Phenomenological Modelling of Four-Stroke Compression Ignition Engine Processes with Dissociation Effect

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Abstract-- **In present work, simulation has been done for four stroke compression ignition engine for Ideal cycle and Progressive combustion. Simulation was modified to Progressive combustion with dissociation effect. Result of Progressive combustion simulation was validated with result available in literature. Plotting of P-θ and T-θ diagrams was done for Progressive combustion with dissociation. It was observed that maximum temperature was 3455.30 K, 2824.488 K, 2749.254 K at crank angle in degree 384.77, 381.61, 381.15 for Ideal cycle, Progressive combustion without and with dissociation respectively. Indicated power, Brake power, indicated thermal efficiency and Brake thermal efficiency obtained from the simulation was good in agreement with the literature results for progressive combustion. The difference between present work and literature was 2.51%, 3.02%, 5.24% and 4.73% respectively. It was observed that dissociation phenomenon reduce the temperature after combustion about 75 K to 150 K and maximum dissociation constant was 13.0. Result of Progressive combustion simulation without and with dissociation presented by plotting performance curve. Variation in power, efficiency, mean effective pressure by changing speed are presented in graphical form. Indicated power and Indicated thermal efficiency was compared between results obtained from simulation of Progressive combustion without and with dissociation. It was observed from comparison that the value of Indicated power and Indicated thermal efficiency obtained from simulation of Progressive combustion without and with dissociation was 10.207 kW,10.007 kW and 46.373%, 45.4335% respectively.**

Key Words-- **Phenomenological Modeling, Progressive combustion, Dissociation**

I. Introduction

In engineering, simulation process mean developing and using proper combination of assumption and equation that permit critical features of the process to be analyzed. Computer simulation can give major contribution to engine design at different levels of general studies, or detail, corresponding to a different stages of model development. [1] As of now two basic types of model: Thermodynamic and Fluid Dynamic. Thermodynamic model on base of energy conservation are categorized as: zero-dimensional, phenomenological and quasi-dimensional. Fluid Dynamic model are often called as multi-dimensional model due to their inherent ability to provide detailed geometrical information on the flow field, based on the solution of the governing flow equation.

The objective of the present work is to analyze the performance of a CI engine using a computational thermodynamic model by the Progressive Combustion. A modeling of single cylinder for four stroke direct injection diesel engine has been developed including the effects of heat losses, dissociation and temperature-dependent specific heats.. The analysis of model covers of compression, power and expansion processes. This new developed model predicts in-cylinder temperatures and pressures as functions of the crank angle (θ). These features can be very useful in providing more realistic estimations of the main performance parameters, such as the thermal efficiency and the break mean effective pressure. .

II. Nomenclature

A_c	Cylinder surface area
A_h	Cylinder head area
BDC	Bottom dead center
BMEP	Brake Mean Effective Pressure
BP	Brake Power
BRTHEFF	Brake thermal efficiency
CI	Compression Ignition
C_v	Specefic heat at constant volume
C_p	Specefic heat at constant pressure
D,d_i	Bore of cylinder
D	Displacement
DN	No. of steps in combustion during progressive combustion
FMEP	Friction Mean Effective Pressure
IC	Internal Combustion
IP	Indicated Power

