogen internal combustion engines, which convert hydrogen's chemical energy to electricity using a hydrogen piston engine coupled to a generator in a hybrid electric vehicle. Onboard restructuring for fuel cells, using catalytic

reactions to convert conventional hydrocarbon fuels, such as gasoline or methanol, into hydrogen that fuel cells use to produce electricity to power vehicles.

d. Unlike internal combustion engines, hydrogen fuel cells do not emit carbon dioxide. But according to Michael Hordeski [1], extracting hydrogen from natural gas, gasoline or other products requires energy and involves other by-products.

Obtaining hydrogen from water through electrolysis consumes electric energy. Electric energy can be generated via; nuclear, hydrocarbon or solar means. The only way to avoid a clean production of Hydrogen gas is to use electrolysis where electricity used in electrolysis is produced by solar means.

e. Building a Hydrogen Infrastructure. Current fuel infrastructure; beginning with transport of crude oil, refining, transporting to petrol stations or power plant has been based on hydrocarbon fuels. To create suitable infrastructure to support the usage of Hydrogen fuel will need a new infrastructure.

The Center for Energy Environmental and Economic Systems Analysis at Argonne National Laboratory near Chicago estimates that building a hydrogen economy would take more than \$500 billion, as presented by Michael Hordeski [1].

Storing Hydrogen fuel can be either in its gaseous form consuming large amount of storage space, or in liquid

form which needs special storage conditions. An example of this given by Michael Hordeski [1]; The GM liquid-fueled HydroGen3 goes 250 miles on a tank about twice of size of a typical gasoline tank. The car must be driven every day to keep the liquid hydrogen chilled to -253°C or it boils off.

f. Sources of H<sub>2</sub> production:

Table (a) shows current production sources of Hydrogen, given in Michael Hordeski [1].

Origin	Percent (%)
Natural gas	48
Oil	30
Coal	18
Electrolysis	4

Starting with a hydrocarbon based fuel; high temperature steam is used to separate Hydrogen from Carbon. If the cost of the natural gas is \$4 per million British thermal units (MMBtu), the cost of the gaseous hydrogen will be about \$10.00 per MMBtu. If the hydrogen is liquefied, an additional \$8.00 to \$10.00 per MMBtu must be added to the cost of the gaseous hydrogen, making the cost of liquid hydrogen produced by this method about \$20.00/MMBtu. If hydrogen is manufactured from water with electrolysis

Table 1. Data Inputs for Numerical Analysis and Results

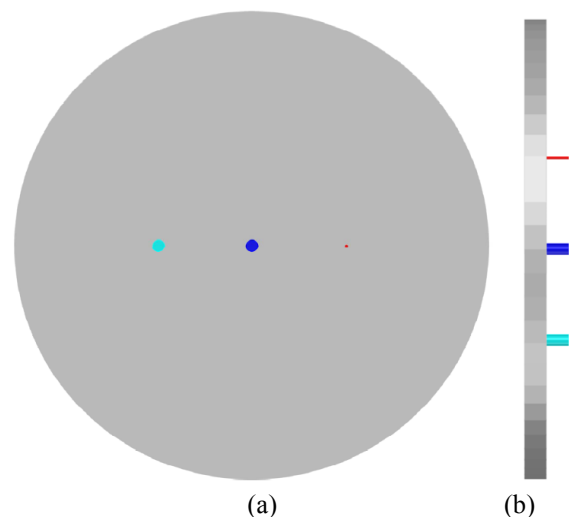
Air kg/s (lb/s)	Diesel kg/s (lb/s)	%	H <sub>2</sub> kg/s (lb/s)	Condi tion	Total Energy J/kg (Btu/lb)	Total Temp K	CO <sub>2</sub>	CO	NO <sub>x</sub>
0.0145 (0.032)	0.001 (0.0022)	0	0	Min	-	297.99	0	0	0
1.48e-02 (3.27e-02)	9.90e-04 (21.8e-04)	1	1.00e-05 (2.2e-05)	Max	438894.2 (189)	2269.37	0.171174	0.145827	0.00055
1.49e-2 (3.28e-02)	9.80e-04 (21.61e-4)	2	2.00e-05 (4.4e-05)	Min	-1529758 (-659)	298	0	0	0
1.55e-02 (3.41e-02)	9.50e-04 (20.94e-4)	5	5.00e-05 (11e-05)	Max	961962 (414)	2363.27	0.156	0.151	0.0054137
1.65e-02 (3.63e-02)	9.00e-04 (19.84e-4)	10	1.00e-04 (2.2e-04)	Min	-1520854 (655)	298	0	0	0
1.74e-02 (3.84e-2)	8.50e-04 (18.74e-4)	15	1.50e-04 (3.3e-04)	Max	2217545 (955)	2368.34	0.170	0.151	0.0045625
1.84e-02 (4.07e-02)	8.00e-04 (17.64e-4)	20	2.00e-04 (4.4e-04)	Min	-1510947 (-651)	297	0	0	0
				Max	2241187 (965)	2383.47	0.158	0.151	0.0051221
				Min	-1492070 (-643)	297	0	0	0
				Max	2341960 (1009)	2402.41	0.140	0.150	0.0052961
				Min	-1473853 (-635)	293	0	0	0
				Max	2607940 (1123)	2414.33	0.123	0.146	0.0053608
				Min	-1453636 (-626)	292.77	0	0	0
				Max	3116242 (1342)	2399.92	0.108	0.135	0.00424478

