International
Journal
Of Advanced Research in Engineering & Management (IJAREM)
ISSN: 2456-2033 || PP. 39-47

Di-Methyl Ether (DME) as a substitute for Diesel fuel in compress ion ignition engines

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Abstract: Compression ignition engines operated on diesel fuel have high emission rates of Nitric oxides (NOx) and particulate matters (PM) despite being the most fuel efficient engines ever developed for trans portation purposes thus necissating the need for advancement in engine designs and source for alternative fuels.

Di-methyl ether (DME) burns like diesel in compression ignition engines, and have the advantag e of lower emissions in terms of soot and (NOx) Di-methyl ether (DME) and Reduced N-Heptane (29 spe cies, 52 chemical reactions) which is a representative of Diesel fuel was utilized in the model by importin g from the relevant files into the chemical reaction interface using the relevant governing equations and so lved with COMSOL 5.0 which employs the finite element method of solution. The model was used to co mpare the thermal efficiency and brake mean effective pressure (BMEP) of the fuels.

The thermal efficiency derived while employing di-methyl ether (DME) as fuel was found to be greater than that which is obtainable by using diesel representative as fuel, signifying that the di-methyl et her (DME) fueled engine will be preferable when the derived work that is obtainable from the heat energy inherent in the fuel is of upmost importance

Key Words: Brake mean effective pressure (BMEP), Compression ignition engine, Compression ratio, Di-methyl ether (DME), Initial temperature, Thermal efficiency,

Introduction

Boosting the efficiency of internal combustion engines is one of the most promising and cost-effective approaches to increasing vehicle fuel economy.

The high compression ratio and lack of throttling loses of compression ignition engines makes them the most fuel efficient engines ever developed for transportation purposes. The high emission rates of Nitric oxides (NOx) and particulate matters (PM) of conventional ignition engines which pose a threat to its continuous usage has led to an interest in research in overcoming this, leading to the development of better fuel efficient engines. Homogenous charged compression ignition engine posses the high efficiency values as regards to the conventio nal compression ignition engines and low emission levels in comparison to spark ignition engines, and would ha ve been a possible solution to the problems of conventional compression ignition engines, but it is taken aback b y the effects of rapid pressure rise which is akin to experiencing 'knock' like a spark ignition engine and proble m of combustion timing.

Di-methyl ether is synthetically produced and burns like diesel in a compression ignition engine can ser ve as a zero soot alternative to diesel. This is been looked upon as a possible alternative to diesel fuel because of its excellent emission properties.

The thermal efficiency and break mean effective pressure (BMEP) of a compression ignition engine op erated on Di-methyl ether (DME) was determined in this study, and compared with that of Diesel (N-Heptane) o perated on the same engine using COMSOL 5.0 multi-physics package for the simulation.

Literature Review

It is most likely that conventional jet mixing controlled diesel combustion cannot meet future emission requirements without the attendant fairly expensive after treatment systems. The combined needs of further emi ssions reduction, improved efficiency, and cost, is making engine-combustion researchers to turn towards altern ative forms of compression ignition combustion, (1) which generally is premised on the principle of dilute premi xed or partially premixed combustion to reduce emissions.

Homogenous charged compression ignition (HCCI) is an offshoot of the studies premised on this princi ple, but as potentially promising as it is, it is been limited by issues of operating range; where, at high loads and speeds, the rates of heat release and pressure rise increases leading to knocking, and at low loads misfire may oc cur, hence, further investigations are being undertaken to examine the various parameters that effect HCCI com bustion. (2)

Still in the quest of finding a possible solution to the emission effects of a compression ignition engine and maintaining its relatively high efficiency, the concept of dual fuel usage was conceived.

Dual fuel engines have drawn a considerable research attention in the area of alternate fuels, and the two main a dvantages of this concept are

i) No major modifications are required in the existing engine and

ii) There is a flexibility of engine operation to switch back to the diesel mode of operation as and when need ari se. (3) Using different combinations of Uppage Oil (UOME) and compressed natural gas (CNG) in dual fuel mo de of operation gave results of inferior performance compared to single mode of operation using diesel. Howeve r, lower smoke and NOX were observed with dual fuel mode of operation compare to conventional mode of ope ration.

