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EXERGY DESTRUCTION AND CHEMICAL IRREVERSIBILITIES DURING COMBUSTION IN SPARK – IGNITION ENGINE USING OXYGENATED AND HYDROCARBON FUELS

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Abstract - The growing concern for energy, economy and environment calls for efficient utilization of natural resources in developing useful work. Second law of thermodynamics provides different perspective compared with first law. This paper provides an overview of the quantitative levels of exergy destruction and chemical irreversibilities during the combustion. For the adiabatic combustion at constant volume, entropy generation approach with second law of thermodynamics is applied. The result of this study is based on a spark ignition, single cylinder combustion engine with stoichiometric condition. Iso-octane, methane, methanol and ethanol are the fuels examined. This study shows that exergy destruction during combustion decreases with the increase in reactant temperature and compression ratios, for all the fuels. Exergy destruction during combustion using *entropy balance* approach for compression ratio range of 7 to 11 found to vary between 16.18 to 21.52%. Chemical irreversibilities calculated at the restricted dead state are found to be in the range of 2.99 to 3.6% for different fuels.

Keywords - Combustion, Compression ratio, Exergy, Chemical exergy, Ethanol, Methanol, Iso-octane, Methane

I. INTRODUCTION

Combustion plays a very important role in energy utilization process. Modern society is heavily dependent on fossil fuels as a source of energy. Most of the world energy needs are completed by the combustion of fossil and other fuels. Combustion of fuels finds its importance in different fields such as power production, heating, transportation, process heating, petroleum, chemical, glass, sugar industries and metal casting. During combustion chemical energy of the fuel is converted into thermal energy. The losses in a combustor that accounts for the decrease in the thermal efficiency are due to unburned fuel, incomplete combustion, and heat loss to the surrounding across the combustor wall. Complete and adiabatic combustion of fuel will increase the output of the engine. The transportation sector and electricity generating plants use the energy obtained from the combustion for the generation of work [1].

Combustion of fuels is a very complex phenomenon and it is highly thermodynamically irreversible process and limits the conversion of fuel energy into useful energy [2, 3,4,5,6,7]. Most of the combustion irreversibility is contributed to the internal heat transfer from burned fuel to the unburned fuel that is from products to the reactants. Such heat transfer is inevitable in premixed and diffusion flames where highly energetic molecules are free to exchange energy with un-reacted fuel and air mixture. For typical atmospheric combustion systems, about $1/3^{\text{rd}}$ of the fuel exergy becomes unavailable due to inherent irreversibility in the

combustor. Internal heat transfer, chemical reactions and mass transfer during combustion generates entropy and reduces the potential of the products gases to do useful work but it is not a direct energy loss from the combustion zone to the surrounding. The losses due to process irreversibility can be calculated using the second law analysis either from the rate of entropy generation or from the unbalanced rate of energy input [8].

Many works are available in the literature advocating the importance of exergy based analysis for the performance evaluation of thermodynamic systems[9,10,11,12]. According to them, energy based performance are often misleading as they fail to identify deviation from reality. The practical processes generate thermodynamic irreversibilities internal to them and results in a loss of exergy even when there is no loss of energy external to the system. Although a large amount of work has been done on availability analysis of engines, turbines and power plants, relatively little work has been done towards the ideal combustion processes and a very less work has been done in finding out the exergy destruction during combustion of spark ignition engines by varying the compression ratio and fuels.

1.1 Previous work:

Dunbar and Lior [9] examined the case of constant pressure adiabatic process. Dunbar and Lior examined the various contributions to the destruction of availability by dividing the number of processes into a number of hypothetical sub-processes. The sub-processes considered in the analysis were (a) combined diffusion/fuel oxidation, (b) internal thermal energy exchange (heat transfer), and (c) the

product constituent mixing process. The largest contribution to the destruction of availability was found to be due to the internal energy exchange within the system. The fuel considered by Dunbar and Lior during their analysis were hydrogen and methane.

Caton conducted an analysis of constant volume combustion, with particular emphasis on the implications of the results as applicable to the internal combustion engines. Caton analyzed the combustion of iso-octane for a range of reactant temperatures, pressures and equivalence ratio. In general, the destruction of availability decreased with increasing reactant temperatures and increasing equivalence ratios. The effect of reactant pressure on the destruction of availability was relatively modest, when compared with the other parameters.