IMEP	Indicated Mean effective pressure
ITHEFF	Indicated Thermal Efficiency
K	Kelvin
K_a	Thermal conductivity of air
K_c	Thermal conductivity of cylinder material
K_p	Chemical Reaction constant
l	Connecting Rod Length
MECHEFF	Mechanical efficeincy
MEP	Mean Effective Pressure
m_s, m_d	Intake and Exit mass flow rate respectively
N	Speed in Revolution per Minute
P, T	Pressure and Temperature respectively
PCS	Progressive Combustion Simulation
P_1, T_1, V_1	Pressure, Temperature and Volume of charge before the compression respectively.
P_2, T_2, V_2	Pressure, Temperature and Volume of charge after the compression respectively.
P_3, T_3, V_3	Pressure, Temperature and Volume of charge at the end of combusiion respectively
P_4, T_4, V_4	Pressure, Temperature and Volume of charge at the end of expansion rrespectively
P_5, T_5, V_5	Pressure, Temperature and Volume of exhaust gases (charge) at end of exhaust respectively
Q	Heat transfer rate through cylinder walls and head
R_c	Compression Ratio
R	Universal gas constant
RAF	Relative Air Fuel Ratio
s	Stroke length
t_h	Thickness of cylinder head
t_c	Thickness of cylinder
T_{ca}	Air temperature at near cylinder head
T_{cw}	Cooling water temperature
T_{new}	New temperature for next cyclere
TDC	Top dead center
θ	Crank angle
U	Total internal energy
U_h	Overall heat transfer coefficient of cylinder head
U_c	Overall heat transfer coefficient of walls
V	Volume
V_c	Cylinder Volume
VR	Cut- off ratio
w	Angular speed
W_{comp}	Work done during compression
W_{comb}	Work done during combustion
W_{exp}	Work done during expansion
Wnet	Net work done during cycle

III. THERMODYNAMIC ANALYSIS

As regards compression ignition engines, these models range from overall engine simulation to ideal cycle simulation and to the more frequently applied phenomenological filling and emptying models. [2] Consider the air and residual gas as control volume which is trapped between the cylinder and piston. If we neglect the potential and kinetic energy then, first law for Control Volume [3],[4]

$$\dot{Q}_{in} + \dot{W}_{in} = \frac{dU}{dt} + \dot{m}_d h_d - \dot{m}_s h_s \quad (1)$$

1) *Mathematical Formulation of Compression Process*

$$\dot{Q} = A_c U_c \left(T - T_{cw}\right) + A_h U_h \left(T - T_{ca}\right) \quad (2)$$

Assuming the cylinder walls are cooled by water and cylinder heads is cooled by air

$$AU = \frac{1}{\sum Rt} \quad (3)$$

Where

$$\sum Rt = \frac{1}{h_i A_i} + \frac{\ln \frac{R_o}{R_i}}{2\times\pi\times k\times l} + \frac{1}{h_o A_o} \quad (4)$$

$$\frac{1}{A_c U_c} = \frac{1}{h_i A_{ci}} + \frac{\ln \frac{R_o}{R_i}}{2\times\pi\times K_c\times l} + \frac{1}{h_o A_{co}} \quad (5)$$

Simplifying the equation (5)

$$\frac{1}{U_c} = \frac{1}{h_i} + \frac{\ln \frac{d_o}{d_i}}{2\times\pi\times K_c\times l} + \frac{d_i}{h_o d_o} \quad (6)$$

Take $d_o = d_i + 2t_c$ = outer diameter of cylinder, d_i=d and $h_i = h_c$ into equation (6)

$$\frac{1}{U_c} = \frac{1}{hc} + \frac{d}{2\times kc}\ln\left(1 + \frac{2\times tc}{d}\right) + \left(\frac{d}{d+2\times tc}\right)\frac{1}{h_o} \quad (7)$$

t_c = cylinder wall thickness

h_o = heat transfer coefficient at outside (water side) approximately (150 W/m^2 K).

h_c = heat transfer coefficient at inside given by Mc Adam correlation for heating and cooling fluid in turbulent flow through pipes/tubes. [5]

Hence overall heat transfer coefficient is determined

$$A_c = \frac{\pi\times d\times V_{tdc}}{A_h} + \pi\times d\times s\left[\frac{1-\cos\theta}{2} + \frac{1}{s}\left(1 - \sqrt{1 - \frac{s^2}{4\times l^2}\times\sin^2\theta}\right)\right] \quad (8)$$

$$A_h = \frac{\pi\times d^2}{4} \quad (9)$$

$$AU = \frac{1}{\sum Rt} \quad (10)$$

$$\sum Rt = \frac{1}{h_i A_i} + \frac{t_h}{k\times A} + \frac{1}{h_o A_o} \quad (11)$$

But $A_i = A_o = A$ and by using the equation (9), (10) and (11)

$$\frac{1}{U_h} = \frac{1}{h_c} + \frac{t_h}{k_c} + \frac{1}{h_h} \quad (12)$$

h_h = outside (air side) heat transfer coefficient of head (approximately 20 W/m^2 K).

