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SIMULATION OF OTTO CYCLE FOR MULTI FUEL

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Abstract There is a continuing demand for increased combustion efficiency and an intuitive concern over problems related to the environment, energy available in utilizable form and specially the economy which is of utmost importance throughout the whole world. For the aforementioned scenario stimulated effort has been accomplished in the field of combustion of both conventional and alternative fuels. To improve the combustion efficiency and hence to save energy or to reduce energy loss the following effort has been accomplished to detect the real behavior of combustion. Subsequent study is to analyze the different effects of thermodynamic properties of reactant and product, specific heat ratio, gas constant R, initial temperature, initial pressure, adiabatic maximum combustion temperature, equivalence ratio PHI, compression ratio and type of fuel on the combustion process. Considering all these mentioned factors the following study estimates the equilibrium product composition, maximum adiabatic combustion temperature and the P-v nature of eleven different individual fuels or any mixture thereof employing iteration technique. The code employed here is able to analyze combustion nature of octane, methane, methanol, ethanol, acetylene, propane, butane, benzene, heptanes, hydrogen, carbon dioxide carbon dioxide and any percentage mixture thereof .

INTRODUCTION

In recent years, the deepening concern over problems related to energy, economy, and environment have prompted tremendous burst of research activities in the field of combustion. At present one target is to make the best use of renewable energy sources and another is to improve the efficiency of the energy utilization methods. Major share of energy production is related to combustion, directly or indirectly. In the view of increasing combustion efficiency for all the fuels that are subjected to combustion, present paper study has emphasized or executed the exact thermodynamic analysis to consider the ideal combustion phenomena that is strictly speaking far deviated from the real behavior.

During the expansion and compression process the isentropic relation is used normally to evaluate the unknowns. While doing this job the specific heat capacity and gas constant is taken as constant which in actual practice changes with temperature. The concentration of the study is towards the elementary effects of these factors on combustion. To analyze all these factors of combustion both the internal energy of combustion and enthalpy of combustion has been focused briefly.

The paper study is carried out for different equivalence ratios at 300 K, at three initial pressures of 101.325 KPa, 200 KPa, 300 KPa, and for different compression ratio of 8, 10, 12. Effect of initial temperature also has been included. To represent an example of the study for any percentage mixture of different fuels a typical result has been shown for a composition of 55% methane and 45% carbon dioxide. P-v nature of four different fuels has been compared or analyzed there also.

ESTIMATION OF PRODUCT COMPOSITION

Estimation of adiabatic combustion temperature require the estimation of the product composition. Product composition is determined by mixture stoichiometry as well as thermodynamic properties. In the present study, NASA data base (Burcat and McBridge, 1997) is used to estimate the thermodynamic properties as required to estimate the equilibrium product compositions.

Combustion stoichiometry: General stoichiometric reaction can be written as

$$\sum \nu_i \mathbf{R_i} \rightarrow \sum \nu_j \mathbf{P_j}$$

where,

ν_i stoichiometric coefficient of reactant species, i
ν_j stoichiometric coefficient of product species, j
R_i reactant species
P_j product species

In general fuels contain carbon, hydrogen, oxygen and nitrogen and some amount of minor species. When fuel is burnt completely, general stoichiometric reaction can be written as

$$\varphi\varepsilon\, C_\alpha H_\beta O_\gamma N_\delta + [O_2]\, O_2 + [N_2] N_2 = \nu_o\, CO_2 + \nu_1\, H_2O + \nu_2 N_2 + \nu_3\, O_2 + \nu_4 CO + \nu_5 H_2 \text{ -----------(1)}$$

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Since atoms are conserved , using atom balance of equation (1) we get

C : $\varepsilon\alpha = \nu_o$
H : $\varepsilon\beta = 2\nu_1$
O : $\varepsilon\gamma + 2[O_2] = 2\nu_o + \nu_1$
N : $\varepsilon\partial + 2[N_2] = 2\nu_2$

The following four relations can be solved and using the convenient approximations for lean ($\varphi<1$) and rich combustion ($\varphi>1$) following species expressions are obtained.