A significant contribution to second law analysis was given by Caton in several research works. He used second law of thermodynamics to study spark- ignition engine and his work was based on the use of a comprehensive thermodynamic cycle simulation. In one part of his study, he examined the effects of engine load and speed on a number of performances, energy and availability terms. He reported that availability displaced to the cylinder wall through heat transfer (as percentage of the fuel availability) range between 15.9% and 31.5%. The net availability expelled with the exhaust gases ranged between 21.0% and 28.1%. The availability destroyed by the combustion process ranged between 20.3% and 21.4%. In addition, his study showed that the mixing of the inlet charge with existing cylinder gases was an additional mechanism for the destruction of availability.

Heywood [4] also contributed to the combustion process analysis. He introduced a zero – dimensional, quasi-dimensional and multi-dimensional model for a combustion process modeling and calculation and he focused especially on scavenging air inlet process and its effects on overall combustion process.

Shapiro and Gerpen [13] extended their previous work introducing a two-zone combustion model and applied this model to both compression –ignition and spark –ignition engines. This new model also included chemical availability considerations and simplifications done in previous work as chemical availability increases in significance with increasing temperatures and richer equivalence ratios due to increased concentrations of incomplete products of combustion such as carbon monoxide and hydrogen.

Caton examined the exergy destruction during the combustion process as a function of operating and design parameters for a spark ignition engine for eight fuels. The results of this study were based on spark ignition automotive engine. Caton analyzed the combustion of iso-octane, methane, propane, hexane, methanol, ethanol, hydrogen, and carbon mono oxide as a function of speed, load,

equivalence ratio, start of combustion, combustion duration, combustion rate parameters, exhaust rate recirculation, inlet oxygen concentration, and compression ratio. The exergy destruction was different for different fuels. The lowest destruction (8.1%) was for carbon monoxide and highest destruction (20.8%) was for iso-octane.

To structure our discussion, we define a conceptual isochoric combustion process. The objective of the present study is to evaluate the exergy destruction during combustion of four fuels that is ethanol, methanol, Iso-octane and methane. The effect of the type of fuel used and change in compression ratio is observed on combustion irreversibilities.

II. SYSTEM DESCRIPTION:

An actual four stroke fuel-air cycle for spark ignition has been considered for the analysis. The analysis carried out is for the exergy destruction during combustion only. The complete SI engine cycle is shown in Figure.1. Process 1-2s is a reversible adiabatic compression, while process 1-2 is real compression process. The process 2-3 represents combustion and process 3-4s is a reversible adiabatic expansion, while 3-4 is an irreversible adiabatic process. The exhaust is at a constant volume process 4-1.

The constant volume combustion process is assumed to be adiabatic. Since the process is considered to be adiabatic, no exergy is transferred due to heat transfer. As the system volume is closed; so no exergy is transferred because of mass flows. Therefore, there is no exergy is transferred during work transfer. Therefore, any change in the exergy, during a change of state is solely attributed to the combustion process. The analytical approach used in this study follows from related work with engine cycle calculations with the change is compression

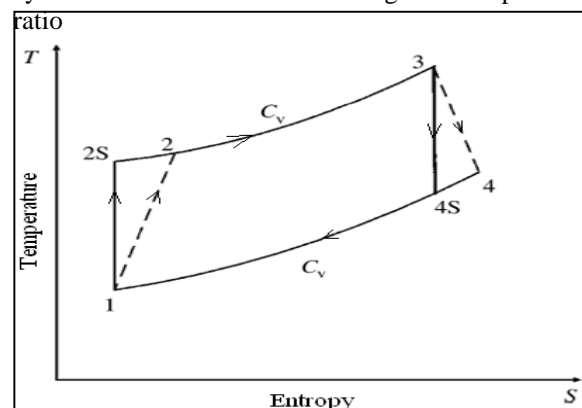


Fig. 1: Four stroke SI cycle

Engine Specification Table 1.0:

Bore	100mm
Stroke length	74mm
Engine Speed	3000rpm

Length of connecting rod	160mm
Inlet valve opening	30° BTDC
Inlet valve closes	40° BTDC
Equivalence ratio	1
Fuels	Various
Compression Ratio	Various
Spark Time	26°BTDC

2.1 Assumptions

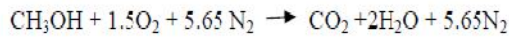
The following assumptions are made during constant volume adiabatic combustion.

