

# Numerical Simulation of Tubular Combustion Chamber Using Kerosene-Methanol Blend

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**Abstract**— Traditional methods like modification of the firing system or post combustion treatment of the flue gas to reduce emissions of CO, CO<sub>2</sub>, and NO<sub>x</sub> are very expensive methods. Due to presence of limited reserve of conventional fuels and to reduce the emissions, scientist is continuously searching for the alternative fuels. Many study shows that partial replacement of conventional fuel by biomass based alternative fuels is good option to reduce the emissions. The present work aims to study effect of methanol on temperature and emissions when it is blended with kerosene. Four fuels are considered for numerical analysis kerosene and three blends of methanol (10%, 20% and 30% by volume). Two dimensional axi-symmetric combustor model is considered for numerical study. Ansys fluent 16 is used as CFD for numerical analysis. P1 gray radiation model, K-ε turbulence model, non-premixed combustion model, thermal NO<sub>x</sub> model and mass brooks model for soot are considered for analysis. Numerical results are compared with experimental results of literature taking kerosene as base line fuel. Numerical results show good agreement with the experimental results. Further numerical analysis is carried out to study the effect of methanol on emissions and combustor centerline temperature with blends. Result reveals reduction in emissions like CO, CO<sub>2</sub>, and NO<sub>x</sub>. Temperature distribution and flame length are affected by use of methanol blend.

**Keywords**— axi-symmetric, alternative fuel, blends of fuel, combustor, CFD, emissions, kerosene, methanol, non-premixed combustion.

## 1 INTRODUCTION

DAY by day increasing the consumption of fossil fuels imposed burden on conventional energy resources. Currently globe is facing problem like acid rain, climate change and global warming due to high pollutants emitted by fossil fuels. Looking towards crises of conventional fuels and problem concerning to high pollutants the momentum has shifted towards alternative fuels. The major alternative fuels currently used are bioethanol, alcohol and biomass [1]. Methanol has provided significant solution for emissions reduction due to its unique constituents and combustion characteristics [3]. Methanol is produced from various carbon based products like wood, biomass, natural gas and coal by the process of steam reforming [2]. Methanol is successfully reduced the emissions of CO, CO<sub>2</sub> and NO<sub>x</sub> due to lower C/H ratio, higher oxygen content and lower calorific value.

Methanol has huge potential to reduced emissions due to its unique physical and chemical properties. Many researchers have carried out experimental investigation to study effect of methanol blends on engine emission characteristics and performance. "yanju and canaksi [5], [6]" tested experimentally methanol-gasoline blend in SI engine. The results revealed that CO and NO<sub>x</sub> emissions shows reduction with the increase of methanol fraction in the gasoline. "sayin et al.[7]" experimentally studied effect of diesel-methanol blend on emissions of diesel engine by considering three blends of methanol. Result revealed that emissions of CO and NO<sub>x</sub> shows decrement

and emissions of CO<sub>2</sub> shows increment due to better combustion due to presence of methanol. "levy et al.[8]" Presented experimental study on swirl stabilized spray combustor to compare combustion characteristics of methanol and kerosene. It was found that emissions of CO is higher in case of methanol as compared to kerosene. These results clarify that to burn 100% methanol required longer combustor due to its slower burning rate. "chundnovsky et al. [4]" experimental study has shown that 50% reduction in NO<sub>x</sub> emission when light fuel is replaced by methanol and more than 80% reduction in NO<sub>x</sub> can be achieved by replacing the heavy fuel oil by methanol.