Put value of equations (7), (8), (9) and (12) all values into equation no. (2) to determine heat flow rate.

$$\dot{W} = -P\frac{dV_c}{dt} = -p\times w\times\frac{dV_c}{d\theta} \quad (13)$$

$$\frac{dU}{dt} = \frac{d(mu)}{dx} = m\frac{du}{dt} + u\frac{dm}{dt} \quad (14)$$

But net mass flow rate in Control Volume

$$\dot{m}_s - \dot{m}_d = \frac{dm}{dt} \quad (15)$$

But during compression $\frac{dm}{dt}=0$

$$\frac{dU}{dt} = m\frac{du}{dt} \quad (16)$$

According to first TdS equation [3]

$$TdS = C_v dT + \left[T\left(\frac{dp}{dT}\right)_v\right]dv \quad (17)$$

But for closed system $TdS = du + pdv$ (18)

$$du + p.dv = C_v dT + \left[T\left(\frac{dp}{dT}\right)_v\right]dv \quad (19)$$

$$du = C_v dT + \left[T\left(\frac{dp}{dT}\right)_v - p\right]dv \quad (20)$$

But $\left[\left(\frac{dp}{dT}\right)_v\right]=0$ (21)

$$du = C_v dT \quad (22)$$

So $\frac{du}{dt} = C_v . \frac{dT}{dt}$ (23)

hence

$$\frac{dU}{dt} = mC_v . \frac{dT}{dt} \quad (24)$$

First law applicable to cylinder during compression process and equation (1) replaced to

$$\dot{Q}_{in} + \dot{W}_{in} = \frac{dU}{dt} \quad (25)$$

By use of equation (24) and (25)

$$mC_v . \frac{dT}{dt} = \dot{Q} - \dot{W} \quad (26)$$

$$w\frac{dT}{d\theta} = \frac{\dot{Q} - \dot{W}}{mC_v} \quad (27)$$

$$\frac{dT}{d\theta} = \frac{\dot{Q} - \dot{W}}{w \times m \times C_v} = \frac{\dot{Q} - \dot{W}}{M \times C_v \times n \times w} \quad (28)$$

Where $\dot{W} = p \times w \times \frac{dV_c}{d\theta}$ (29)

Hence Temperature is determined by solving equation numerically by using Euler's principle

$$T_{x+1} = T_x + \frac{dT}{d\theta} \times stepsize \quad (30)$$

Pressure can be calculated by equation

$$P_{x+1} = \frac{(N_a + N_x) \times R \times T_{x+1}}{V_c} \quad (31)$$

Where N_a = no. of moles of air and N_x = No. of moles of exhaust residual gases

2) Mathematical Formulation of Progressive Combustion Process

We begin with pressure and temperature at the end of compression and if the Air-Fuel ratio is known, we can compute the adibatic flame temperature (T_3') at constant volume by Newton Raphson technique [6] and N_p and N_r found by the applying the chemical theory. [1] Calculate the Volume at the end of combustion by following equation [1]

$$P_3' = \frac{p_2 \times T_3' \times N_p}{N_r \times T_2} \quad (32)$$

P_3' =is the pressure that would be reached if all fuel burned instaneously at TDC (i.e. at constant volume)

$$V_3 = V_{tdc}\left(1 + \frac{p_3' - p_2}{k \times p_2}\right) \quad (33)$$

Where

k=is the ratio of specific heats & n = amount of fuel burned

Time rate of burning is given by

$$\frac{dn}{dt} = \frac{dn}{dV}\frac{dV}{d\theta}\frac{d\theta}{dt} = \frac{1}{V_3 - V_{tdc}} V'\theta \frac{d\theta}{dt} \quad (34)$$

