NUMERICAL INVESTIGATION FOR EXHAUST GAS EMISSIONS FOR A DUAL FUEL ENGINE CONFIGURATION USING HYDROGEN AND COMPRESSED NATURAL GAS (CNG)

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ABSTRACT

A simulation for numerical analysis of internal combustion engines, both spark-ignited and compression-ignited systems, running on duel fuel of Hydrogen and any hydrocarbon developed is presented in this report. The program coded using Matlab is used to simulate various engine conditions and discern its effect on the emissions. The engine emissions, including species like NOx, CO, and CO_2, in accordance with the extent of hydrogen fraction, the equivalence fuel-air ratio, combustion equilibrium temperature and pressure are simulated. The paper focuses on simulation of exhaust emissions while using H-CNG blend. Simulation attempts to find an optimum extent of dual-fuelling, equivalence ratio, combustion temperature with regard to quality of emissions.

Key words:Hydrogen,Matlab,CNG,emissions etc

1. Introduction

Our history tells us one thing that all along the past men was consistently tending to go wrong, as if he always beholds to the Murphy's Law which says, 'if anything can go wrong, then it will'. Such an error made by man was his incorrect assessment on availability of petroleum fuels. Till the early 1970s, petroleum was considered as the eternal fuel source when it was realized that the petroleum-based fuels were dwindling fast and at the same time, the rate of consumption of these fuels was increasing at a much faster rate and this presents the trillion dollar quest today, for the best alternative fuel [1].Looking at this problem, we have a broader aim than just an alternative to the present fuels, but a better one in terms of its emissions. Considering the effect of global warming which has already made big impact giving us serious warning of its effects has led to the need for an alternative fuels which produce minimum emissions. But there also lies another big problem in terms of economic viability. So, taking all these factors, we look for an environment friendly, economically viable alternative fuel for the existing internal combustion engines.Over the years, liquefied petroleum gas (LPG), alcohols (both ethanol and methanol), compressed natural gas (CNG), Bio-fuels (including biodiesel), hydrogen and so many other fuels has been investigated as alternative fuels for both the spark ignition (SI) and compression ignition (CI)engines[1]. Performance studies were done in engines running on these fuels and many methods have been implemented to improve the emissions as well as engine performance. CNG is one fuel which had been able to replace gasoline in spark ignited engines. In order to reduce the emissions from these engines, lean burn strategy is being implemented. But this has a setback on the engine power output. It is clear that the lower flame speed of CNG significantly reduce the power output available. It has additional drawbacks as they are difficult to ignite, which results in misfire and increases un-burned hydrocarbon emissions, and wastes fuel. Adding hydrogen as a blend with CNG helps in reducing these defects. Hydrogen's high flame speed (high burning speed), low ignition energy makes the hydrogen-CNG mixture easier to ignite, thus avoiding misfire and improving the emissions [7]. It also improves the mixture's energy density at lean zone which improves the power output.

Far sighting the potential of H-CNG dual fuelling, studies have been done on various fields in view of developing this concept. It is, however a necessity that we have to optimize all the factors that affects the performance of the engine. Conducting experiments is the obvious way of doing this, but it always has its own limitations as many of the possible combination of factors may not be brought up practically. So, an intelligent way of doing this is by theoretical analysis.There was a time when analytical methods were time consuming and extremely challenging. But today, the scenario is different. With the development of technology, there are enormous and effective ways of theoretically analyzing situations. This paper attempt to numerically analyze the exhaust gas emissions from an engine run on duel fuel involving Hydrogen-CNG blends. The paper involves an indigenously developed simulation program with graphical user interface which is capable of calculating the mole fraction of different components in exhaust emission.

2. THE PROGRAM

The developed program is capable of simulating the effects of various factors, such as extent of dual-fuelling, the equivalence fuel-air ratio, combustion equilibrium temperature and pressure, on the emission properties as well as calculating the emission properties for a specific set of input values. The species which could be analyzed in the exhaust are CO, NO, CO_2, H_2O, O_2, H_2, O, H, OH and N_2.