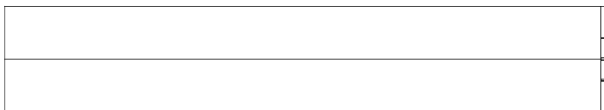
The first four columns from left represent data entered in the numerical combustion software. The six columns to the right refer to data obtained from numerical combustion software. Above data was used to plot the graphs shown in Figs 6 to 10.

Table 2: Expected CO<sub>2</sub> Data – Theoretically

Maximum CO <sub>2</sub> %	Air Values			
	0	0	60%	
Hydrogen	0	0	0	0
Liquid fuel No 1 and 2	15	12.3	10.5	9.1

Data obtained from ASHRAE 2009 [2]. Percentage CO<sub>2</sub> decreases as excess air increases. *Liquid fuels No 1 and 2, are similar to Diesel fuels grades; 1-D and 2-D respectively with the exception of the cetane number which is part of the Diesel specification.*





(c)

Fig.1. Drawing showing a disk with three injectors; Air injector in the middle in blue color, 5 mm (0.2 inch) in diameter. To the right the Diesel injector marked in red color, 1mm (0.04 inch) in diameter. And to the left Hydrogen fuel gas injector in light blue color, 5 mm (0.2 inch) in diameter. View (a) represents top view, and (b) side view. View (c) represents the cylindrical form, 1000 mm (40 inch) in length of meshed combustion flame, shown in Fig 2.

equipment, its cost is roughly equivalent to \$5 / MMBtu per 10 mills (\$5/kWh/cent/kWh), details from Michael Hordeski [1].

The above table shows that current production practices of Hydrogen do actually contribute to the depletion of fossil fuels and can increase the carbon footprint. With the exception of electrolysis if solar or nuclear powered electric energy was the source of electric energy.

Considering the above mentioned challenges, the sudden switching to Hydrogen fuel is clearly not feasible at present. Therefore, a gradual shift towards Hydrogen fuel might be more practical. Such as the gradual introduction of Hydrogen fuel in a combustion process with another fuel. This is the main reason behind this research paper. Gradually introduce Hydrogen fuel with Diesel, and study the benefits.

#### Hydrogen dosing - effects

Recent research in Hydrogen / Diesel internal combustion engines, indicate; improved energy output, completed Diesel combustion, and higher combustion temperatures. However, higher combustion temperatures are known to cause an increase in NO<sub>x</sub> emissions, as discussed in section IV of this paper. In general higher temperatures and the displacement of carbon elements with Hydrogen can reduce the presence of CO and CO<sub>2</sub> in the combustion output. Thus reducing the amount of wasted un-burned fuel flowing in a relatively fast flow combustion flow rate. The advantages in having higher combustion temperatures are clear. The aim will be and as shown in section IV is to optimize the combustion process in energy production.

In this paper the numerical combustion analysis was aimed to investigate such fuel mixtures in a combustion nozzle. With no external pressure applied to the combustion process, as in the case of an internal combustion engine. Emissions were recorded and tabulated.