For lean combustion :
$\nu_0 = [O_2] \times \alpha / (\alpha + 0.25\beta - 0.5\gamma)$
$\nu_1 = ([O_2]/2) \times \beta / (\alpha + 0.25\beta - 0.5\gamma)$
$\nu_2 = [N_2] + ([O_2]/2) \times \delta\beta / (\alpha + 0.25\beta - 0.5\gamma)$
$\nu_3 = [O_2](1-\varphi)$
$\nu_4 = \nu_5 = 0$

For rich combustion:
$\nu_0 = [O_2] \times \alpha / (\alpha + 0.25\beta - 0.5\gamma) - \nu_4$
$\nu_1 = ([O_2]/2) \times \beta / (\alpha + 0.25\beta - 0.5\gamma) + \nu_4$
$\nu_2 = [N_2] + ([O_2]/2) \times \delta\beta / (\alpha + 0.25\beta - 0.5\gamma)$
$\nu_3 = 0$
$\nu_4 = (-B1 + \sqrt{(B1^2 - 4 \times A1 \times C1)}) / (2 \times A1)$
$\nu_5 = [O_2] \times 2 \times (\varphi - 1) - \nu_4$

where,
$\varepsilon = [O_2] \times \alpha / (\alpha + 0.25\beta - 0.5\gamma)$
$T_o = T/1000$
$K = \exp(2.743+T_o(-1.761+T_o*(-1.611+T_o*0.2803)))$
$A1 = 1.0 - K$
$B1 = [O_2] - PHI \times \varepsilon \times (2\alpha - \gamma) + K \times ([O_2] \times (PHI - 1) + \alpha \times PHI \times \in)$
$C1 = -[O_2] \times \alpha \times PHI \times \varepsilon \times (PHI-1) \times K$

The summery may be written as in the following table.

Table: low temperature combustion products (moles / mole of air)

I	Species	$\varphi \le 1$	$\varphi > 1$
1	CO_2	$\varepsilon\alpha\varphi$	$\varepsilon\alpha\varphi - \nu_4$
2	H_2O	$\beta\phi\varepsilon$	$2[O_2] - \varepsilon\phi(2\alpha-\gamma) + \nu_4$
3	N_2	$[N_2]+\delta\phi\,\varepsilon/2$	$[N_2] + \delta\phi\varepsilon/2$
4	O_2	$[O_2](1-\varphi)$	0
5	CO_2	0	ν_4
6	H_2	0	$[O_2](\varphi-1) - \nu_4$

THERMODYNAMIC PROPERTIES

Thermodynamic properties both for the individual fuel and mixture fuel or for any other gases may be calculated by evaluating the polynomials at desired temperature. The functions employed for any given species are----

$$\frac{c_p}{R} = a_1 + a_2T + a_3T^2 + a_4T^{33} + a_5T^4$$

$$\frac{h}{RT} = a_1 + \frac{a_2}{2}T + \frac{a_3}{3}T^2 + \frac{a_4}{4}T^{33} + \frac{a_5}{5}T^4 + \frac{a_6}{T}$$

“ a ” values are polynomial coefficients, that may be found from Burcat and McBridge (1997) data-base.

In the main code these constants have been read as conf [i] for single fuel and as con_fuels [j][i] for mixture fuel. Properties of mixture fuel can also be computed introducing their relative percentages. For example mixture fuel enthalpy can be calculated as below ---

Hfuel=Σ (ho_fuels [i] * fuel_percent [i] /100.0)
[i stands for different individual fuel components]

Hence the mixture fuel properties can be calculated after computing the individual fuel properties and introducing their relative percentages in their respective expressions. Gas properties are computed in the similar way as for the individuals using the same polynomials but different coefficients where the coefficients are written as con [j][i] and properties as ho[i] , cpo[i].