For simulating the effects of input parameters on exhaust emissions, we considered three main input parameters, Temperature, equivalence ratio, and extent of dual fuelling, on the exhaust species CO, NO, and CO_2. Out of the different methods possible of simulating the effect, we found three-dimensional surface plots as the apt one in our analysis. In two-dimensional plots, when simulating the effect of two factors on output, there is a limitation that there can be only one variable factor and the effect of other has to be analyzed for various constant values. Surface plots give a wider scope of simulation, since in addition to what is possible in two-dimensional plots, we can simulate the effect of two factors, both being variables at a time on the exhaust properties. And this approach makes it more comparable with real engine simulations.

Table 1.Notations used

p	Number of carbon atoms in primary fuel
q	Number of hydrogen atoms in primary fuel
r	Number of oxygen atoms in primary fuel
s	Number of nitrogen atoms in primary fuel
t	Temperature (K)
x	Fraction of Hydrogen in blend
Pres	Pressure (atm)
equ	Equivalence ratio
sto	Stoichiometric fuel-air ratio
K	Equilibrium constant
ni	Concentration of 'i'th product

2.1 PROGRAM INTERFACE

A user friendly interface is given to the program as seen in **Fig.1** that enables the user to control the hydrocarbon fuel data (the number of Carbon, Hydrogen, Nitrogen, and Oxygen atoms), fraction of Hydrogen in the fuel blend, combustion conditions including equilibrium combustion temperature and pressure, and the equivalence fuel-air ratio. According to the user's choice, the output will be the mole fractions of the compounds CO_2, H_2O, N_2, O_2, CO, H_2, H, O, OH, and NO corresponding to the input set of values or the simulated change in mole fraction of the species with the change in input parameters.

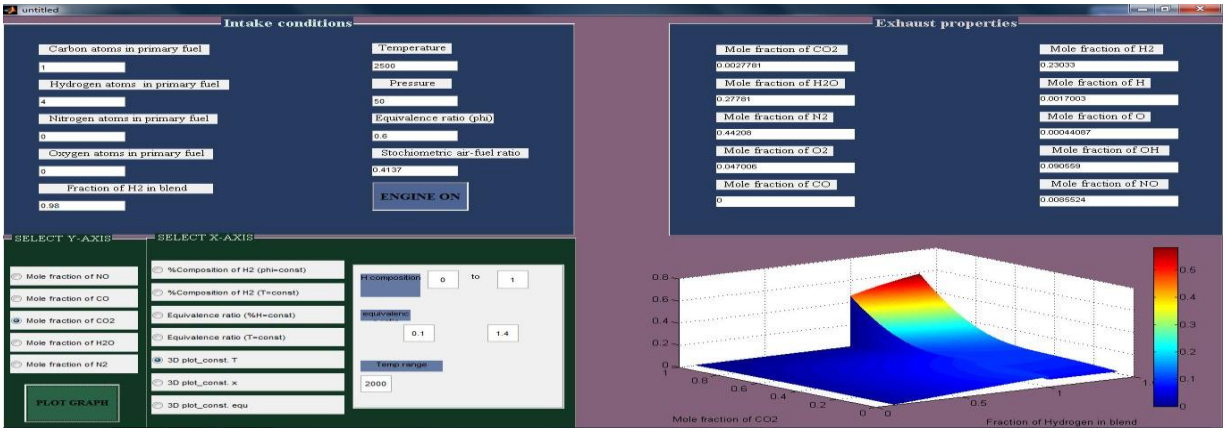

Fig.1: Interface of the program

3. SIMULATIONS

Mole fractions of NO, CO, H_2O, N_2 and CO_2 can be simulated against varying

- Extent of blending (fraction of hydrogen in blend) for five different values of combustion temperature with equivalence fuel-air ratio kept as a constant in a 2- dimensional plot.
- Extent of blending for five different values of equivalence fuel-air ratio with combustion temperature kept as a constant.
- Equivalence fuel-air ratio for five different values of combustion temperature with extent of blending kept as a constant.
- Equivalence fuel-air ratio for five different values of extent of blending with combustion temperature kept as a constant.

- Equivalence fuel-air ratio and extent of blending for a constant value of temperature in a three dimensional surface plot.
- Equivalence fuel-air ratio and Temperature for a constant value of composition of hydrogen in a three dimensional surface plot.
- Temperature and composition of hydrogen for a constant value of equivalence fuel-air ratio in a three dimensional surface plot.