Combustion is complex phenomenon. It is difficult to understand by experimental study because ample amount of money and latest advanced technologies are required. The development in computer technology and availability of high speed computer has made easier to understand complex reacting combustion phenomenon, with the help of computation fluid dynamics (CFD) tool. "Ilbas et al. [9]" Investigated numerically turbulent diffusion flame in non-premixed combustion system. Reported results shows good agreement with the experimental data. "Shah et al. [10]" numerically studied the effect of swirler vane angle on thermal and emission characteristics of CAN combustor by solving RNG- k-ε model for turbulence and non-premixed combustion model with Probability Distribution Function (PDF) approach for combustion. They reported that RNG- k-ε model captured better flow physics for near wall flows, separated flows and rotating flow. "datta et al. [11]" considered Standard k-ε model with wall function treatment for near wall for turbulence and spray parameters are specified using PDF size distribution. Absorption of thermal radiation by various species has been modeled using first order moment method and formation of thermal NO<sub>x</sub> is governed by Zeldovich mechanism. "aliyu et al. [12]" has used discrete ordinate model (DO) for radiation. Combustion che-

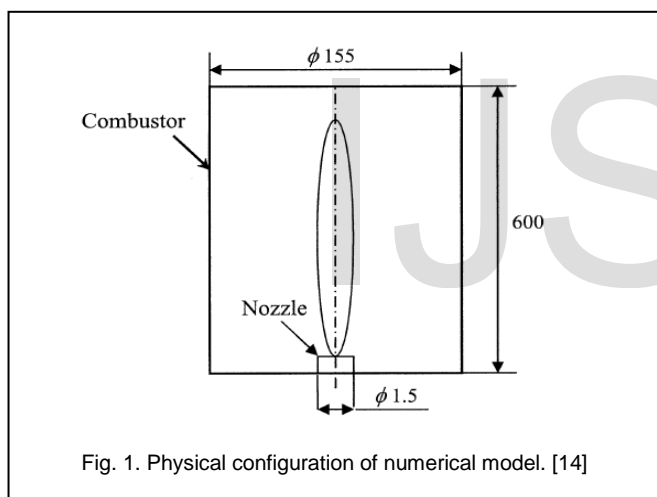
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mistry has been modeled using species transport model, and for turbulence standard  $k-\epsilon$  model is used.

From compiled summary of literature review it is conclude that intensive research is going on methanol as alternative fuel for internal combustion engine but minimal work has done on methanol as alternative fuel for combustor. Objective of present work is to develop computational domain for combustor, and study effect of methanol blend on emission characteristics and temperature distribution within combustor.

## 2 MODEL FORMULATION

Fig.1 shows physical configuration of numerical model. The combustor is comprised of 1.5 mm diameter cylindrical nozzle surrounded by coaxial annulus having outer diameter 155 mm. In present study [14] model is used for numerical simulation. "wen et al. [14]" has considered kerosene is a mixture of 20%  $C_7H_8$  and 80%  $C_{10}H_{22}$  and thus has a C/H ratio of 0.49. Present study has considered standard kerosene fuel present in fluent database having chemical formula  $C_{12}H_{23}$  and thus C/H ratio is 0.51. Boundary condition at inlet and outlet of fuel



and oxidizer are given separately. The velocity of inlet fuel and air is 22.28 m/s and 0.234 m/s respectively [14]. It is also note that prevaporized fuel is given at inlet and pilot flame is not included in numerical simulation. Detailed boundary conditions are given in table 1. The axi-symmetric condition is applied at central axis of a tube.

### 2.1 Numerical Methodology

In present study Turbulence chemistry is modeled using  $k-\epsilon$  turbulence model because this model gives good agreement between experimental and numerical results [16]. Thermal radiation absorption by various species has been modeled using P-1 radiation gray model. Soot formation is modeled using acetylene based Mass Brooks model [15]. Turbulence-combustion chemistry interaction has been modeled using non-premixed combustion model with PDF approach considering the chemical equilibrium condition. Thermal model are

TABLE 1  
BOUNDARY CONDITION OF CFD MODEL. [14]