1. The thermodynamic system is the closed chamber content.
2. The cylinder content is assumed to be spatially homogeneous and to occupy one zone.
3. The fuel is assumed to be completely vaporized and mixed with the reactant air.
4. The thermodynamic properties (including pressure and temperature) are spatially uniform.
5. Variation of specific heat with temperature at different process points has been incorporated.
6. Combustion takes place instantaneously.

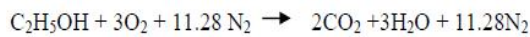
2.2 Chemical equations:

The following chemical equations are used during combustion of fuels at stoichiometric condition.

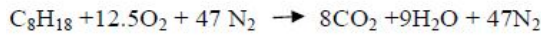
(i) Methanol Fuel



(ii) Ethanol Fuel



(iii) Iso-octane Fuel



(iv) Methane Fuel



III. THERMODYNAMIC MODEL:

3.1 Entropy balance approach:

An entropy generation analysis was applied to SI engine and an entropy generation calculation model was developed. Mathematical formulation of the principle of the non-conservation of entropy for a non- steady flow process in a time interval t_1 to t_2 following the second law of thermodynamics can be written as

$$\sum_i m_i s_i - \sum_e m_e s_e + \sum_r \left(\frac{Q_r}{T_r}\right)_{1-2} + S_{gen, 1-2} = S_2 - S_1$$

Where m_i and m_e respectively denote the amount of mass across input port i and exiting across port e ; $(Q_r)_{1-2}$ denotes the amount of heat transferred into the control volume r on the control surface. $S_{gen, 1-2}$ denotes the amount of entropy generated in the control volume and S_1 and S_2 are the amounts of entropy in the control volume at t_1 and t_2 .

Comparison of the properties of selected fuels (methanol, ethanol, iso-octane, and methane) is provided in Table 2.0.

Table 2.0 Comparison of selected fuels properties:

Property	Methanol	Ethanol	Iso-octane	Methane
Chemical formula	CH ₃ OH	C ₂ H ₅ OH	C ₈ H ₁₈	C ₃ H ₈
Molecular weight(Kg/kmol)	32.04	46.07	114.228	44.14
Oxygen present (wt %)	49.9	34.8	-	-
Stoichiometric air/fuel ratio (AFR)	6.47	9.0	15.2	15.6
Lower heating value of the fuel (kJ/Kg)	20000	26900	44300	46350
Fuel exergy (kJ/Kg)	21100	28400	45500	47100

The entropy generation during the four key processes of the SI engine is calculated after applying the equation (1) and the consequent exergy destruction is evaluated after using the Gouy – Stodola theorem as

$$E_{dest} = T_0 S_{gen} \tag{2}$$

The entropy balance for any system (including reacting systems) undergoing any process is expressed as

$$S_{in} - S_{out} + S_{gen} = \Delta S_{sys} \tag{3}$$

$S_{in} - S_{out}$ is net entropy transfer by heat and mass. S_{gen} is entropy generation and ΔS_{sys} is the change in entropy.

$$\sum Q_k/T_k + S_{gen} = S_{prod} - S_{react} \tag{4}$$

Where T_k is the temperature at the boundary where Q_k crosses it.

But for an adiabatic process ($Q = 0$) so entropy generation for an adiabatic process is given by

$$S_{gen} = S_{prod} - S_{react} \tag{5}$$

Absolute entropy values at pressures other than 1 atm for any temperature T are obtained from the ideal gas entropy change relation.

$$\bar{s}(T,P) = \bar{s}^0(T,P_0) - \bar{R} \ln P/P_0 \tag{6}$$

For the component i of an ideal gas mixture,

$$\bar{s}(T,P_i) = \bar{s}^0(T,P_0) - \bar{R} \ln y_i P_m/P_0 \tag{7}$$

Where P_i is the partial pressure, y_i is the mole fraction of the component, and P_m is the total pressure of the mixture.