Various Hydrogen gas percentages by mass were carried out. Starting with; 0, 1, 2, 5, 10, 15, and 20% in equivalent mass of displaced Diesel fuel.

Combustion air requirements were calculated on the basis of Air to Fuel ratios for each fuel type.

### III. CALCULATIONS AND METHODOLOGY

This section is divided into two parts.

In preparing data for numerical software analysis; Table 1 was produced starting with an assumed 0.001kg/s (0.0022 lb/s) Diesel mass flow rate, without H<sub>2</sub>. The next row of data in table 1, represent; 9.9e-4 and 1e-5 kg/s (21.78e-4 and 2.2e-5 lb/s) of Diesel and H<sub>2</sub> fuels respectively. An example of these calculations can be seen below. Data in table 1 was completed as explained. Refer to the four columns to the left of table 1.

Amount of air in kg/s for combustion requirements was calculated as shown in the following example;

Note: Chemical formula for common diesel fuel is C<sub>12</sub>H<sub>23</sub>. Diesel fuels can range approximately from C<sub>10</sub>H<sub>20</sub> to C<sub>15</sub>H<sub>28</sub>. In this example C<sub>12</sub>H<sub>23</sub> was selected from Fluent fuels data base. This range is divided in ASTM into three grades of diesel oil; 1-D, 2-D, and 4-D, ASHRAE 2009 [2].

Air to Fuel ratio for Hydrogen gas in this case is 34.28:1, ASHRAE 2009 [2].

Air to Fuel ration for Diesel 14.5:1, from Wikipedia.

1% of Diesel in mass calculated as follows: -

$(1 \div 100) \times 0.001\text{kg/s} = 1\text{e-}5$  (2.2e-5 lb/s), this represents the mass which will be replaced by Hydrogen gas or H<sub>2</sub> in this example.

Remainder Diesel after replacing 1% in mass with H<sub>2</sub>, gives;

$0.001 - 1\text{e-}5 = 9.9\text{e-}4\text{kg/s}$  (21.78e-4 lb/s) of Diesel.

Air required for H<sub>2</sub> combustion;

$$34.28 \times 1\text{e-}5 = 34.28\text{e-}5 \text{ kg/s} \quad (1)$$

Air required for Diesel combustion;

$$14.5 \times 9.9\text{e-}4 = 0.0145 \text{ kg/s} \quad (2)$$

Total air required for combustion by the two fuels mentioned above, add (1) and (2), gives;

$$34.28\text{e-}5 + 0.0145 = 0.01484 \text{ kg/s} (0.03265 \text{ lb/s}).$$

Details of combustor nozzle model can be seen in Fig 1.

Assumptions made in the Fluent software tools; all parameters at the setup stage were kept at default. With the exception of the following;

P1 = P1 Radiation Model,

k epsilon = a common turbulence model with default settings, and also for inlets and outlets boundary conditions,

Non-adiabatic analysis,

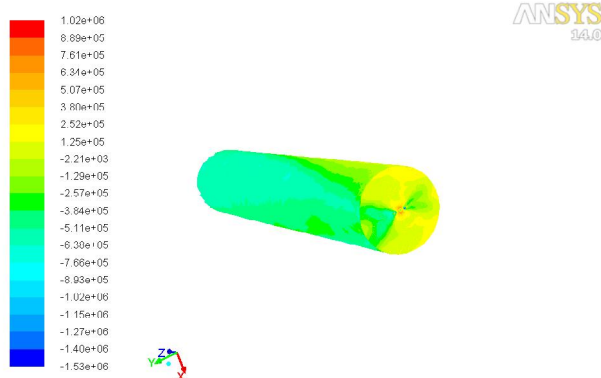
Select Standard Initialization in the Initializations Task Page.

Fuels and air entering temperatures = 300K.

Medium sized mesh was selected using automatic meshing.