Fuel	<ul style="list-style-type: none"> <li>Inlet velocity(m/s) = 22.28</li> <li>Turbulent intensity = 0.03</li> <li>Eddy length scale = 0.02</li> <li>Temperature(K) = 598</li> <li>Mole fraction of kerosene = 1, 0.9, 0.8, 0.7.....</li> <li>Mole fraction of methanol = 0, 0.1, 0.2, 0.3.....</li> </ul>
Air	<ul style="list-style-type: none"> <li>Inlet velocity(m/s) = 0.232</li> <li>Turbulent intensity = 0.03</li> <li>Eddy length scale = 0.02</li> <li>Temperature(K) = 288</li> <li>Mole fraction of oxidizer = 0.21</li> </ul>
Outlet	<ul style="list-style-type: none"> <li>Outlet pressure(bar) = 1</li> <li>Mole fraction of oxidizer = 0.21</li> </ul>
Wall	<ul style="list-style-type: none"> <li>No slip, adiabatic, stationary</li> </ul>

considered for the evaluation of NO containing in flame. Thermal NO formation is modeled following Zeldovich mechanism with steady state assumption for N-atoms, partial equilibrium between O-atoms and  $O_2$  molecules [11]. Numerical solution is based on finite volume method. Grid is generated using ICEM cfd, and ANSYS fluent 16 is used to solve the all transport equation. The SIMPLE algorithm is used for pressure-velocity coupling. The governing transport equations are solved iteratively at each and every node across computational domain. Mixture of fuel and air is ignited at 2500 K. The convergence criterion of all equations is solved at  $1 \times 10^{-6}$

### 2.2 Grid Independence Study

Validation of code and grid independence is important aspect of CFD simulation. Grid independence is carried out so that refinement in grid size does not change the result of simulation. Present study considers three Grids Grid A, Grid B and Grid C having number of cells 64692, 100181, 147382 respectively. Simulations are carried out for three different grid sizes

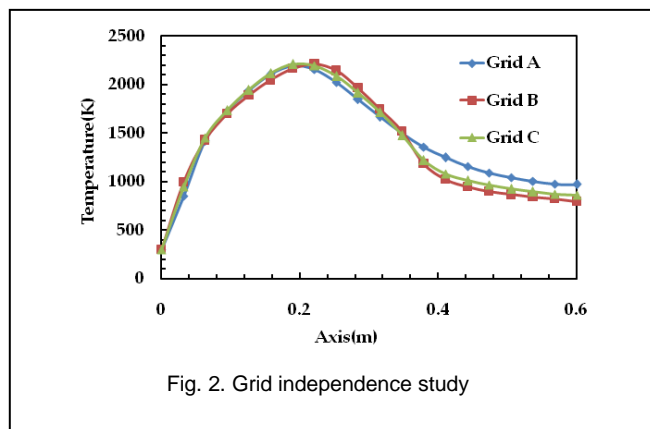


Fig. 2. Grid independence study

to arrive at independent grid for the combustor geometry. Variation of temperature along axis is considered as grid sensitive parameter. Variation of temperature along the axis is presented in fig.2. The grid sensitive parameter for Grid B and

Grid C almost overlaps each other so Grid B is taken for further numerical simulation.

### 3 VALIDATION OF NUMERICAL MODEL

The accuracy of any predicted result depends upon the accuracy of numerical computation. Numerical results of present study are compared with the experimental results of literature [14] by considering kerosene as fuel to validate numerical model.

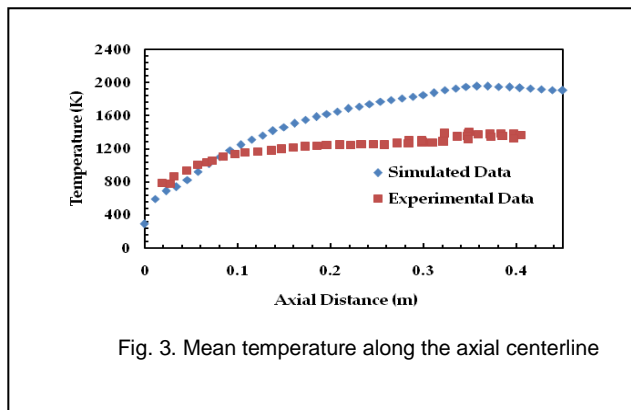


Fig. 3. Mean temperature along the axial centerline

Fig.3 Shows variation of mean temperature along the centerline of combustor. Numerical result shows good agreement with experimental results near the nozzle exit and over prediction in the region extending from an about 100 mm along length of combustion chamber due to exclusion of pilot flame in the numerical simulation and considering the chemical equilibrium condition during formulation of non-premixed model.