Exergy destroyed with a chemical reaction is determined by

$$e_{Dest,comb} = T_0 S_{gen} \tag{8}$$

3.3 Chemical exergy destruction:

At the restricted dead state the system is in thermal and mechanical equilibrium with the environment. However, no chemical equilibrium exists, which means that some work recovery is possible due to differences between the composition of the system at the restricted dead state and that of

the environment. If the system at the restricted dead state is also permitted to pass into but not react chemically with, the surrounding environment. Then for ideal gas mixture, the chemical availability is defined as

$$A_{ch} = T_0 \sum_i R_{si} m_i \ln (x_i/x_i^0) \quad (9)$$

Where x_i and x_i^0 are the mole fraction of species i in the mixture (restricted dead state) and the environment (true dead state). This chemical availability is a measure of maximum work when the system comes to equilibrium with the environmental composition

Standard air compositions (Mole fraction)

$$N_2 = 0.7565, O_2 = .2029, H_2O = .0313, \\ CO_2 = .0003, T_0 = 300K, P_0 = 1.0325 \text{ bar}$$

IV. RESULTS AND DISCUSSION:

4.1 Exergy destruction during combustion (Entropy balance approach):

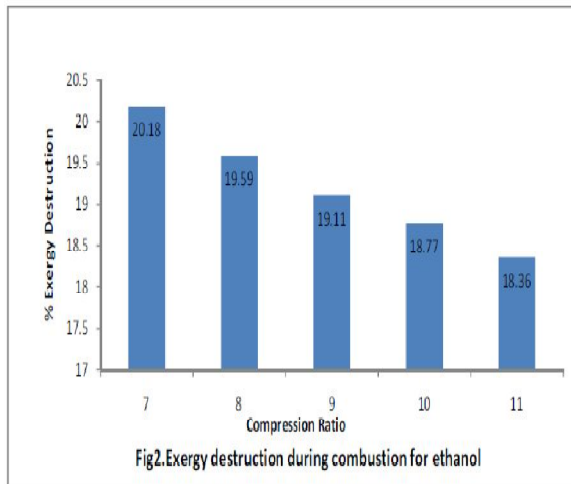


Fig.2 shows the exergy destruction during combustion for ethanol with the change in compression ratio. It is found that exergy destruction during combustion decreases with the increase in compression ratio and this is due to the reason that ethanol fuels have rich oxygen content and it burns smoother which results in less exergy destruction. Exergy destruction during combustion varies from 20.18% to the 18.36%.

Fig.3 shows the exergy destruction during combustion for iso-octane with the change in compression ratio. It is found that exergy destruction during combustion decreases with the increase in compression ratio and this is due to the reason that Iso- octane fuels have higher temperature which results in less exergy destruction. But exergy destruction during combustion for iso-octane is significantly higher than ethanol, methanol, methane and this is because of the reason that iso-octane have complex molecular structure. Exergy destruction during combustion varies from 21.52% to the 19.89%.

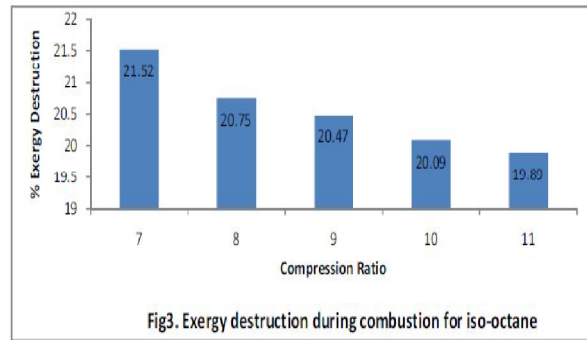


Fig.4 shows the exergy destruction during combustion for methanol with the change in compression ratio. It is found that exergy destruction during combustion decreases with the increase in compression ratio and this is due to the reason that methanol fuels have rich oxygen content and it burns smoother which results in less exergy destruction. Exergy destruction during combustion varies from 21.06% to the 19.01%.