Using pongamia oil and liquefied petroleum gas in dual fuel mode; brake thermal efficiency was increa sed from medium to higher load operations, optimal specific fuel consumption was observed for substitution of LPG-biodiesel dual fuel mode and NOx emission was decreased with increase of LPG flow rate. The HC and C O emissions were observed in optimized level in dual fuel mode. (4)

A relevant increase in CO production occurs in the whole range of dual fuel mode when natural gas and diesel a re utilized, but with a reduction in the CO_2 indices. Natural gas rates up to 50% of the dual fuel gives an engine behaviour which is almost similar to that in full diesel operation, both in terms of lean combustion development and as regards the nitric oxide formation. (5)

Di-methyl ether (DME) offers the advantage of reduced emission in all ramifications for use in compre ssion ignition engines, and an advantage is the high cetane number of 55, compared to that of diesel from petrole um, which is 40–53, thus requiring only moderate modifications to convert the engine to burn di-methyl ether. (6) The simplicity of this short carbon chain compound leads to very low emissions of particulate matter, NO_x, a nd CO during combustion coupled with it's been sulfur free, it has a CO2 reduction potential of 68 – 101% in co mparison to diesel (7) making it to meet even the most stringent emission regulations in Europe. The clean burni ng properties of di-methyl ether (DME) eradicates the need for diesel particulate filter (DPF) hence reducing the cost required for after-treatment equipment and associated maintenance. (7)

Adding of ethanol to di-methyl ether have a pronounced effect on the indicated mean effective pressure (IMEP) for advanced in-cylinder injection timing than around the top dead center (TDC) conditions, but it has o nly little effect on the IMEP for same ignition timing. Significant reduction in indicated specific Nox without de terioration of indicated specific soot was also observed with the use of di-methyl ether-ethanol dual fuel combus tion strategy.(8)

The engine's compression ratio and initial inlet temperature and pressure have a significant effect on th e delay period of di-methyl ether, just as it does for diesel fuel. (9) Higher compression ratios ensures shorter ign ition delay period provided the initial temperature is sufficient enough for its self-ignition.

Methodology

The parameters used in the modeled engine are depicted in table 1 below;

Table 1 Model Parameters

ENGINE SPECIFICATION	VARIABLE	VALUE
Cylinder Bore	D	0.0875m
Stroke	S	0.11m
Connecting rod length	Lc	0.2m
Crank arm	La	0.055m
Engine speed	RPM	2500
Equivalence ratio	ϴ	0.5
Compression ratio	CR	15 & 18
Initial Pressure	P_initial	100000N/m^2

The chemical reaction mechanism of di-methyl ether (DME) was utilized in the model by importing it from the relevant files into the chemical reaction interface for case one, while the chemical reaction mechanism of reduced N-Heptane a diesel representative was utilized in case two by importing it to the chemical reaction interface on the other hand.

Energy and mass balances describing the combustion of the di-methyl ether (DME) and N-heptane in a variable-volume system were solved.

The combustion of the fuels in each case is governed by the generalized Navier Stokes equation;

ρ + ρ (ϴ . Δ) ϴ = Δ. [- ρl + μ (Δϴ + (Δu) ^{T})] + F 1

Where ϴ is a dependent variable such as momentum, energy, turbulence e.t.c

F is the source term for the ϴ variable

The reactor energy balance is;

Vr = Q + Qext +Vr 2

Where Cp,i is the species molar heat capacity (J/(mol·K)), T is the temperature (K), and p gives the pressure (Pa). Q is the heat due to chemical reaction (J/s)

Q = - Vr 3

Where Hj is the enthalpy of reaction (J/(mol·K)), and rj equals the reaction rate (mol/ (m^3·s)). Qext denotes heat added to the system (J/s), and for this model it is zero as adiabatic conditions is assumed.