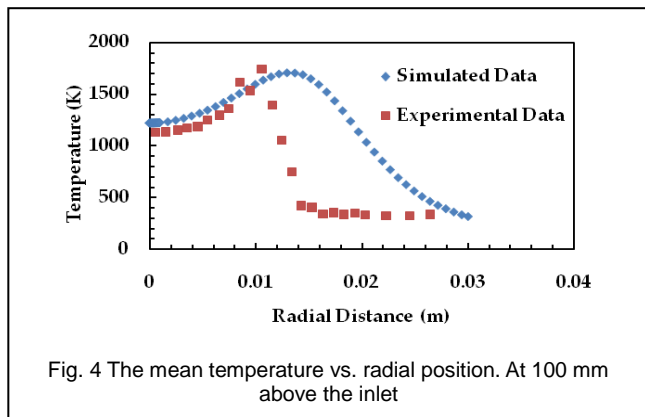


Fig. 4 The mean temperature vs. radial position. At 100 mm above the inlet

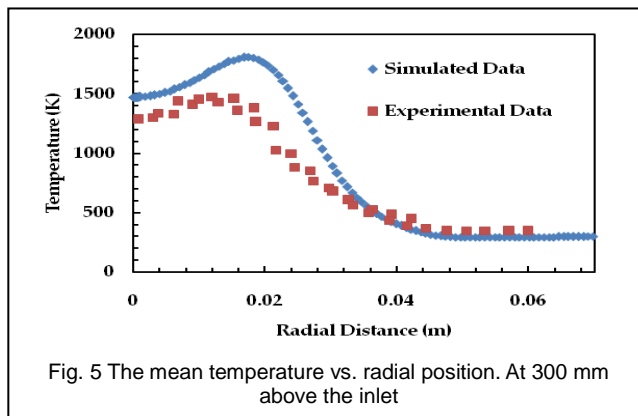


Fig. 5 The mean temperature vs. radial position. At 300 mm above the inlet

Fig. 4 and fig. 5 shows variation of mean temperature field along radial position at 100 mm and 300 mm above the inlet. In fig. 4 numerical result shows good agreement with the numerical result near the centerline and result are over predicted as move towards wall. In fig. 5 numerical result shows good agreement near the wall region and slightly over predicted near centre line. This behavior is attributed due to exclusion of various losses that occurs in experimental condition and considering chemical equilibrium condition.

### 4 RESULT AND DISCUSSION

Numerical analysis of axi-symmetric combustor has done and results of temperature and emissions along axial direction are presented. This section is mainly focused on impact of methanol addition on emissions and temperature.

#### 4.1 Effect of Methanol on Temperature

The exhaust gas temperature is an indication of energy content. Exhaust gas temperature gives pattern factor which determines the life of blades of gas turbine. Fig. 6(a), fig. 6(b), fig. 7(a) and fig. 7(b) are representing contours of temperature for non-premixed kerosene and kerosene methanol blends. Maximum Flame temperature is occurred for kerosene that is 1940 K and drops in temperature occurs with the addition of methanol. Drop in flame temperature for kerosene and M10 is about 46 K. However further increasing the share of methanol