4. Formation Of Equations

The program uses a modified version of equilibrium constant method applied by Olikara and Borman to find the solution for the properties of equilibrium gas phase products of combustion of Hydrocarbon fuels. [3] The coding is done for any general dual fuel blend involving hydrogen. The reactant mixture is a blend of a primary fuel of formula CpHqOrNs and H2 and air. Lagrange multiplier approach [3] is done with the help of NASA simulation program [5] to restrict the number of species to be considered in the equilibrium constant method. The data showed that if fuel-air ratio is less than 3, the only species of importance because of dissociation are O, H, OH, and NO. In accordance with the results, we considered only 10 products of combustion.

The combustion reaction is hence written as:

$$equ\times sto\times\{(1-x)\times C_pH_qO_rN_s+(x\times H_2)\} + (0.21\times O_2) +(0.79\times N_2) \rightarrow n_1CO_2 + n_2H_2O + n_3N_2 + n_4O_2 +n_5CO + n_6H_2 + n_7O + n_8H + n_9OH + n_{10}NO \quad (1)$$

Here, stoichiometric fuel-air ratio:

$$sto = 0.21\times\left(\frac{1-x}{p+0.25q-0.5r} + 2x\right) \quad (2)$$

Balancing of atoms leads to:

$$C: equ\times sto\times(1-x)\times p = n_1 + n_5 \quad (3)$$

$$H: equ\times sto\times(1-x)\times q + 2x = 2n_2 + 2n_6 + n_8 + n_9 \quad (4)$$

$$O: equ\times sto\times(1-x)\times r + 0.42 = 2n_1 + n_2 + 2n_4 + n_5 + n_7 + n_9 + n_{10} \quad (5)$$

$$N: equ\times sto\times(1-x)\times s + 1.58 = 2n_3 + n_{10} \quad (6)$$

Applying the following approximations, we developed the equations:

$$\text{For } equ < 1: n_5 = 0 \quad (7)$$

$$\text{For } equ > 1: n_4 = 0 \quad (8)$$

The equations of products for equivalence fuel-air ratio < 1 are:

$$n1 = (1-x)\times p\times equ\times sto \quad (9)$$

$$n2 = 1\times q\times equ\times sto/2 \quad (10)$$

$$n3 = 1\times 0.79 + (1-x)\times s\times equ\times sto/2 \quad (11)$$

$$n4 = (1)\times 0.21\times(1-equ) \quad (12)$$

$$n5 = 0 \quad (13)$$

$$n6 = 0.42x \quad (14)$$

And for equivalence fuel-air ratio > 1;

In this case, considering the equilibrium constant for the water gas reaction [3] and taking values from JANAF tables [7] we get the following equations:

$$K= e^{0.273 - (1.761 \div \frac{t}{1000}) - (1.611\div(\frac{t}{1000})^2) + (0.283\div(\frac{t}{1000})^3)} \quad (15)$$

$$a = 1\times(1-K) \quad (16)$$

$$b = (1-x)\times(0.42-equ\times sto\times(2-r) + k\times(0.42\times(equ-1)) + p\times equ\times sto) + x\times(0.42-2\times equ\times sto + K\times 0.42\times(equ-1)) \quad (17)$$

$$c = -(1-x)\times(0.42\times equ\times sto\times p\times(equ-1)\times k) \quad (18)$$

$$n_5 = \frac{-b\pm\sqrt{b^2-4ac}}{2a} \quad (19)$$

$$n_1 = (1-x)\times(p\times equ\times sto - n_5) + x\times n_5 \quad (20)$$

$$n_2 = (1-x)\times(0.42+equ\times sto\times(2p-r) + n_5) - x\times(0.42+n_5) \quad (21)$$

$$n_3 = (1-x)\times(0.79+s\times equ\times sto/2) + 0.79x \quad (22)$$

$$n_4 = 0 \quad (23)$$

$$n_6 = (1-x)\times(0.42\times(equ-1)-n_5) + 0.42x \quad (24)$$

Mole fractions of these products are found out using the equation:

$$y_i = n_i / \sum n_i \quad (25)$$

The six gas-phase reactions are introduced which include the dissociation of hydrogen, oxygen, water, carbon dioxide, and equilibrium OH and NO formation [3]. The equilibrium constants of these reactions [3] had been curve fitted to JANAF table by Olikara and Borman for $600 < t < 4000$ K. Their expressions are of the form:

$$\log_{10} K_i = A_i \times \ln\frac{t}{1000} + \frac{Bi}{t} + C_i + D_i \times t + E_i \times t^2 \quad (26)$$

The values of A, B, C, D, E are obtained from JANAF table [7].