The mass balances describing a perfectly mixed reactor with variable volume are summarized by

= VRi 4

Where ci represents the species concentration (mol/m^3), and Ri denotes the species rate expression (mol/ (m^3·s)).

The stoichiometric requirement of the oxidizer (air) to combust DME is found from the overall reaction:

$CH_3OCH_3 + 3 (O_2 + 3.76N_2) \longrightarrow 2CO_2 + 3H_2O + 11.28N_2$ 5

Assuming that the composition of air is 21% oxygen and 79% nitrogen, the stoichiometric air-fuel ratio is;

(A/F)stoic = ()stoic = 6

Also for the diesel representative, the stoichiometric requirement of the oxidizer (air) required for its combustion is found from the overall reaction;

$C7H16 + 11(O_2 + 3.76N_2)$ $7CO_2 \rightarrow 8H_2O + 41.36N_2$ 7

And following the same trend as for di-methyl ether, the stoicihometric air-fuel ratio is;

(A/F)stoic = ()stoic = 8

Working with the under listed following assumptions;

- The heat energy, generated by combustion, is added uniformly over the domain.
- The convection effects in the combustion chamber are neglected.
- All the equations are solved on the original domain, and the effect of change in the cylinder volume is accounted for manually in the equations.

The engine was modeled using Comsol 5.0 in 2-D axi-symmetry coordinates and utilizes the finite element method in solving the governing equations.

The initial cylinder volume 'V0' = 2*π*r 9

The cylinder volume, *V* at any instance is computed by subtracting the piston swept volume from the initial cylinder volume. ($V = V0-\pi*rp^2*xp$) 10

The piston displacement, *xp*, as a function of crankshaft rotation, θ, can be written as

$xp = l^2 – (rcSinϴ)^2) – rcCos ϴ – (l – rc)$ 11

Where *xp*, *rc*, *l* and θ represent the piston displacement, crank radius, connecting rod length and crank angle, respectively.

The swept volume of the cylinder, Vs = 12

D is the cylinder bore and S is the engine piston stroke.

The thermal efficiency is gotten from the expression;

ƞ = *100% 13

The brake mean effective pressure (BMEP) is derived from the expression;

BMEP = 14

Results and Discussions

The combustion in a compression ignition engine was analyzed numerically in this study. Using compression ratios of 15 and 18 at 2500rev/min and equivalence ratio of 0.5with initial temperatures ranging from 300 – 400^{o}C, computations were carried out for the thermal efficiency, the brake mean effective pressure (BMEP) . Cylinder bore D = 0.0875m, stroke length S = 0.11m, connecting rod length Lc = 0.2m and crank arm length La = 0.04375m, equivalence ratio = 0.5. Di-methyl ether (DME) and N-Heptane were used as fuel.
In the model engine under study the swept volume, Vs = = 6.6145 E – 4 m^{2}.
Pressure-Volume (PV) plots were obtained for both fuels at engine compression ratios (CR) of 18 and 15 with initial temperatures of 300^{o}C, 350^{o}C and 400^{o}C respectively, and the plots are depicted in figures; 1a, 1b to 5a, 5b. At a compression ratio of 18 and 15, the thermal efficiency for both fuels; di-methyl ether (DME) and diesel have peak values for thermal efficiency and brake mean effective pressure at an initial temperature of 300^{o}C as evidenced in figures 1a, 1b and . Di-methyl ether (DME) performed better in terms of efficiency at this initial temperature, but there is a significant difference in the values of their brake mean effective pressure (BMEP); the value obtained for the diesel representative being hundreds of percentage greater than that for di-methyl ether (DME) meaning that for the same engine parameters, the torque and power that is obtainable from a compression ignition engine operating on diesel as fuel far outweighs that which is operated on di-methyl ether (DME). Similar trends of superior performance in terms of brake mean effective pressure (BMEP) values was obtained for diesel fuel as against di-methyl ether for all values of initial temperatures and compression ratios as depicted in figures 2a, 2b, 3a, 3b, 4a, 4b, 5a and 5b respectively.
A high drop in efficiency value was noticed for di-methyl ether while using an initial temperature of 350^{o}C as against 300^{o}C at a compression ratio of 18 (figures 1a and 2a), but this was not the case with a compression ratio of 15 (figures 4a and 5a), indicating that a compression ratio of 15 will be suited for di-methyl ether (DME) combustion in an internal combustion engine.
The efficiencies values derived for diesel fuel representative at compression ratios of 18 and 15 are not markedly different at the same initial temperatures as depicted in figures 1b, 2b, 3b, 4b and 5b, but same cannot be said for the brake mean effective pressure (BMEP) values, as there is a wide margin. Using a compression ratio of 18 will thus lead to better engine performance for diesel combustion in compression ignition engines than that of 15.