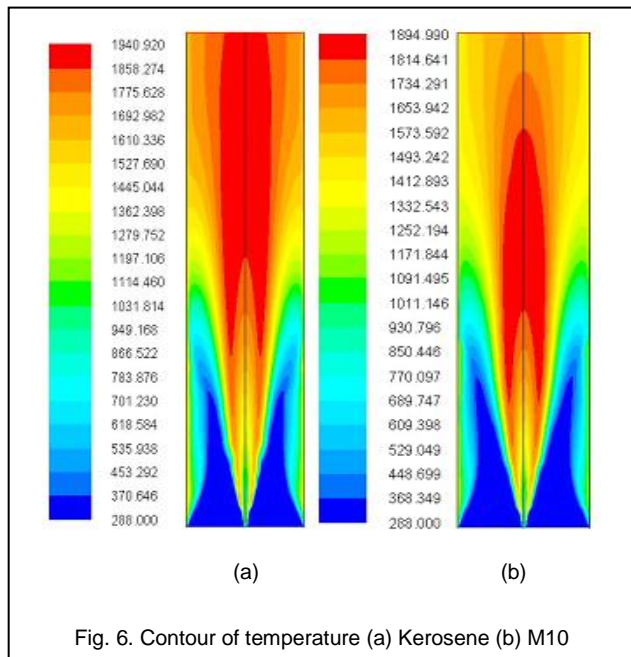


Fig. 6. Contour of temperature (a) Kerosene (b) M10

to 20% and 30% drop in temperature is only 11K. Looking towards temperature contours it is found that maximum flame length occur for the kerosene and Flame length shows decrement with methanol blends. Lower calorific value of methanol is responsible for reduction in temperature.

Fig. 8 shows variation of temperature along axial direction. It is observed that temperature shows increment from inlet to outlet because combustion proceeds to completion from inlet to outlet due to availability of more coflow air. Initially temperature shows little variation with addition of methanol and temperature shows decrement from 0.3 m distance from inlet with addition of methanol. This phenomenon takes place due to lower calorific value and cooling effect produced by methanol.

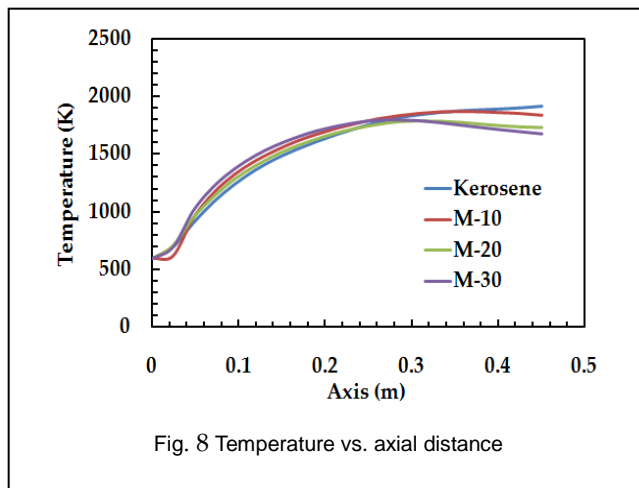


Fig. 8 Temperature vs. axial distance

#### 4.2 Effect of Methanol on Emissions of CO

Emissions of CO are hazardous and must be restricted. It is produced by incomplete combustion of fuels. Fig. 9 shows the variation of mole fraction of CO with axial distance along the combustion chamber. It is observed that maximum concentration of CO present at inlet and decreases as move towards the outlet. Reason for this behavior is that, incomplete combustion present near the inlet and proceeds to complete combustion towards outlet due to presence of more air for combustion. It is also observed that concentration of CO decreases with increase in percentage of methanol. This behavior is attributed due presence of oxygen content in methanol which help for complete combustion [13].