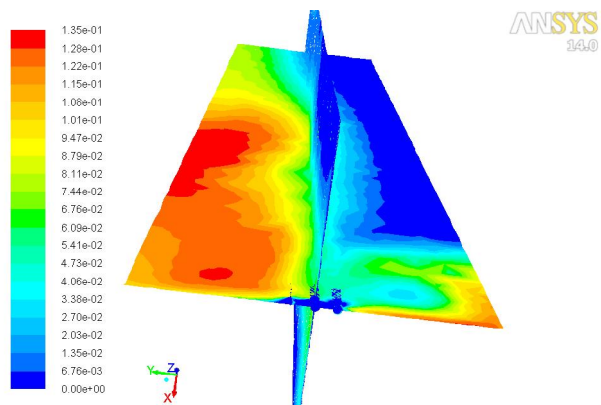
### IV. RESULTS AND DISCUSSIONS

Examples of graphic results can be seen in Figs 2 to 5 showing the software contour plots for 1% and 20% Hydrogen injection. Covering the combustion output in terms of; CO, CO<sub>2</sub>, and NO<sub>x</sub> mass fractions. Graph plots can be seen in



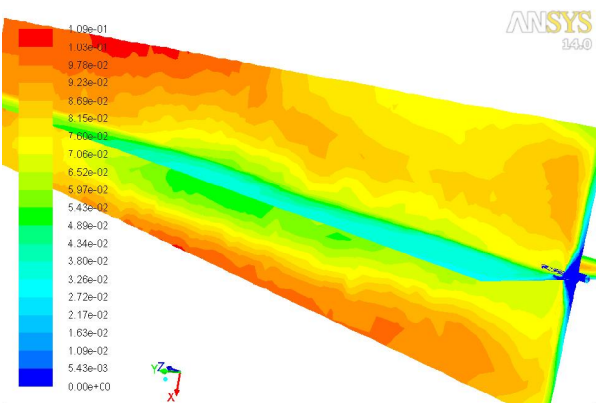
Contours of Total Energy (J/kg) Nov 17, 2013  
ANSYS FLUENT 14.0 (3d, dp, pbns, pdf20, ske)

Fig.2. Graphical display of Total Energy for a 1% Hydrogen injected separately with Diesel fuel in a combustion process, within a cylinder. The middle injector represents the air inlet. Injector to the right represents the Hydrogen injector. To the left the Diesel injector can be seen



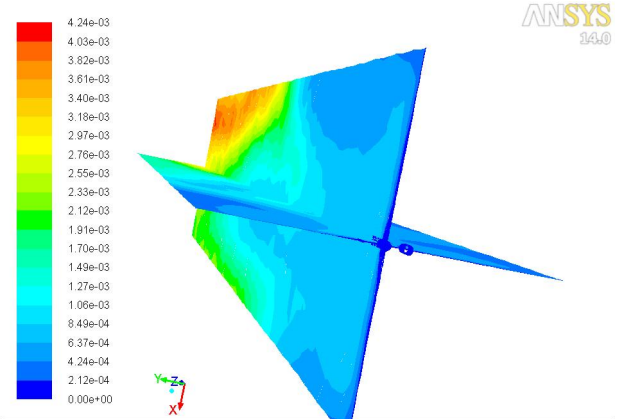
Contours of Mass fraction of co Nov 13, 2013  
ANSYS FLUENT 14.0 (3d, dp, pbns, pdf20, ske)

Fig.3. Graphical display of CO mass fraction with 20% Hydrogen dosage. The middle inlet represents the air inlet. To the right the Hydrogen injector. To the left the Diesel injector. Longitudinal sectional planes were captured to view the internal combustion process.



Contours of Mass fraction of co2 Nov 13, 2013  
ANSYS FLUENT 14.0 (3d, dp, pbns, pdf20, ske)

Fig.4. Graphical display of CO mass fraction without 20% Hydrogen dosage. Longitudinal sectional planes were captured



Contours of Mass fraction of Pollutant no Nov 13, 2013  
ANSYS FLUENT 14.0 (3d, dp, pbns, pdf20, ske)

Fig.5. Graphical display of NOx mass fraction with 20% Hydrogen dosage. Higher levels of NOx were observed this could be explained due to the effects of higher combustion temperatures as shown in Fig 10. Higher combustion temperatures can increase the levels of NOx mass fraction, as discussed in section IV.

Figs 6 to 10 representing data shown in the five columns to the right of table 1.

Notes:

Total Energy measured in J/kg of combustion output. CO, CO<sub>2</sub> and NO<sub>x</sub> measured as fraction of mass in the nozzle combustion output.