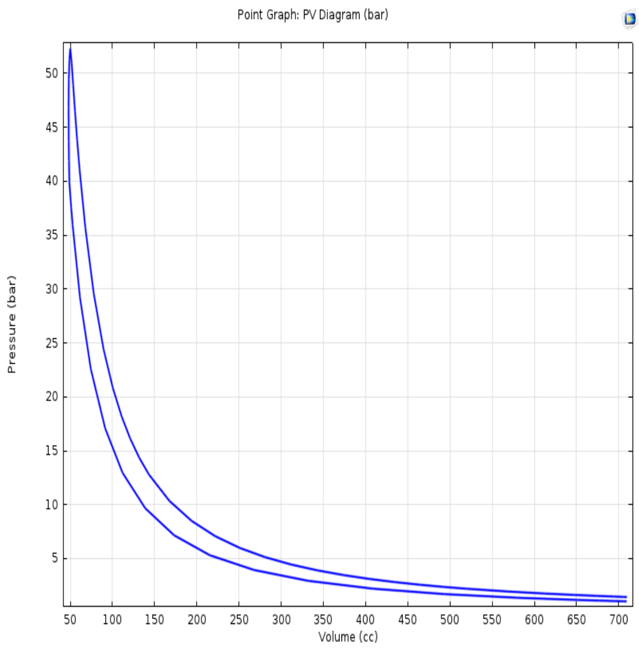

Figure 1a Initial Temperature; 300K, CR; 18, RPM; 2500

Mechanical energy output = 130.05J
η = = 63.7%
BMEP = = 196.61KN/m^{2}

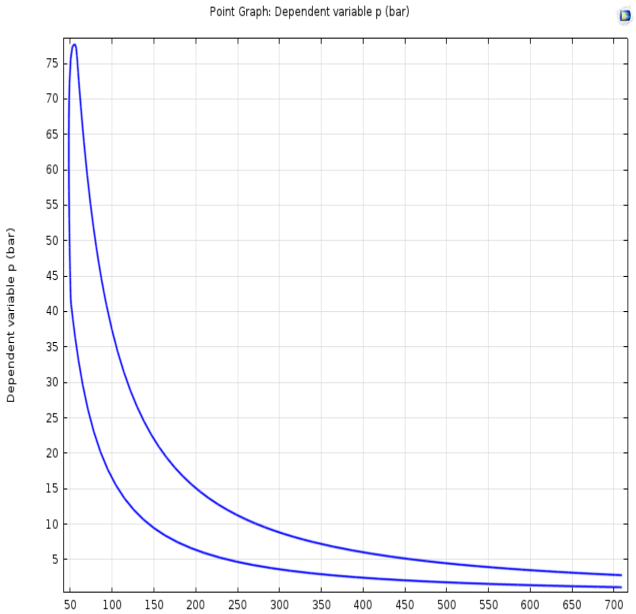

Figure 1b Initial Temperature; 300K, CR; 18, RPM; 2500

Mechanical energy output = 476.59J

ɳ = = 59.9%

BMEP = = 720.52KN/m^2

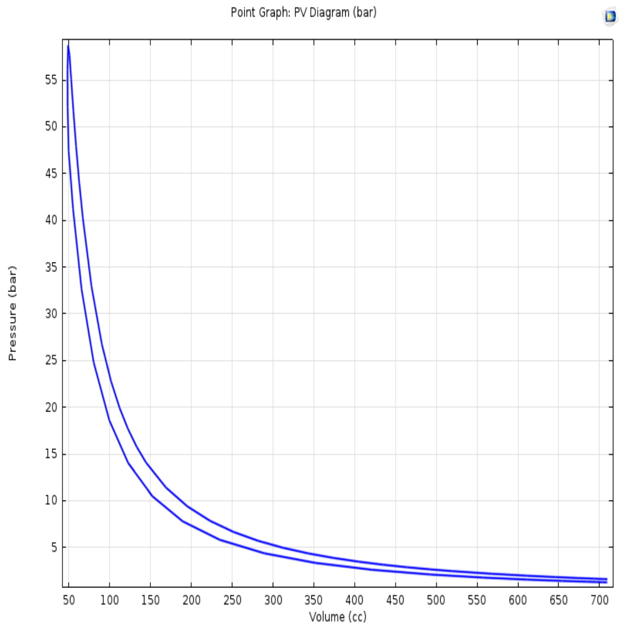

Figure 2a Initial Temperature; 350K, CR; 18, RPM; 2500

Mechanical energy output = 107.22J

ɳ = = 53.5%

BMEP = = 162.1KN/m^2

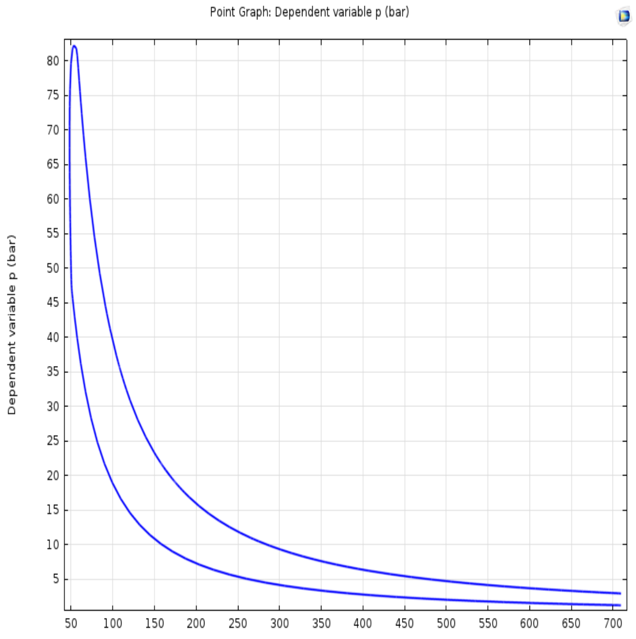

Figure 2b Initial Temperature; 350K, CR; 18, RPM; 2500