Suppose the maximum burning rate is known or some hypothetical value is agreed upon, we can find θ_3, the crank angle corresponding to V_3

We can compute by equation (33) and (34)

$$\left(\frac{dn}{dt}\right)_{\theta=\theta_3} \quad (35)$$

We compared it with the maximum allowable burning rate. If rate is not exceeding, then we can know the entire combustion process will proceed at the constant pressure. Hence we can found temperature at the end of combustion by

$$T_3 = \frac{p_2 \times V_3}{N_p \times R} \quad (36)$$

On the other hand if the burning rate (calculated by equation (36)) shows that it is more than maximum allowable burning rate then whole combustion process does not happened at constant pressure and it flowed in step fashion. Consider combustion happened in DN steps

$$\Delta\theta = \frac{\theta_3 - 180}{DN} \quad (37)$$

Using equation

$$\Delta V = V'_\theta \Delta\theta \quad (38)$$

And as long as the maximum burning rate is not exceeded,

$$\Delta n = \frac{\Delta V}{V_3 - V_{tdc}} \quad (39)$$

Once the burning rate reaches maximum allowable,

Take

$$\Delta n = \left(\frac{dn}{dt}\right)_{max} \Delta t \quad (40)$$

For all subsequent increment in time. The integration is completed when

$$\sum \Delta n = 1 \quad (41)$$

The work of expansion during combustion is calculated from

$$W_{comb} = \sum\left(p + \frac{\Delta p}{2}\right)\Delta V \quad (42)$$

Where the summation applies for the entire combustion process. Dissociation effect understands by chemical reaction constant and basic chemical reaction during combustion.

3) Mathematical Formulation of Expansion Process

All the steps are same as that of compression process in expansion process but have to be started from crank angle at which combustion ends.

Exhaust temperature found by

$$T_5 = T_4 \left(\frac{P_1}{P_4} \right)^{\frac{n-1}{n}} \quad (43)$$

Where n is index of expansion

Amount of exhaust residual gases found by

$$N_x = \frac{p_1 \times V_{tdc}}{R \times T_5} \quad (44)$$

$$N_a = \frac{p_1 \times V_{bdc}}{R \times T_1} - N_x \quad (45)$$

New temperature for the next cycle

$$T_{new} = \frac{R_c \times T_1}{R_c - 1 + \left(\frac{T_1}{T_5} \right)} \quad (46)$$

4) Mathematical Formulation of Performance Parameter

$$W_{net} = W_{exp} + W_{comb} - W_{comp} \quad (47)$$

$$IMEP = \frac{W_{net}}{V_{disp}} \quad (48)$$

$$ITHEFF = \frac{W_{net} \times 100}{m_f \times 40} \quad (49)$$

The mean effective losses of power due to friction in different moving parts are calculated by using the empirical relations. [6]

Brake Mean Effective Pressure (BMEP) can be calculated

Brake MEP = IMEP – FMEP (50)

$$IP = \frac{Wnet \times N \times 0.001}{120} \quad (51)$$

$$BP = \frac{BMEP \times Vdisp \times N \times 0.001 \times 100000}{120} \quad (52)$$

$$MECHEFF = \frac{BP \times 100}{IP} \quad (53)$$

$$BRTHEFF = \frac{MECHEFF \times 100}{ITHEFF} \quad (54)$$

Engine specification are taken for the Simulation are given below

1. Bore (d_i) = 0.08 m and Stroke length (s) = 0.11 m
2. Connecting Rod Length (l) = 0.23 m
3. Compression Ratio (R_c) = 16.5
4. RPM (N) = 1500 and Fuel is injected at 360^0
5. Temerature of air (Ta)= 300 K and Pressure of air (Pa)= 1.01325 bar
6. Fuel : $C_{10}H_{22}$ and Molecular Weight of Fuel (WT)= 142
7. No of Piston rings (NPR) = 3
8. Piston Skirt Length (PSL) = 9.0 mm
9. No. of Intake valve per cylinder GH = 1
10. Inlet and Outlet Manifold Pressure = 1.01.325 bar
11. Area of Exhaust valve (AEV) =3.0 cm^2
12. Area of Intake valve (AIV) =2.5 cm^2