R<sup>2</sup>, or regression description.

Assessing integrity of formulas developed by regression. With a low R<sup>2</sup>= 0 none of the variances on the Y axis can be explained against % H<sub>2</sub> shown on the X axis. With high R<sup>2</sup>=1, all of the variances on the Y axis can be explained against % H<sub>2</sub> on the X axis.

Hydrogen fuel used in the following equations was represented by H<sub>2</sub> in percentage mass out of the equivalent Diesel fuel. Refer to table 1 for fuel mixture breakdowns.

Total Energy:

Total Energy increased as percentage H<sub>2</sub> increased in the fuel mixture. Reference is made to Fig 6.

Curve fitting techniques were employed using Excel 2010. A polynomial equation was developed as shown: -  

$$\text{Total Energy J/kg} = 26.901(\text{H}_2)^5 - 1502(\text{H}_2)^4 + 31288(\text{H}_2)^3 - 296761(\text{H}_2)^2 + 1\text{E}+06(\text{H}_2) + 322302$$

With a regression, R<sup>2</sup> = 0.9532. This represents a good level of curve fitting approximation.

The Total Energy increase can be explained due to the fact that Hydrogen fuel has a higher heating value, ASHRAE [2]; LHV 120,075MJ/kg (51.7 MBtu/lb), and HHV 142,107 MJ/kg (61.2 MBtu/lb). This compared with Diesel fuels which can be approximately 48MJ/kg (20.7 kBtu/lb).

Total Temperature:

Reference is made to Fig 7. The graph shows an increase in temperature starting from 0% Hydrogen and rising sharply towards 1% Hydrogen in mass. Then gradually increasing towards 15% in Hydrogen. A drop in

temperature was observed at 15% to 20% Hydrogen dosage. Equation developed;

$$\text{Total Temperature (K)} = 0.0629(\text{H}_2)^3 - 2.499(\text{H}_2)^2 + \frac{29.884(\text{H}_2) + 2302.4}{}$$

With a regression,  $R^2 = 0.7907$ . This represents an acceptable level of accuracy in curve fitting.

This increase in combustion temperature was expected and is due to the higher heating energy value, as discussed above.

*Carbon monoxide, CO by mass fraction:*

Reference is made to Fig 8. Employing curve fitting tools using Excel 2010 spread sheet. Equation developed as shown below;

$$\text{CO mass fraction} = -1\text{E-}06(\text{H}_2)^4 + 4\text{E-}05(\text{H}_2)^3 - \frac{0.0006(\text{H}_2)^2 + 0.0031(\text{H}_2) + 0.1468}{}$$

With a regression,  $R^2 = 0.9744$ . This represents a high level of accuracy in curve fitting.

The high spread of the red contour plots representing CO shown in Fig 3 was expected and is due to the presence of Carbon atoms in the Diesel fuel. This area is closer to the Diesel injector. The second explanation can be related to the lack of air supply. It is common practice in industry to provide excessive air supply for combustion. Higher A/F than specified in stoichiometric [2] calculations are recommended to allow for imperfect fuel mixtures. For maximum efficiency, combustion at low excess air is desirable according to ASHRAE [2]. Figure 3 indicates a lower CO level at the nozzle outlet, and therefore, an overall complete combustion of fuels.

*Carbon Dioxide, CO<sub>2</sub> by mass fraction:*

Reference is made to Fig 9. Employing curve fitting tools using Excel spread sheet. Equation developed as shown below;

$$\text{CO}_2 \text{ mass fraction} = -0.003(\text{H}_2) + 0.1697$$

With a regression,  $R^2 = 0.9505$ . This represents a high level of accuracy in curve fitting.

Contour plots of mass fraction for CO<sub>2</sub> show that concentration begins at the higher part of the nozzle and continues towards the outlet. The CO<sub>2</sub> concentration gradually drops as Hydrogen dosage increases, displacing Diesel mass and subsequently reducing the presence of Carbon atoms.

ASHRAE [2] provide information on how CO<sub>2</sub> can be reduced with excess air. In this example, and liquid fuels; No 1 and 2, are similar to Diesel grades; 1-D and 2-D with the exception of the exception of the cetane number which is an additional Diesel specification, according to ASHRAE [2]. Refer to table 2.