Mechanical energy output = 471.27J

η = = 58.9%

BMEP = = 712.48KN/m^2

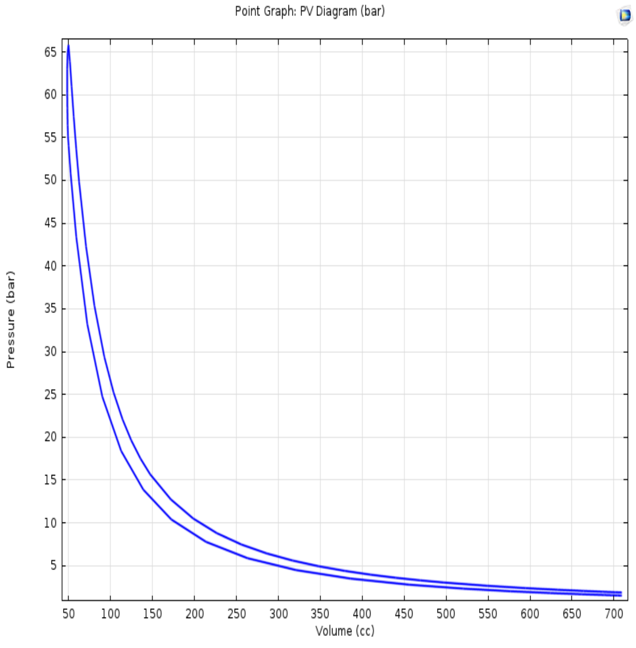

Figure 3a Initial Temperature; 400K, CR; 18, RPM; 2500

Mechanical energy output = 109.77J

η = = 56.5%

BMEP = = 165.9KN/m^2

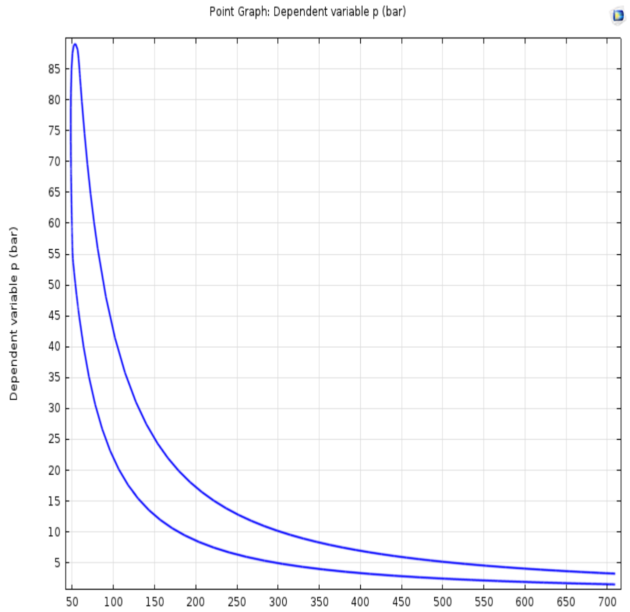

Figure 3b Initial Temperature; 400K, CR; 18, RPM; 2500

Mechanical energy output = 472.31J

η = = 57.9%

BMEP = = 714.05KN/m^2

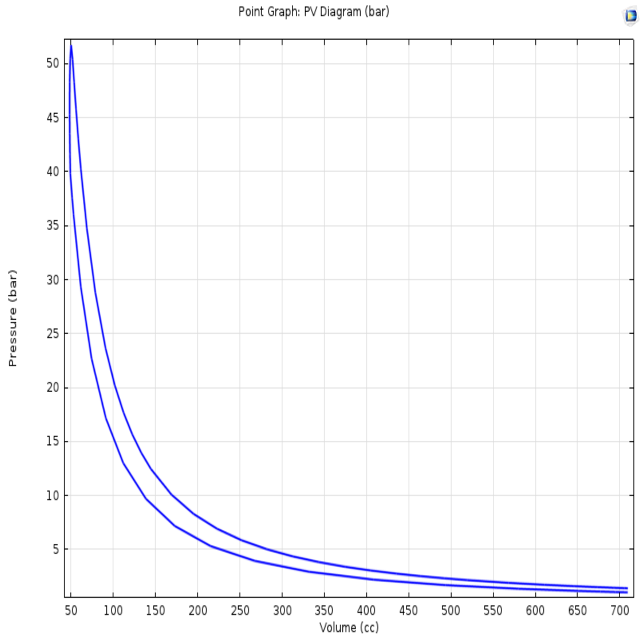

Figure 4a Initial Temperature; 300K, CR; 15, RPM; 2500

Mechanical energy output = 123.15J

η = = 63.3%

BMEP = = 186.18KN/m^2

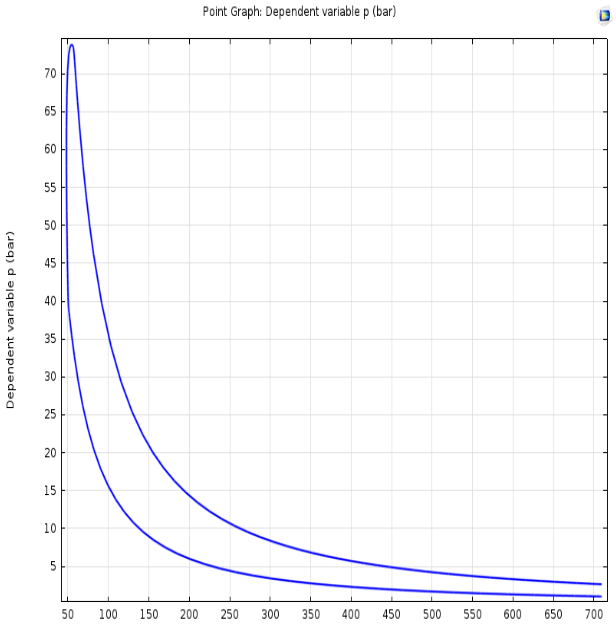