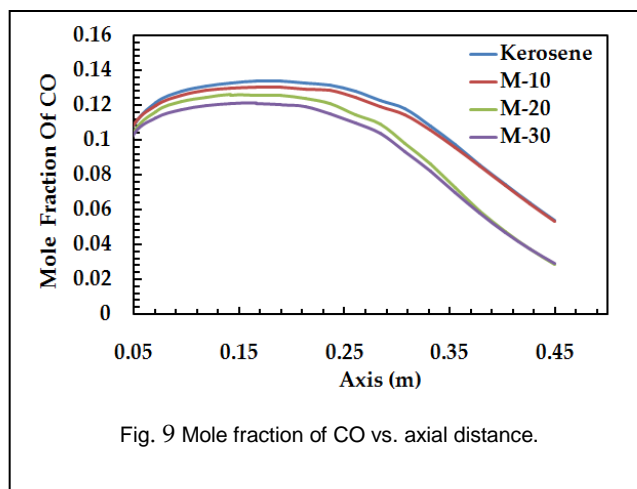


Fig. 9 Mole fraction of CO vs. axial distance.

#### 4.3 Effect of Methanol on Emissions of CO<sub>2</sub>

Formation CO<sub>2</sub> is normal during process of combustion. It is responsible for global warming that's why its emission must be reduced. Fig. 10 presents variation of mole fraction of CO<sub>2</sub> along axial direction. It is observed that concentration of CO<sub>2</sub>

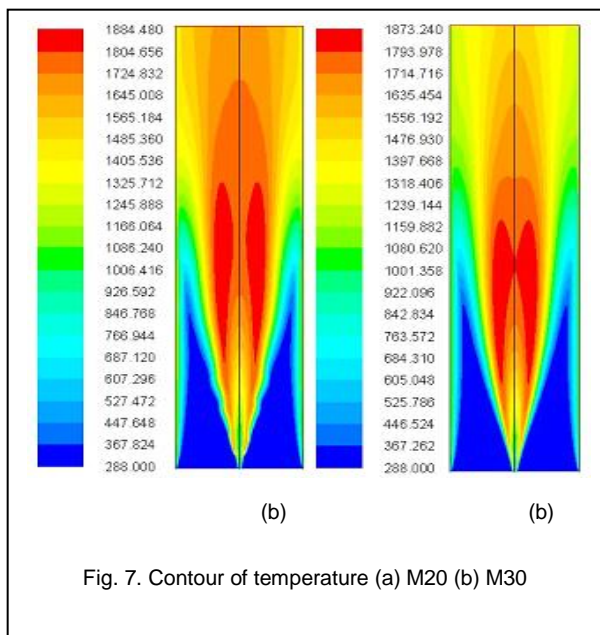


Fig. 7. Contour of temperature (a) M20 (b) M30

is minimum at inlet and increases to maximum towards outlet due to complete combustion as proceed towards outlet. Concentration of CO<sub>2</sub> decreases with percentage of methanol due to lower C/H ratio of methanol compared to kerosene [13].

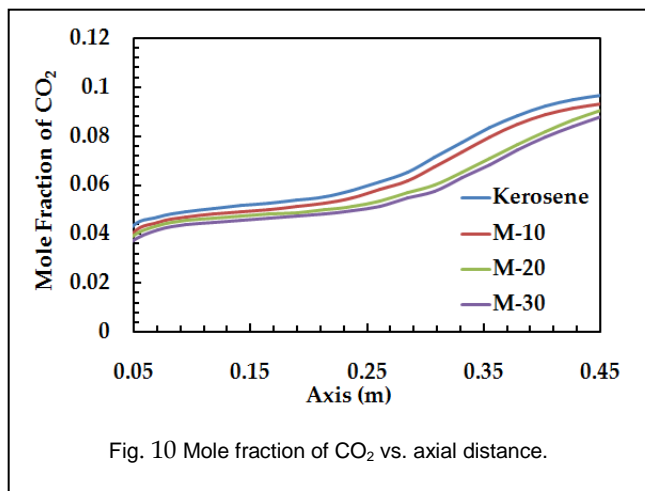


Fig. 10 Mole fraction of CO<sub>2</sub> vs. axial distance.