*Nitrogen Oxides, NO<sub>x</sub> by mass fraction:*

Reference is made to Fig 10. Employing curve fitting tools using Excel spread sheet. Equation developed as shown below;

$$\text{NOx mass fraction} = -8\text{E-}07(\text{H}_2)^4 + 3\text{E-}05(\text{H}_2)^3 - \frac{0.0005(\text{H}_2)^2 + 0.0025(\text{H}_2) + 0.0016}{}$$

With a regression,  $R^2 = 0.7064$ . This represents an acceptable level of accuracy in curve fitting.

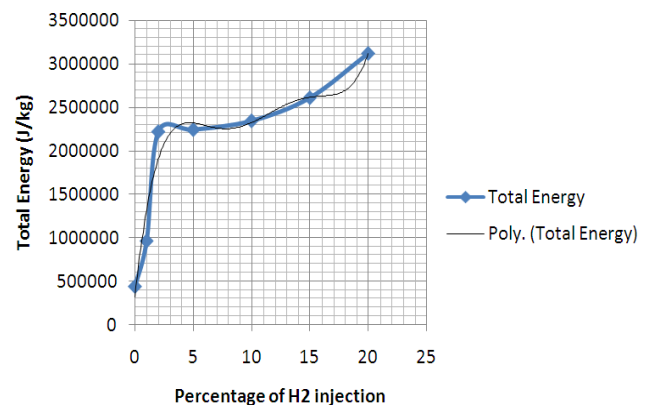


Fig.6. Graph of Total Energy against injected percentage 20% dosage.

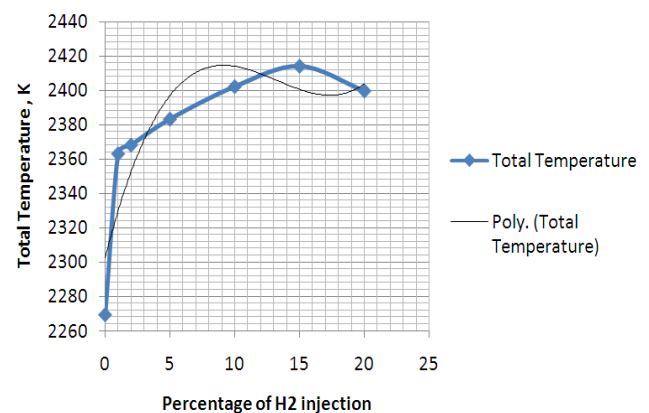


Fig.7. Graph of Total Temperature against injected percentage Hydrogen dosage.

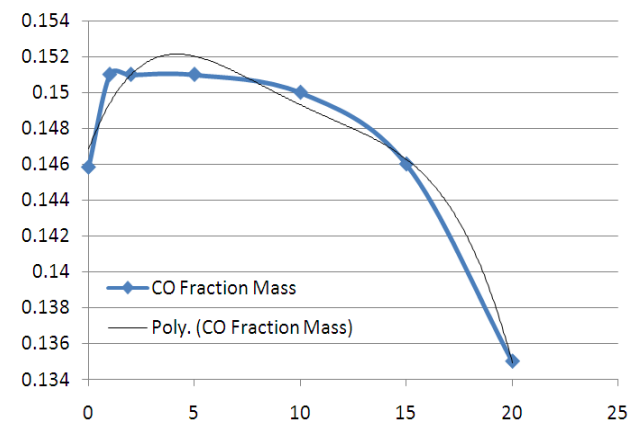


Fig.8. Graph of CO against injected percentage Hydrogen.

This is expected as increases in Hydrogen can cause the CO levels to decrease. Hydrogen fuel does not contain any Carbon atoms.

In general NO<sub>x</sub> concentrations are higher with Hydrogen dosing between 1% and 15%. Combustion reactions at higher temperatures produce nitrogen oxides [4]. Limiting the production of NO<sub>x</sub> can be done with a precise control of excess air in a combustion process, according to Wikipedia.

NO<sub>x</sub> concentration were observed at the upper part of nozzle and towards the outlet, as shown in Fig 5.