For the purpose of simulation, the following expression has been chosen to represent flowing property [1]

$$h(T) = A + BT + C\ln(T) \quad \text{(kJ/mol)} \quad (55)$$

$$C_p(T) = B + C/T \quad \text{(kJ/mol.K)} \quad (56)$$

$$C_v(T) = B - 8.314 + C/T \quad \text{(kJ/mol.K)} \quad (57)$$

$$K_p = \exp\left[\frac{a}{T} + \left(b + \frac{c}{T} \right) \ln(T) + d \right] \quad \text{(P in atm)} \quad (58)$$

The coefficient A, B, and C for calculation of h(t) and $C_v(t)$ and the coefficient a, b, c and d for calculation of the reaction constant K_p are taken for temperature range 400 K to 1600 K and above 1600 K. [1]

IV. RESULT AND DISCUSSION

Assumption taken during simulation given below

1. The intake valve open at TDC and Exhaust valve open at BDC.
2. The suction and exhaust process happened at constant pressure.
3. Neglecting gas exchange process during intake and exhaust and neglecting the blow by losses.
4. The fuel mass injected instaneously and calculation of fuel mass that takes part in chemical reaction during combustion is based on complete combustion of the fuel. Combustion started at TDC.
5. No delay period and uniform distribution of fuel with air.
6. Cylinder head wall contains homogeneous air & Spatial homogeneity of pressure and temperature (for the whole cylinder or for each zone considered).
7. Air-fuel mixture) is considered an ideal gas.
8. Gas properties (enthalpy, internal energy, etc.) are modeled using polynomial relations with temperature (and pressure).
9. Heat released from combustion is distributed evenly throughout the cylinder.
10. Enthalpy associated with pressure of injected fuel is usually not significant and hence ignored.
11. No heat transfer and work transfer occurs between burned and unburned zones.

According to table I, the Difference in power and efficiency can be arising due to difference in inlet pressure condition and in combustion efficiency. In present work combustion efficiency taken 100% and in literature taken 80%. This difference can be ignored as differences are small.

TABLE I
CODE VALIDITATION AT RAF=1.0, R_C=16.5 AND VR=3.75

Variables	ICS by Literature	ICS by Present Code	Difference in %	PCS by Literature	PCS by Present Code	Difference in %
P_1[bar]	1	1.01325	1.31	1	1.01325	1.31
V_1[m^3]	0.00059	0.00059	0.07	0.00058859	0.000589	0.07
T_1[K]	300	300	0	314.353	314.593	0.08
P_2[bar]	50.638	51.3492	1.39	50.34	51.12703	1.54
V_2[m^3]	0.00036	0.00036	0.91	0.00035672	0.00036	0.91
T_2[K]	920.693	921.413	0.08	959.139	962.053	0.30
P_3[bar]	50.638	51.3492	1.39	50.342	51.12703	1.54
V_3[m^3]	0.00013	0.00013	0.17	0.00011236	0.000111	1.23
T_3[K]	3452.6	3455.3	0.08	2572.085	2824.488	8.94
P_4[bar]	6.363	6.44942	1.34	6.365	6.266890	0.43
V_4[m^3]	0.00059	0.00059	0.07	0.00058859	0.000589	0.07
T_4[K]	1908.82	1909.52	0.04	1752.61	1855.797	5.56
P_5[bar]	—	—	—	1	1.01325	1.31
V_5[m^3]	—	—	—	0.00035672	0.00036	0.91
T_5[K]	—	—	—	1216.472	1278.671	4.86
Wnet[J]	964.552	962.523	0.21	837.575	816.59	2.505
IP[kW]	12.057	12.032	0.21	10.47	10.207	2.51
η_{ith} (%)	54.613	54.638	0.05	43.943	46.373	5.24
IMEP[bar]	17.217	17.408	1.1	14.95	14.769	1.21
BMEP[bar]	17.217	17.408	1.1	12.577	12.357	1.75
BP[kW]	12.057	12.032	0.21	8.807	8.541	3.02
η_{bth} (%)	54.613	54.638	0.05	36.966	38.802	4.73
η_m (%)	100	100	0	84.123	83.673	0.53

