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Numerical Investigation for Exhaust Gas Emissions for a Dual Fuel Engine Configuration Using Diesel and Hydrogen

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ABSTRACT: *A SIMULATION FOR NUMERICAL ANALYSIS OF INTERNAL COMBUSTION ENGINES, BOTH SPARK-IGNITED AND COMPRESSION-IGNITED SYSTEMS, RUNNING ON DUAL FUEL OF HYDROGEN AND ANY HYDROCARBON FUEL 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-DIESEL BLEND. SIMULATION ATTEMPTS TO FIND AN OPTIMUM EXTENT OF DUAL-FUELLING, EQUIVALENCE RATIO, COMBUSTION TEMPERATURE FOR HYDROGEN-DIESEL BLEND WITH REGARD TO QUALITY OF EMISSIONS.*

Key Words*: Dual Fuel, Diesel Hydrogen, Numerical Investigation, Matlab*

I. Introduction

Our history tells us one thing that men always tends 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 diminishing 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, hydrogen and a horde of other alternatives were investigated as alternative fuels for both the spark ignition (SI) and compression ignition (CI) engines [1]. Among this, considering Hydrogen's work experience as fuel of the stars and its exceptional properties like high flame speed, high diffusivity, wide flammability limits, and high calorific value etc., researchers do have a glimpse of hope for it as the answer to the present quest. Hydrogen supplementation was done with fuels like diesel, petrol in order to exploit its properties. Results from Hydrogen supplementation to diesel show improvements in BTFC, Brake power, and emissions [2].

It is a necessity that we have to judge all the factors and its effects on the performance of the engine, when being run by alternative fuels. Conducting experiments is a way of achieving the above said, but it always has its own limitations since many of the possible conditions may not be realized practically. So, a better 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 advances in technology, there are enormous and effective ways of theoretically analyzing situations. This paper includes numerical analysis of the exhaust gas emissions from an engine run on dual fuel involving Hydrogen-Diesel 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.

II. 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.

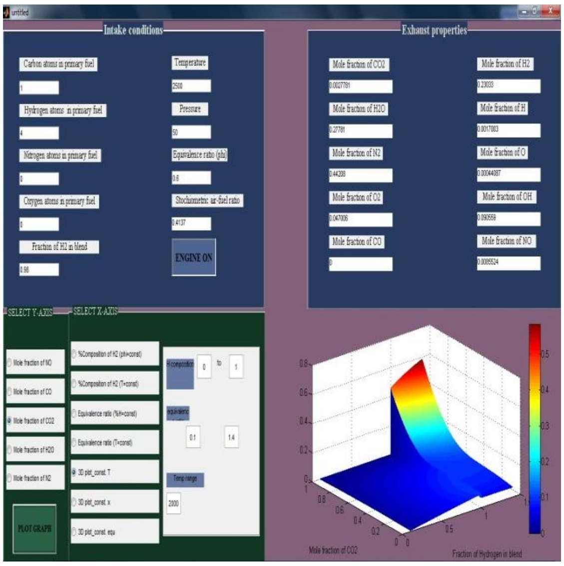

Fig.1 Interface of the program

2.2 Simulations

Mole fractions of NO, CO, H_2O, N_2 and CO_2 can be simulated against varying the factors such as

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.

2.3 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:

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

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

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

$n4 = (1)\times 0.21\times(1\text{-equ})$ (12)

$n5 = 0$ (13)

$n6 = 0.42x$ (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:

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

$a = 1\times(1\text{-K})$ (16)

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

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

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

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

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

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

$n_4 = 0$ (23)

$n_6 = (1\text{-x})\times(0.42\times(\text{equ}-1)\text{-}n_5) + 0.42x$ (24)

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

$y_i = n_i / \sum n_i$ (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:

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

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

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

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

III. Results

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

3.1 CO Emissions

It can be observed from Fig.2 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 the highest for T=2500K and equ=1.5 in the plot.

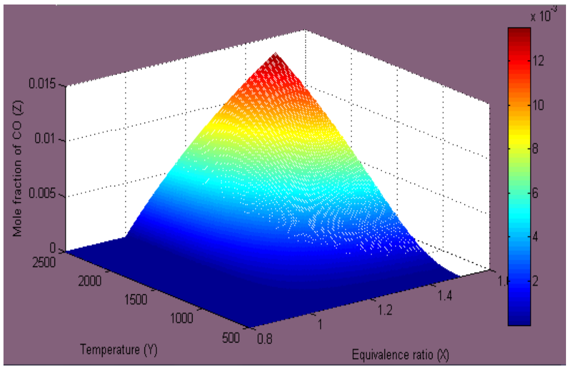

Fig.2: effect of temperature and equivalence ratio on co emissions at x=0.3

Fig.2 also 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.

