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Effect of Ferrocene as a Fuel Additive on Four Stroke Diesel Engine Performance

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ABSTRACT: *Ferrocene is used as an antiknock additive to replace lead alkyls. The Anti knocking and soot suppressing property of Ferrocene ($Fe(C_5H_5)_2$) catalytic action, lightened a method for the manual coke clean up which increase the effective fuel combustion and life time of the combustion parts of the engine without effecting the process but energizing the purpose. The metastable Ferrocene nucleate enables further burnout of the carbon deposits in the combustion chamber. This paper presents the evaluation and positive effect of adding the optimal percentage of ferrocene in the diesel. The performance of the diesel engine is tested and compared with different blends of ferrocene in the diesel. The Experimental results show that the addition of the ferrocene optimal percentage to the fuel will enable to increase the break thermal efficiency, decrease the specific fuel consumption of the engine and pinking tendency.*

Keywords: *Diesel engine, ferrocene, pinking tendency.*

I. INTRODUCTION

Engine technologies are increasing very fast and also the education level of the people for a professional way to operate the engine. The only parameter that cannot be influenced directly is the availability of a good and economical fuel. Especially for modern four stroke engines with high output, the combustibility of the fuel is of paramount importance to achieve reliable operation of the engine. One way to improve the combustion of the fuel in the engine, without altering the specification of the fuel, is to introduce a chemical additive. Ferrocene has the formula $(C_5H_5)_2Fe$, a molecular weight of 186.04, and is an orange crystalline substance that is insoluble in water but soluble in organic solvents and fuels.

Ferrocene -- Preparation:

Ferrocene, $(C_5H_5)_2Fe$, was first discovered in 1951. Until this time organometallic compounds containing Metal-Carbon bonds were restricted to Grignard Reagents (R-MgBr), Zeise's Salt and a few miscellaneous others. Attempting to prepare Fulvalene via a Grignard Reagent, T.J. Kealy and P.L. Paulson formed Dicyclopentadienyl Iron, or Ferrocene, instead:

$$2\ (C_5H_5)\text{-}MgBr + FeC_{l2}\ (C_5H_5) \rightarrow Fe\text{-}(C_5H_5)_2 + MgBr_2 + MgC_{l2}$$

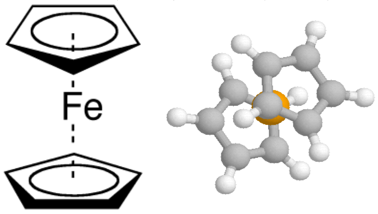

Fig 1: Image of Cyclopentadienyl Iron

Ferrocene and its numerous derivatives have no large-scale applications, but have many niche uses that exploit the unusual structure (ligand scaffolds, pharmaceutical candidates), robustness (anti-knock formulations, precursors to materials), and redox (reagents and redox standards).

John J. Kracklauer [1]has observed a method of conditioning diesel engines. The diesel fuel containing dicyclopentadienyl iron thereof for a period of time sufficient to eliminate carbon deposits from the combustion surfaces of the engine and to eliminate carbon deposits from the combustion surfaces of the engine and to deposit a layer of iron oxide on the combustion surfaces, which layer is effective to prevent further buildup of carbon deposits. In Effect of Ferrocene on catalysis combustion [2] experimental results show that ferrocene can increase the combustion rate effectively and reduce kindling temperature by 50^0C. Results [3]obtained with an acetylene diffusion flame show that iron oxide incorporated in the soot particles acts as catalyst to promote soot burnout at the tip of the flame. As per the conclusions[4] the addition of ferrocene to the laminar jet diffusion flame acted as expected by reducing the number and mass of soot particulate. The ferrocene acted as a catalyst in oxidizing the soot and fuel, the more ferrocene added to the flame the more it aided in oxidation to the point that virtually all hydrocarbons and soot had been oxidized.

i) Nucleates before and after soot inception. The catalysis combustion process can be explained as the transition metal ion Fe^{2+} attaches to the surface of the coke particles and the internal surface of the tiny holes at the coke surface, which makes the coke active surface increasing, The transition metal ion Fe^{2+} reacts with the oxygen in the gas flow and forms the meta stable oxidized state. The meta stable oxidized state acts as a oxygen carrier, letting the oxygen travels to the surface of the coke particle by absorption and digression process. The coke particle breaks to nano scale carbon clusters and the coke combustion process can be extremely accelerated and forms CO_2 The deoxidized Fe element reacts with the oxygen in the flu and again repeats the above catalysis process. During this reaction cycle, the transition metal ion Fe^{2+} as the function of oxygen transferring. iii) Addition of aromatic rings the remained part of ferrocene $(C_2H_5)^-_2$ let the engine to decrease the knocking tendency. Decreasing knocking tendency order is paraffins, napthenes, and aromatic hydrocarbons.