THERMO CHEMICAL ANALYSIS OF CONSTANT VOLUME SYSTEM

If a chemical reaction occurs in a closed system maintained at constant volume then the basic energy balance can be expressed as

$$Q = \Delta U = U_{product} - U_{reactant} = \sum(N_iu_i)_{product} - \sum(N_iu_i)_{reactant} \text{ ------------(2)}$$

Recalling $u_{i,T} = (h - pv)_{i,T} = \Delta h^0_{f,298} + h_T - h_{298} - (Pv)_T$

Hence,

$$Q = \sum(N_i\Delta h^0_{f,298,i})_{prod} - \sum((N_i\Delta h^0_{f,298,i})_{reac}) + \sum N_i(h_T - h_{298})_{prod} - \sum[N_i(h_T - h_{298})_i]_{reac} - \sum[N_i(Pv)_{i,T}]_{prod} + \sum[N_i(Pv)_{i,T}]_{reac}$$

Furthermore the volume of solid and liquid components in a chemical reaction is usually negligible in comparison to the volume occupied by the gaseous components. Hence in the summations above which involves P, V terms can be replaced by RT. Consequently the conservation of energy principle for the constant volume process can be written in the following forms:

$$Q = \sum[N_i(\Delta h^0_{f,298} + h_T - h_{298})_i]_{prod} - \sum[N_i(\Delta h^0_{f,298} + h_T - h_{298})]_{reac} - \sum(N_iRT)_{prod} + \sum(N_iRT)_{reac}$$

$$H_{product} = \Sigma(y_i \, ho_i - y_i \, RT)_{prod}$$
$$= \Sigma[N_i\,(\Delta h^0_{f,298} + h_T - h_{298})_i\,]_{prod}$$

$$H_{reactant} = \Sigma(y_i \, ho_i - y_i \, RT)_{reac}$$
$$= \Sigma\;[\,N_i\,(\Delta h^0_{f,298} + h_T - h_{298}\,)_i\,]_{reac}$$

$$Q = (H_{product} - H_{reactant}) - \Sigma(N_i\,RT)_{prod} + \Sigma(N_i\,RT)_{reac}$$

ESTIMATION OF ADIABATIC COMBUSTION TEMPERATURE

To obtain adiabatic combustion temperature under constant volume combustion process it can be assumed that there is no heat loss. Hence Q = 0 and adiabatic temperature is the temperature for which

$$H_{product} = H_{reactant}$$

To get the value of adiabatic combustion temperature of the mixture in complete combustion process iteration has been performed with known initial temperature and incremental change of temperature dt. Estimation of maximum combustion temperature made on this basis is normally conservative. That is, the calculated value frequently will be several hundred degrees higher than the measured value. In actual practice, the combustion is seldom complete. Secondly, heat losses may be minimized but not eliminated. Thirdly, some of the products of combustion may dissociate into other chemical species as a result of higher temperatures present. These dissociation reactions normally are endothermic and consume some of the energy released by the overall reaction.

THE CODE FOR SIMULATION OF OTTO CYCLE FOR MULTI FUEL

The code has been developed mainly to analyze P-V characteristic of eleven individual fuel or any mixture thereof in different conditions. Further modifications or another development of the following code would be able to analyze P-V characteristic in constant pressure process.

While expansion and compression the value of specific heat ratio and gas constant R for any species are not essentially remain constant. The effect of this change has been encountered during developing the code. The specific heat capacity γ decreases with the increase of temperature and its mean value for any temperature range (normally encountered in the compression process as well as in the expansion process) is appreciably less than 1.4 even if the gas is air. The mixing of the incoming charge with residual products of combustion results in a lower value of γ for the mixture as the products of combustion contain CO_2 and H_2O which individually have a relatively low value of γ. In SI engines the gas compressed is an air fuel mixture, and this too has a lower value of γ than air. Finally, heat transfers from the cylinder to the gas in the early stages of the compression and the gas to the cylinder in the later stages, mean that the compression does not follow isentropic path. The net result is that the pressure and temperature at the end of the compression are appreciably less than the values predicted by air standard calculations.

To depict very briefly the inclusion of these effects into the code the following description may be mentioned. In case of individual gas combustion the chemical formula can be written as

$$C_\alpha H_\beta O_\gamma N_\delta$$

But in case of mixture combustion (such as bio-gas, mixture of CH_4, CO_2) the formula to be used may be written as below.