Figure 4b Initial Temperature; 300K, CR; 15, RPM; 2500

Mechanical energy output = 452.94J

η = = 60%

BMEP = = 684.77KN/m^2

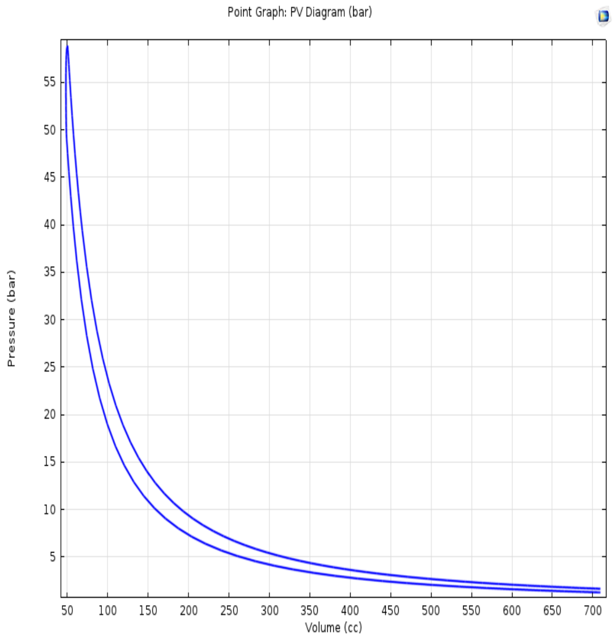

Figure 5a Initial Temperature; 350K, CR; 15, RPM; 2500

Mechanical energy output = 113.06J

η = = 62%

BMEP = = 170.93KN/m^2

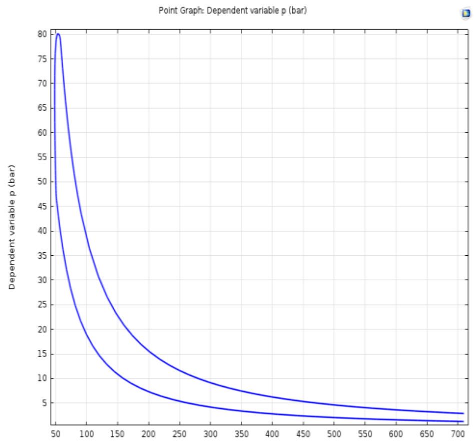

Figure 5b Initial Temperature; 350K, CR; 15, RPM; 2500

Mechanical energy output = 449.53J

ɳ = = 59.3%

BMEP = = 679.61KN/m^2

CONCLUSION

The thermal efficiency of compression ignition engines operated on di-methyl ether (DME) using initial temperature of 300^{o}C is greater than that operated on diesel fuel at the same initial temperature. While the engine operated on di-methyl ether (DME) have better performance in terms of thermal efficiency, the one operated on diesel fuel representative performs exceedingly better in terms of brake mean effective pressure. The compression ignition engine operated on di-methyl ether (DME) will hence be a better alternative to the one operated on diesel fuel when the amount of the work that is obtainable from the heat energy inherent in the fuel is of upmost importance.

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