The complete set of reaction steps and the kinetic parameters have to be known together with all partial pressures to predict the exact behavior of each individual engine and combustion.

Step 1: Combustion of Ferrocene and fuel oil

The combustion of **fuel oil** leads to carbon dioxide, carbon monoxide and carbon (soot)

$$\mathbf{C_mH_n + z\ O_2 \rightarrow CO, CO_2, C_{solid}...}$$

The combustion products of Ferrocene are iron oxides and carbon dioxide

$$\mathbf{Fe(C_5H_5)_2 + O_2 \rightarrow Fe_xO_y + CO_2\ ...}$$

The main combustion product of Ferrocene is iron oxide **Fe2O3** (and slight amounts of **FeO**).

Step 2: Soot reduction activity of Ferrocene

Iron oxides and soot react to carbon monoxide or carbon dioxide and iron

$$\mathbf{2\ Fe_2O_3 + 3C \rightarrow 4\ Fe + 3CO_2}$$

$$\mathbf{FeO + C \rightarrow CO + Fe}$$

Step 3: Reactivation of the catalytic activity

Iron and oxygen react to iron oxide

$$\mathbf{4\ Fe + 3O_2 \rightarrow 2\ Fe_2O_3}$$

and the catalytic cycle can start again. The mechanism described above indicates that the active compound is Fe2O3 that is the base of the catalytic cycle can start again.

Ignition quality is a measure of the ability of fuel to ignite promptly after injection. A fuel which ignites slowly causes diesel knock. The Chemical structure desired in petroleum fuels for CI engines is opposite to that of desirable for spark ignition engines. The best fuels for the CI engine are highly paraffinic with average molecular weights greater than those of gasolines. The antiknock quality and ignition quality are opposed to each other. There seems to exist a simple, linear relation between the characteristic numbers, octane number (ON) and cetane number (CN) is given

ON=120-2CN

ON=150-2.5CN

and it varies around 5%. Gasoline has got antiknock qualities, but does not ignite readily. As such, gasoline is not suitable for use in diesel engines. Sharp oscillations of pressure are noted during combustion. With the addition of ferrocene the calculated cetane index is getting decreased with the increase in percentage of ferrocene.

Therefore a number of additives are added to improve its combustion characters prevents engine knocking by increasing octane number, reacts with carbon and sulphur residue and removes from the cylinder, as an antioxidant prevents gum formation, overcomes catalytic effects of dissolved copper, prevents corrosion , impart color for identification. The addition of ferrocene will increase the combustion rate, decrease the knocking tendency. It is vapourised above 100^0C and hence can be easily added into industrial installations. It is one of the most stable organic metal complexes at high temperatures, which will not be decomposed till 400^0 C. According to some previous report [2], ferrocene and derivatives are very effective in catalysis of liquid and solid fuel. It is non-toxic, which is not common in most organic metal complexes. Compared to other organic metal complexes, it is relatively cheaper.

II. MATERIALS AND METHODOLOGY

Solubility of ferrocene in diesel:

The samples of ferrocene are 0.15g, 0.20g, 0.25g, 0.30g, 0.40g, 0.50g are mixed to 10ml diesel individually. The mixture is stirred and left for a day. At atmospheric temperature the diesel dissolves till 3% of ferrocene completely, for 4% and above the precipitate of ferrocene is observed. Hence the saturated dissolving percentage of ferrocene in diesel is in between 3-4% only.