#### 4.4 Effect of Methanol on Emissions of NOx

NOx is most critical emissions from combustor. In nature it exits in two forms one is oxide form and other is dioxide form. It is mainly responsible for acid rain and its emissions must be restricted. Fig. 11 shows variation of mole fraction of NOx along axial direction. It is found out that concentration of NOx is minimum at inlet and increases to maximum towards outlet due to increase in temperature as move towards outlet as result of complete combustion. Concentration of NOx decreases with increase in the percentage of methanol due to lower flame temperature and the calorific value of methanol is lower than kerosene. It also note that Methanol produces cooling effect on the charge due to its higher latent heat of vaporization as compared to kerosene and Emission of nitrogen oxide is reduced as a result of cooling effect[6].

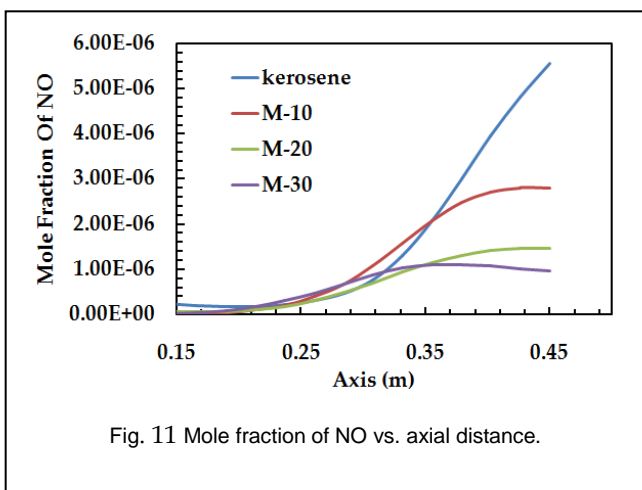


Fig. 11 Mole fraction of NO vs. axial distance.

#### 4.5 Emissions and Temperature Along Radial Direction

Table 2 is comparing emissions like CO, CO<sub>2</sub>, and NOx and also the temperature for different blend of methanol. It is observed that concentration of CO, CO<sub>2</sub>, and NOx is decreased with increased in the percentage of methanol in kerosene. Presence of oxygen content in fuel help for complete combustion which reduces CO emission. Concentration of CO<sub>2</sub> is reduced due to lower C/H ratio of methanol as compared to kerosene. Concentration of NO is reduced due to lower calorific value of methanol which reduces maximum flame temperature. It is also evident from the table that temperature is decreasing with increasing the percentage of methanol due to lower calorific value of methanol.

TABLE 2  
COMPARES EMISSION OF CO, CO<sub>2</sub>, NO AND TEMPERATURE ALONG RADIAL DIRECTION AT AXIAL DISTANCE OF 100 MM

Fuel	Max. mole fraction of CO	Max. mole fraction of CO <sub>2</sub>	Max. mole fraction of NO	Max. Temperature
Kerosene	0.130495	0.064822	1.85×10 <sup>-07</sup>	1761.59
M10	0.127516	0.062566	4.4×10 <sup>-08</sup>	1738.37
M20	0.123497	0.061335	2.98×10 <sup>-08</sup>	1726.79
M30	0.118751	0.060585	3.34×10 <sup>-08</sup>	1717.66

#### 5 CONCLUSION

The major findings of present investigation are:

- In present study numerical result compare with the experimental result from this It is conclude that numerical results shows good agreement with the experimental results. Result of temperature shows over prediction towards exit due to exclusion of pilote flame in numerical simulation and using chemical equilibrium condition during model formulation.
- CO shows reduction with addition of methanol in base line fuel due to presence of oxygen in methanol which helps for complete combustion.
- CO shows reduction with blends of methanol due to lower C/H ratio of methanol (0.25) as compared to kerosene (0.51).
- Temperature shows decrement in value with increase percentage of methanol in kerosene due to lower heating value of methanol
- NOx decreases with addition of methanol in kerosene

due to lower heating value of methanol as compared to kerosene.

- Temperature and emissions shows minimal variation for M20 and M30 so M20 can be used as optimal blend.

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