TABLE II
COMPARISION OF VARIOUS SIMULATIONS FOR ENGINES PROCESSES

Variable	PCS with Dissociation			PCS			ICS		
	P (bar)	V(cc)	T (K)	P (bar)	V(cc)	T (K)	P (bar)	V(cc)	T (K)
START OF COMPRESSION	1.01325	589	314.397	1.01325	589	314.593	1.01325	589	300.00
END OF COMPRESSION	51.1330	36	961.565	51.1270	36	962.053	51.34919	36	921.41
END OF COMBUSTION	51.1330	109	2749.254	51.1270	111	2824.488	51.34919	134	3455.29
END OF EXPANSION	5.99157	589	1779.335	6.26689	589	1855.797	6.44942	589	1909.52
END OF EXHAUST	1.01325	36	1227.304	1.01325	36	1278.671	—	—	—

In table II, result at RAF=1.0, R_c=16.5, N=1500 and shows VR=3.75 shows that temperature at the end of combustion is lowered by nearly 75 K due to dissociation effect.

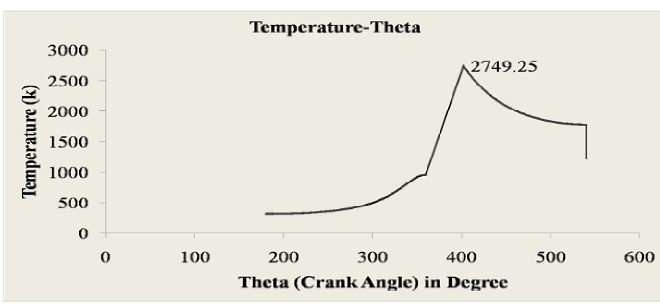

Fig. 1. T-θ Diagram

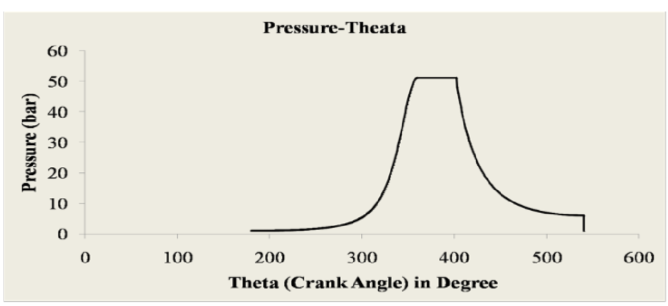

Fig. 2. P-θ Diagram

Fig. 1 and 2 show variation of Temperature and pressure with respect to crank angle for PCS with dissociation at RAF=1.0, N=1500 and compression ratio =16.5 respectively.

Performance of 4 stroke single cylinder CI engine with varying speed at RAF=1 and Compression Ratio =16.5