The mole fraction of rest species are found out using these equilibrium constant values in accordance with the following equations:

$$y_7 = \frac{K_1}{pres^{0.5}} \times y_6^{0.5} \quad (27)$$

$$y_8 = \frac{K_2}{pres^{0.5}} \times y_4^{0.5} \quad (28)$$

$$y_9 = K_3 \times y_6^{0.5} \times y_4^{0.5} \quad (29)$$

$$y_{10} = K_4 \times y_4^{0.5} \times y_3^{0.5} \quad (30)$$

5. RESULTS

Simulations are done for CNG – H_2 fuel blend emissions under various conditions as discussed before. The results are presented below:

5.1 CO EMISSIONS

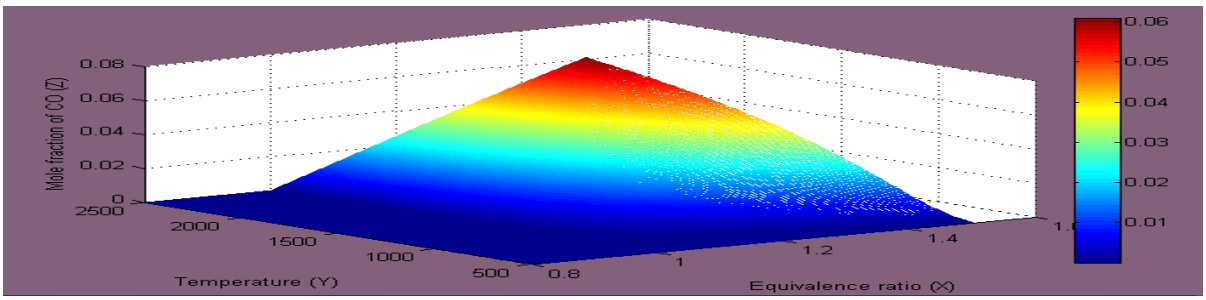

Fig.2: Effect of Temperature and equivalence ratio on mole fraction of CO for x=0.3

Fig.2 shows that for lean mixtures (equ<1), the CO emissions are negligible which is due to complete combustion of fuel. On the other hand for rich mixtures (equ>1), it can be observed that mole fraction of CO increases with increasing equivalence ratio. This can be attributed to the occurrence of incomplete combustion.

It can also be observed that CO emissions increase with increase in temperature. This result is due to the increase in dissociation of CO_2 at higher temperatures which boosts the formation of CO. It can be noted that the emissions of CO are more prevalent for T=2500K and equ=1.4 in the plot.