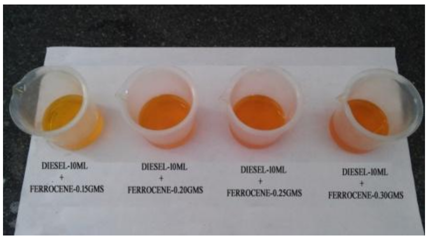

Fig 2: Image of Solubility of Ferrocene

Fig 3: Image of saturated dissolving Percentage of Ferrocene in diesel

The Gross calorific values for different blends of ferrocene were observed to be decreasing from 1% of ferrocene blend to 3% of ferrocene blend in diesel which does not affect the engine performance.

Fig 4: Tabular form of calorific values for the blends.

S.No.	Test Pattern	Diesel Oil	1%ferrocene	2%ferrocene	3%ferrocene
1	Density at 15^0C (g/cc)	0.8264	0.8319	0.8354	0.8387
2	Gross Calorific value (K.cal/Kg)	10430	10190	10060	9950
3	Calculated Cetane Index	55.5	54.0	53.5	52.5

On observing there is a slight increase in density, decrease in the gross calorific and calculated cetane index. It indicates clearly that the blends with the higher percentages of ferrocene are not suitable because there is a much decrease in the calorific value that of from diesel.

Experimentation:

A single cylinder four stroke diesel engine (5HP, 1500 rpm) of kirloskar was run with different percentages of ferrocene from 0% to 3% by weight. The performance of the engine is observed. The Break thermal efficiency, specific fuel consumption and brake power are compared with each blend including diesel.

The above mentioned four stroke diesel engine is run with diesel, 1%, 2% and 3% of ferrocene blends. The Load (KW), speed (rpm), time taken for 10cc of fuel consumption were taken at the variation of the loads from 0 to 10kg and the Break Thermal Efficiency, Specific fuel consumption and break power are calculated and tabled, based on the formulae.

$$1)\ B.P = \frac{2\pi N * w * \frac{(D+d)}{2}}{60} KW$$

Where D= dia of break drum=0.246m
d= dia of rope =0.02m
W= 9.81*mass
N=speed (rpm)

2) SFC= Mfc/BP

3) Break thermal efficiency= BP/heat input

III. RESULTS AND DISCUSSION

Break Power:

The break power of the diesel and 1%ferrocene blend are competitive whereas that of 2 and 3% are having lower power because the calorific value of the ferrocene blended diesel are decreasing with the increase in ferrocene percentage. And Calculated Cetane Index is also decreasing indicating decrease in ignition quality. As a result 1% ferrocene blend is better and suggestible for use.

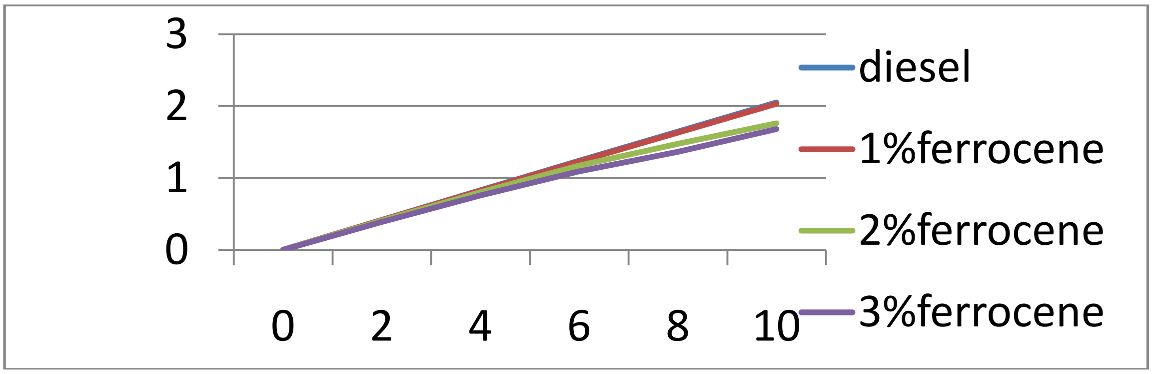

Fig 5: Break Power vs Load (X axis- Load, Y axis- Break Power)

Specific fuel consumption:

The order of decreasing specific fuel consumption is observed to be 2%,3%,diesel,1%ferrocene. Due to the catalytic action of Iron oxide improves the effective fuel combustion. But in the case of 2 and 3% blends is having high SFC because the calorific value of the fuel is low that of from diesel. The cetane index is also low which decrease the Ignition Quality of the fuel.