For two fuel mixture:

$$C_\alpha H_\beta O_\gamma N_\delta \approx (1^{st}\text{ fuel percent}) \times C_{\alpha 1} H_{\beta 1} O_{\gamma 1} N_{\delta 1} + (2^{nd}\text{ 1fuel percent}) \times C_{\alpha 2} H_{\beta 2} O_{\gamma 2} N_{\delta 2}$$

For more than two fuel mixture:

$$C_\alpha H_\beta O_\gamma N_\delta \approx \Sigma\;(i^{th}\text{ fuel percent} \times C_{\alpha i} H_{\beta i} O_{\gamma i} N_{\delta I})$$

Isentropic path can be assumed to be followed by the air-fuel mixture before combustion and the combustion products under expansion. Hence their properties can be evaluated as below.

$$T_2 = T_1 \times (CR)^{\gamma-1}$$
$$P_2 = P_1 \times CR \times T_2 / T_1$$

Where
CR is the compression ratio

Specific heat ratio =

$$\frac{\text{Cp of the mixture}}{\text{Cp of the mixture - R for the mixture}}$$

Specific heat at constant pressure C_p and gas constant R for the mixture can be calculated using the following expression.

R for the mixture =

$$\frac{\text{AF ratio} \times 0.287}{(\text{AF ratio} + 1)} + \frac{8.314}{\text{mass of fuel} \times (\text{AF ratio} + 1)}$$

C_p for the mixture =

$$\frac{\text{AF ratio} \times \text{Cp of air}}{(\text{AF ratio} + 1)} + \frac{\text{Cp of fuel}}{\text{mass of fuel} \times (\text{AF ratio} + 1)}$$

Where,

$$\text{AF ratio} = \frac{[O_2] \times 32.0 + [N_2] \times 28.0}{(\text{Mass of fuel} \times \text{PHI} \times \varepsilon)}$$

$$\varepsilon = [O_2] \times \alpha / (\alpha + 0.25\,\beta - 0.5\,\gamma)$$

$$\text{Mass of the fuel} = \alpha \times 12.011 + \beta \times 1.0079 + \gamma \times 16.0 + \partial \times 14.0$$

C_p for air and C_p for fuel is calculated from the subroutine fuel_property and gas_property employing Burcat and McBridge (1997) data-base.

RESULTS AND DISCUSSION

The code written for P-V diagram analysis corresponds to numerous point evaluation while completing OTTO cycle stages. It is possible to determine various properties such as pressure, temperature, specific-volume at different stages. Exhaust gas temperature and adiabatic combustion temperature are of very extensive importance where ever combustion is a way to convert energy in a utilizable form. Extension of the thesis may result in further more essential elements like work done, heat loss etc. Graph analysis shows the response of P-v diagram and temperature for various factors. Typical results may be given herewith.