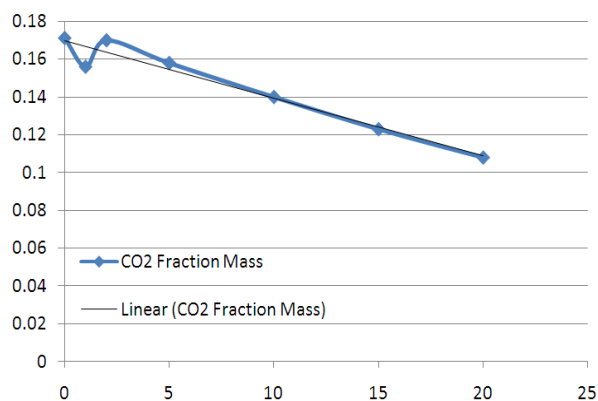


Fig.9. Graph of CO<sub>2</sub> against injected percentage Hydrogen. This is expected as increases in Hydrogen can cause the CO<sub>2</sub> levels to decrease. Hydrogen fuel does not contain any Carbon atoms.

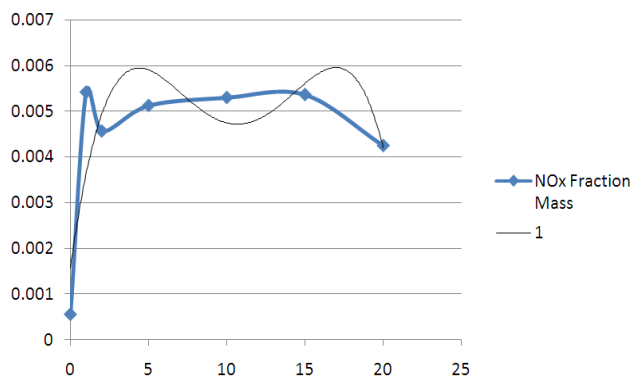


Fig.10. Graph of NO<sub>x</sub> against injected percentage Hydrogen. This increase in NO<sub>x</sub> was discussed in section IV.

## V. CONCLUSION

Software numerical combustion analysis showed that the total energy output per unit mass increases, as Hydrogen dosage increases. Relationship can be described in a polynomial form of equation. This energy increase per a unit mass of fuel can contribute to a reduction in Diesel hydrocarbon fuel consumption. That is if the source of Hydrogen fuel is non-hydrocarbon based.

Combustion temperature begins to increase as the percentage Hydrogen dosage increases. This is expected due to the comparatively higher energy heating value associated with Hydrogen, when compared with Diesel.

The analysis did show an improvement on the lowering of CO as Hydrogen dosage increases. This can be explained due to the fact that Hydrogen fuel does not contain Carbon atoms.

A drop in CO<sub>2</sub> levels was observed with higher Hydrogen dosage, for similar reasons as in the case of the observed CO reductions discussed above.

General increase in NO<sub>x</sub> omissions was observed. This is expected since NO<sub>x</sub> levels are known to increase as the combustion temperature increases.

With the aim of driving down pollutants such as; CO, CO<sub>2</sub>, and NO<sub>x</sub>, it was demonstrated that Hydrogen fuel can drive down the CO and CO<sub>2</sub> levels. On the condition that the source of Hydrogen fuel generation starts from non-Carbon based resources. That is Hydrogen generated by solar means or nuclear generated electricity used for electrolysis. Limiting the production of NO<sub>x</sub> can be done with a precise control of excess air in a combustion process.

## ACKNOWLEDGMENTS

The author would like to thank Dr. Lik F. Sim for setting up and providing access to the FLUENT software.

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- [2] ASHRAE Handbook Fundamentals chapter 28 – 2009.
- [3] wikipedia.org/wiki/Stoichiometric-Stoichiometry of Combustion.
- [4] wikipedia.org –Nitrogen dioxide–Safety and pollution considerations.

## NOTATIONS

C= Carbon. H<sub>2</sub> = Hydrogen. CFD=Computational Fluid Dynamics. ANSYS Fluent=CFD software brand. A/F=Air/Fuel ratio. Kg/s=kilogram per a second. mm=millimeter. m/s=meter per a second. 1inch=25mm. 1m/s=3.3 feet per a second. 1kg=2.2lb.

## AUTHOR'S PROFILE

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