5.2 CO_2 EMISSIONS

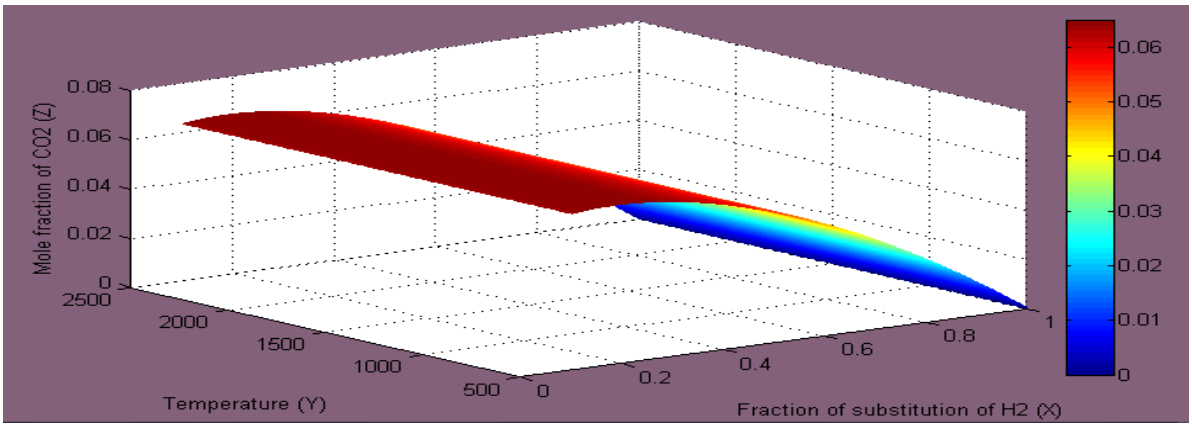

Fig.3: Variation of Mole fraction of CO_2 with change in Temperature and Hydrogen fraction at equ=0.3

In Fig.3, with increase in hydrogen fraction, CO_2 emissions decrease as the carbon content in the fuel (CNG fraction) is decreasing, for a lean mixture (equ=0.3). This trend was found to be the same for all other values of equ less than one. For the hydrogen fraction of 0.2, the value of CO_2 mole fraction is 0.06, and for 0.9 the value of mole fraction is 0.01, which gives an average decrease of 83%.

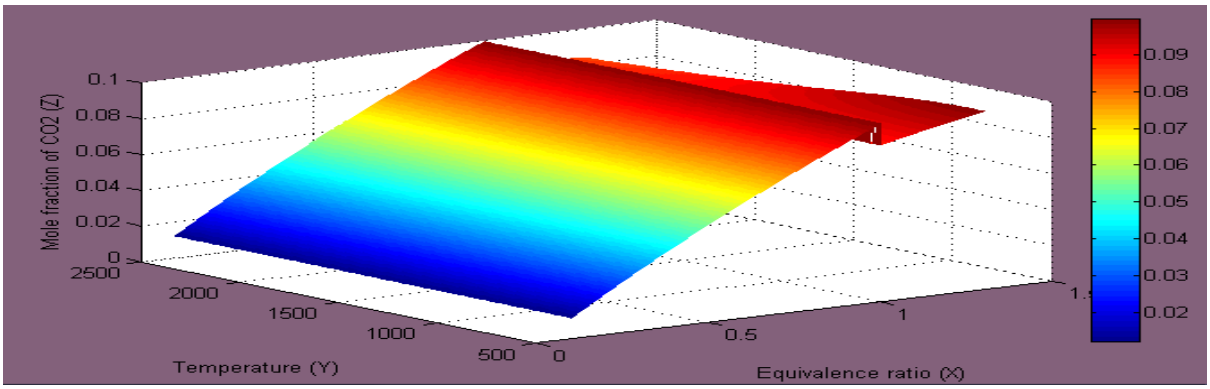

Fig.4: Effect of equivalence ratio and temperature on the mole fraction of CO_2 at x=0.3

In Fig.4, it can be observed that for lean mixtures, the mole fraction of CO_2 is almost independent on temperature. However, for rich mixtures it is seen that the mole fraction decreases with increase in temperature. From the plot, the mole fraction for T= 2500K is much less than T= 500K. This can be explained as temperature increases, dissociation of CO_2 increases which, on the other hand leads to the increase in mole fraction of CO, a product due to incomplete combustion of rich mixtures. It is also noticeable that mole fraction of CO_2 shows an increasing trend with increase in equivalence ratio, which can be accredited to the increase in carbon content (due to increased fuel content).