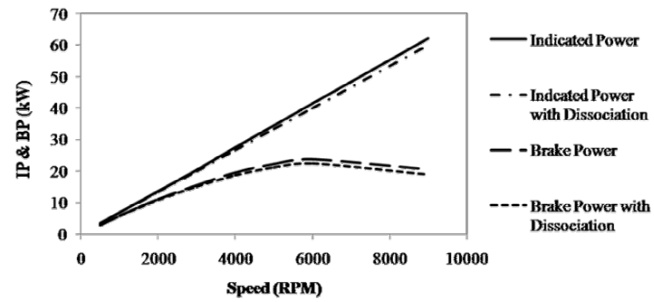

Fig. 3. Power Vs Speed

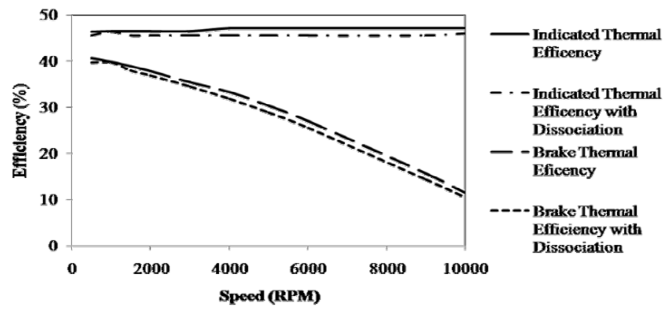

Fig. 4. Efficiency Vs Speed

Fig. 3 shows that the engine speed is at 1500 RPM the Indicated power (IP) of engine is 10.207 kW. If the engine speed is increase, IP also increase. When the engine speed is more than 5000 rpm the brake power (BP) is decrease and go to down because friction power increases. Maximum BP is 23.742 KW on the engine speed is 6000 RPM. The dissociation effect is predominant above the 6000 RPM. Loss of IP is important than BP above the 6000 RPM.

Fig. 4 shows maximum indicated thermal efficiency (ITHEFF) is 47.032%. The change in ITHEFF is negligible but brake thermal efficiency (BTHEFF) reduced as speed increased. When the engine speed is over than 500 RPM the BTHEFF is decrease and go to down from 40.593%. As speed increase, the friction power also increased hence BTHEFF reduced. Dissociation reduced BTHEFF nearly 2.39%.

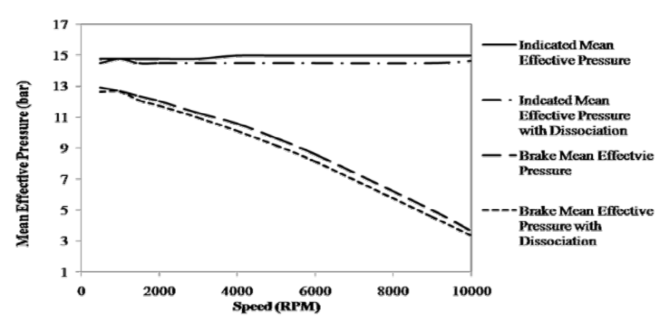

Fig. 5. Mean Effective Pressure Vs Speed

Fig. 5 shows Maximum indicated mean effective pressure is 14.977 bar at high speed. It is constant but brake MEP reduced from 12.92 bar as speed increased. After the engine speed is over than 500 rpm the BMEP is decrease and go to down. Dissociation reduces the brake mean effective pressure efficiency by nearly 2.33%.

V. CONCLUSION AND FUTURE WORK

1. The variation of specific heats and heat transfer are reduce the temperature and pressure of the gases after the compression stroke in I.C. engine.
2. The effect of variable specific heats is to reduce the temperature and pressure of the gases at the end of combustion in I.C. engine due to chemical heat release decrease as C_p increases.
3. The dissociation is not pronounced in CI engine. With dissociation, the maximum temperature is reduced by 100 K to 200 K in diesel engine.
4. The actual physical properties of the gases before compression and after combustion are taken into analysis, a reasonably close value to the actual pressure and temperature in the cylinder during the cyclic process can be achieved. Then the MEP and efficiency calculated by this analysis can be higher only few percent from the actual values.
5. Deviation in efficiency between Progressive Combustion Simulation (with dissociation and without dissociation) with actual engine is partly due to valve operation, incomplete combustion and gas exchange process.

PCS still popular due to their simplicity, low computational cost and reasonable accuracy [7],[8],[9],[10] This model is not however reliable, owing to temperature gradients in the burnt zone and disproportionately high rate of heat transfer from the mixture that burns first during combustion.

Apart from the single-zone models, two-zone [11],[12] , four-zone or even multi-zone models [13] which increased accuracy and flexibility for such complex phenomena as the formation of nitric oxide and soot in engine cylinders. Multi-zone models cover the fluid flow analysis and take care of premixed and diffusive combustion hence a detailed two zone model and three dimensional CFD modeling would be essential to understand the phenomenon. But it fact that it is still a preferred model for its computationally undemanding requirements, while being almost as accurate as more complex models.

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