3.2 CO_2 Emissions

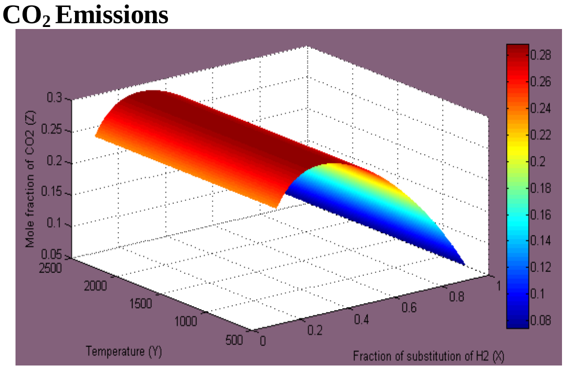

Fig.3: variation of mole fraction of co_2 with change in temperature and hydrogen fraction at equ=0.6

In Fig.3, it can be seen that with the increase in hydrogen fraction, CO_2 emissions first increase and then decrease for equ=0.6. It is observable that maximum CO_2 emissions occur for hydrogen fraction around 0.3. This trend was found to be the same for all other values of equ less than one. For the hydrogen fraction of 0.1, the value of CO_2 mole fraction is 0.24, it is 0.28 for hydrogen fraction 0.3 and for 0.9 the value of mole fraction is 0.1.

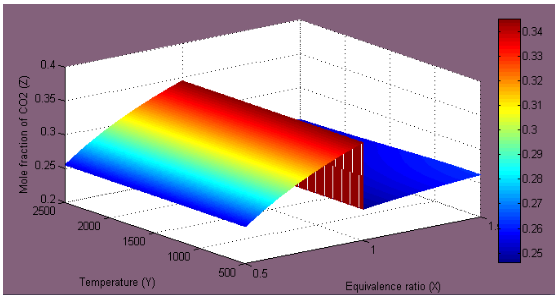

Fig.4: Effect of Temperature and equivalence ratio on CO_2 emissions for x=0.3

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 slightly decreases with increase in temperature. 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 is a result of the increase in carbon content (due to increased fuel content). From the plot, a sudden fall in mole fraction at equ=1 is visible, which can be accredited to the incomplete combustion of fuel after equ=1.

3.3 NO_x Emissions

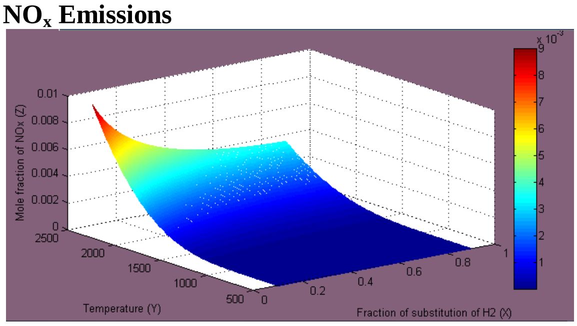

Fig.5: Effect of Temperature and Hydrogen fraction on mole fraction of NO_x for equ=0.6

The Fig.5 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.

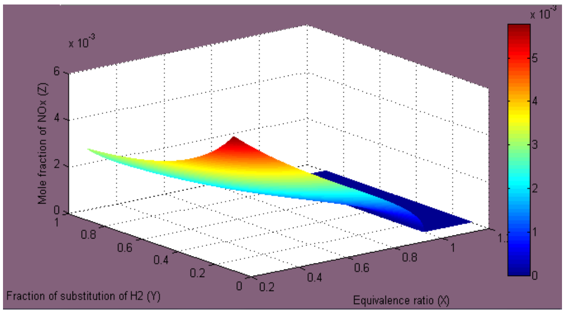

Fig.6: Effect of Equivalence ratio and Hydrogen fraction on mole fraction of NO_x for T=2000K

In Fig.6, the effect of Hydrogen fraction 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 and it becomes negligible after equ=1. This can be explained by the decrease in availability of Oxygen after combustion with fuel as equivalence ratio increases.

IV. Conclusions

The effects of equivalence ratio, Temperature and Hydrogen fraction on emission of different species in an H-Diesel 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 increase with increase in equivalence ratio. But with the increase in Hydrogen fraction, the emissions will increase initially, reaches a maximum at around 0.3, and then it will decrease. 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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