NO_X EMISSIONS

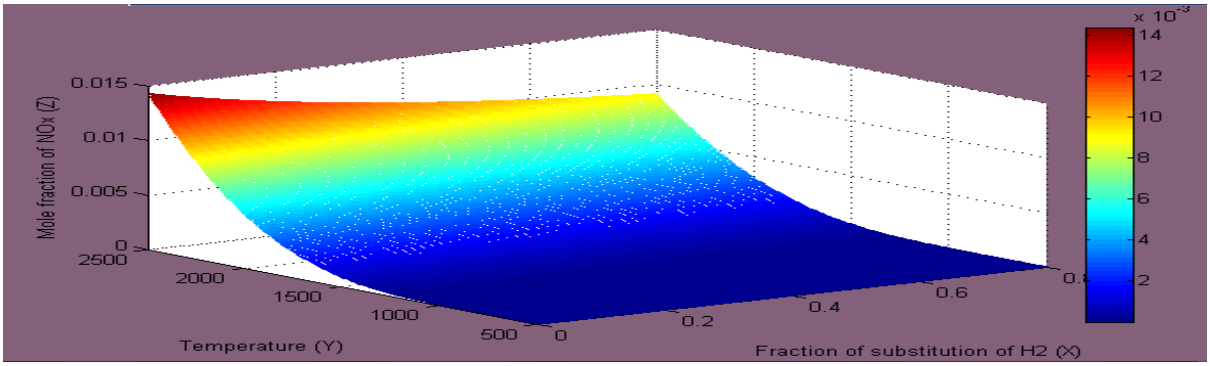

Fig.5: Effect of Temperature and Hydrogen fraction on mole fraction of NO_x at equ=0.6

The Fig.7 shows that for all hydrogen fractions, mole fraction of NO increases with increase in temperature. This is due to the very high dissociation energy of N_2 atoms which demands higher temperatures for its dissociation, which is in turn essential for NO formation. It can also be observed that for a fixed temperature, NO emissions show a slightly decreasing trend with increase in hydrogen fraction.

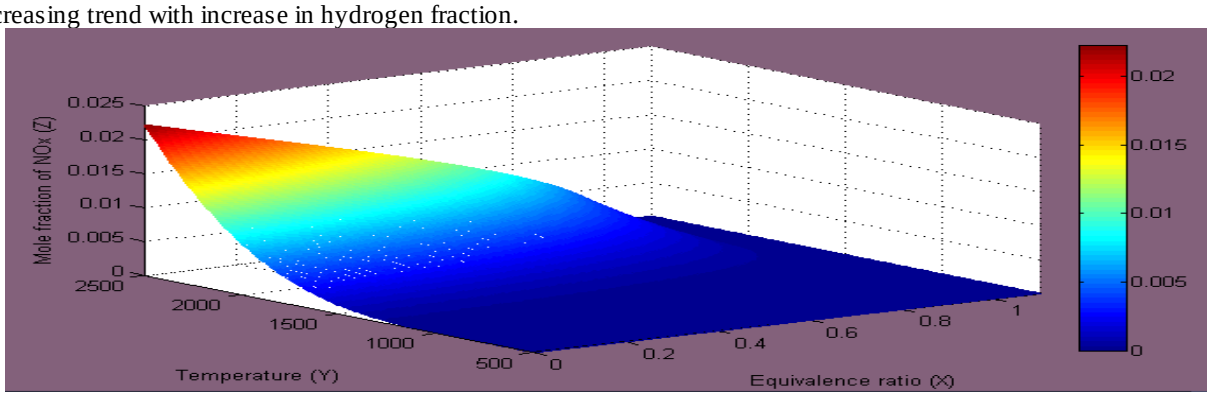

Fig.6: Effect of Temperature and equivalence ratio on mole fraction of NO_x

From the Fig.8, it is clear that effect of temperature on NO emission is consistent with the earlier result. It can also be observed that as equivalence ratio increases for a given temperature, NO_x emissions decrease. This can be explained by the decrease in availability of Oxygen with increase in equivalence ratio.

6. CONCLUSIONS

The results from the simulation were successfully verified with experimental values, which give credibility to the algorithm used. But there are many limitations to the program as it cannot be used for simulating very high temperatures (T> 3000K) due to the assumptions involved in derivation of the formula.

The effects of equivalence ratio, Temperature and Hydrogen fraction on emission of different species in an H-CNG blend can be concluded as follows:

- The emission of CO is negligible for lean mixtures and increases with equivalence ratio for rich mixtures. Also for rich mixtures, the CO emissions increase with increase in combustion equilibrium temperature.
- For lean mixtures, CO_2 emissions decrease with increase in hydrogen fraction and increase with increase in equivalence ratio. It is also independent on temperature for lean mixtures, but decrease with increase in temperature for rich mixtures.
- The emission of NO is negligible for rich mixtures and decreases with equivalence ratio for lean mixtures. NO emissions also decrease slightly with increase in hydrogen fraction. Also, the emissions increase with increase in temperature.

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