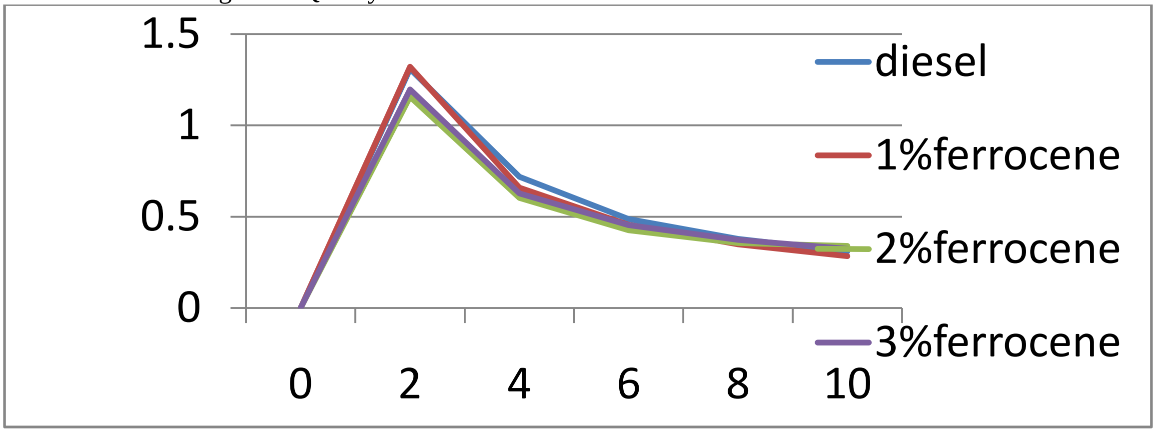

Fig 6: SFC vs Load (X axis- Load, Y axis- SFC)

Break Thermal Efficiency :

The Break thermal efficiency of 1%ferrocene blend got the highest value near to 30% followed by 2% ,3% blends and diesel. And the input power follows the reverse order.

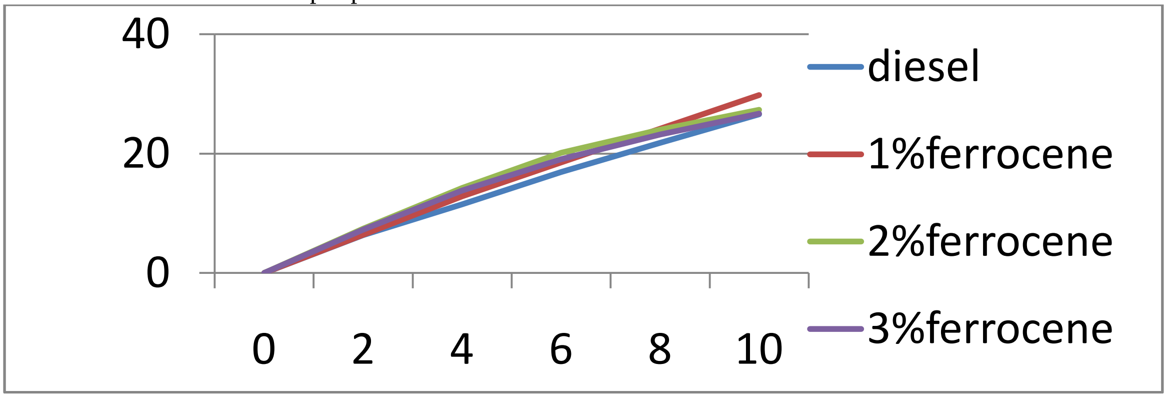

Fig 7: Break Thermal Efficiency vs Load (X axis- BTE, Y axis- Break Power)

IV.CONCLUSION

The experimental results and discussions shows that there is a positive effect of adding the optimal percentage of ferrocene in the diesel. For 1% ferrocene blended diesel has more thermal efficiency (29.77%) and the specific fuel consumption is lower compared to other is 0.283 Kg/KW-hr. Therefore the optimal percentage is in between 1% to 2% that is 10ppm to 20ppm of ferrocene in the fuel. Not only it improves the effective fuel combustion but also decreases the knocking tendency due to the presence of aromatic molecules. The knocking tendency decreases with the increase in the ferrocene percentage. The Break Thermal efficiency improves and the specific fuel consumption decrease.

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