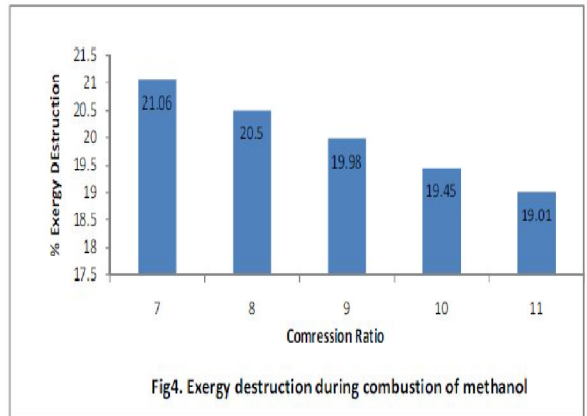
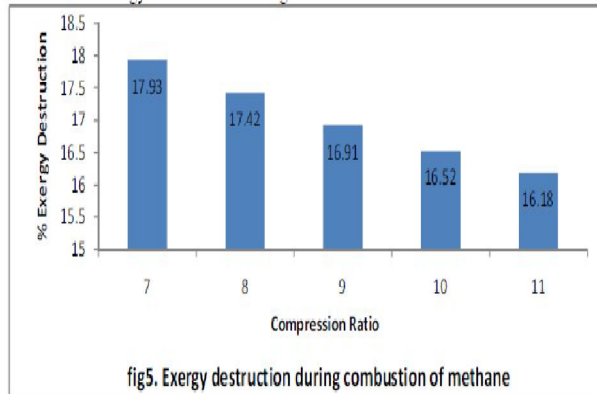


Fig.5 shows the exergy destruction during combustion for methane with the change in compression ratio. It is shown that exergy destruction during combustion decreases with the increase in compression ratio and this is due to the reason that methane fuels have simpler molecules structure and it burns smoother which results in significantly lower exergy destruction. Exergy destruction during combustion varies from 17.93% to the 16.18%.



4.2 Chemical exergy destruction:

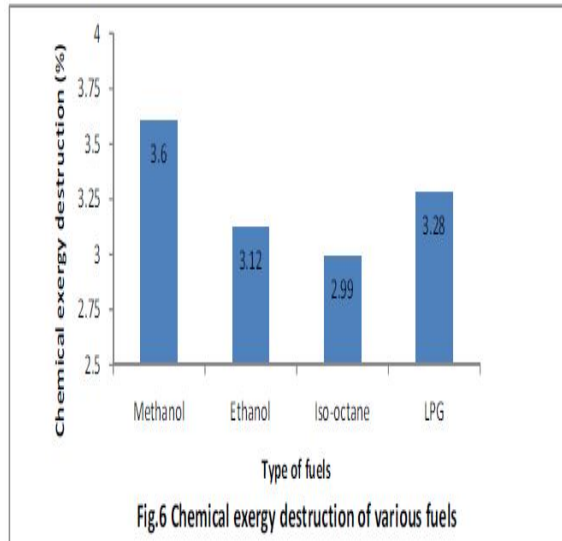


Fig.6 shows the chemical exergy destruction of the various fuels. It is shown that chemical exergy loss of methanol is significantly higher than the other examined fuels and lowest for the iso-octane. A part of the fuel exergy goes waste as chemical irreversibilities and this loss is not recoverable in internal combustion engines.

V. CONCLUSION:

A analytical examination of the exergy destroyed during combustion of methanol, ethanol, LPG, Iso-octane, and methane was completed for constant volume adiabatic process.. The effect of the reactant temperatures and compression ratios on the percentage of exergy destroyed due to combustion process was determined.

It is concluded that exergy destruction during combustion decreases with the increase in reactant temperature and compression ratio for all the fuels in both the approaches. Exergy destruction during combustion was varied between 21.52% to 16.18% with entropy balance approach with a change in compression ratio from 7 to 11. Chemical exergy destruction varies from 2.99% to 3.6% for the different fuels examined.

It is also found that exergy destruction during combustion of iso-octane is highest in both the approaches and it is lowest for the methane. Availability of the products are less than the reactants.

In general, the use of second law and availability analyses provides deep insight and new perspectives on the destruction of available energy due to combustion processes. Significant implications of these results relate to destroying the potential for useful work.

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