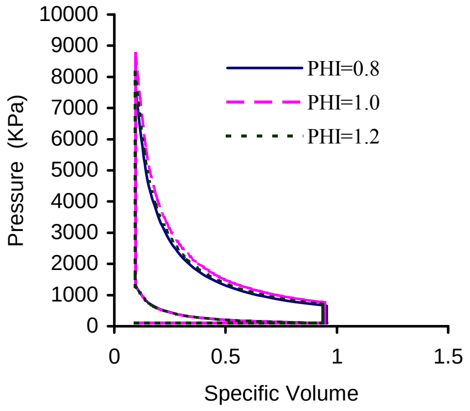

Fig. 1Effect of PHI on P-V diagram

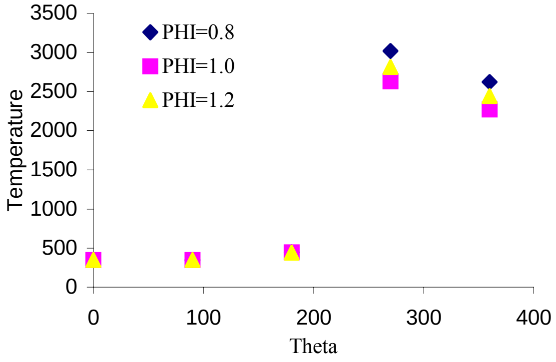

Fig. 2Effect of PHI on adiabatic temperature

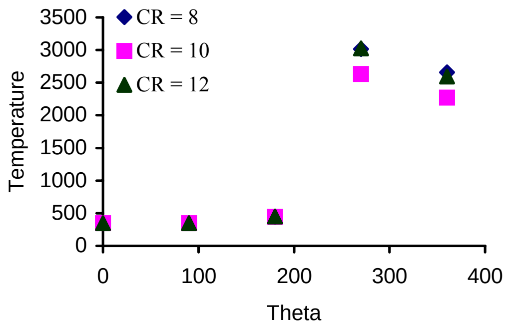

Fig. 3 Effect of compression ratio on adiabatic temperature

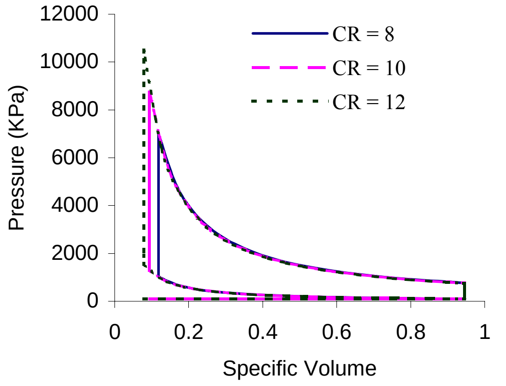

Fig. 4Effect of compression ratio on P-V diagram

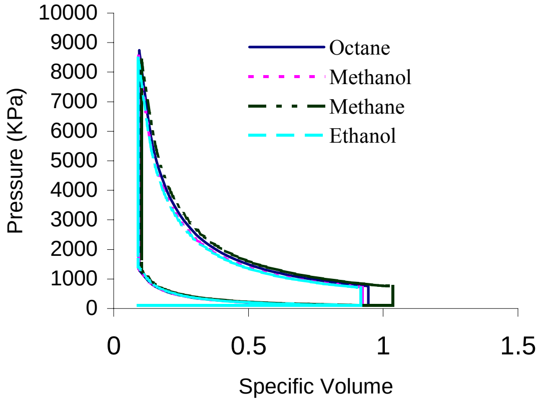

Fig. 5Effect of type of fuel on P-V diagram

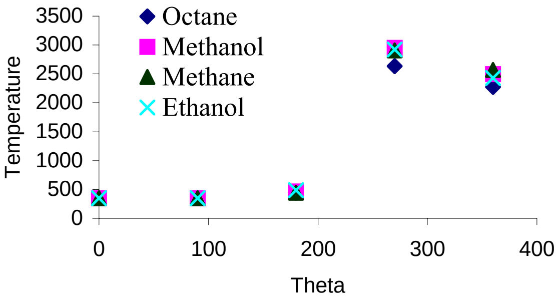

Fig. 6Effect of type of fuel on adiabatic temperature

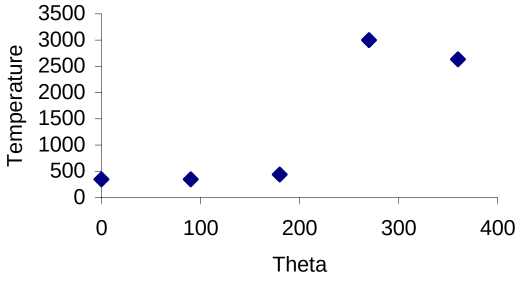

Fig. 7Adiabatic temperature for biogas (55%$CH_4$and 45%CO_2)

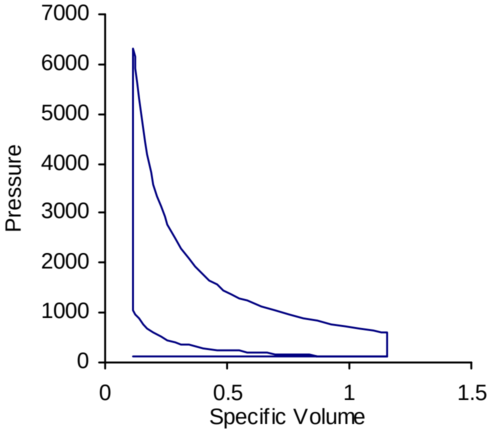

Fig. 8 P-V diagram for biogas (55%CH_4 and 45%CO_2)

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