

# Analysis of Catalytic Converter Performance with Air Box using CFD Technique

<sup>1</sup>Ch.Indira Priyadarsini, <sup>2</sup>Dr.M.V.S.MuraliKrishna, <sup>3</sup>Dr.P.UshaSri

<sup>1</sup>Assistant professor, Mechanical Engg. Dept., CBIT, Gandipet, Hyderabad,

<sup>2</sup>Professor, Mechanical Engg. Dept., CBIT, Gandipet, Hyderabad

<sup>3</sup>Professor, Mechanical Engg. Dept., OU, Hyderabad

## ABSTRACT

*Catalytic converter is one of the import element in reduction of automobile exhaust emissions without changing the basic design of engine. This paper deals with the basic understanding of typical species transportation inside converter using computational fluid dynamics techniques as it is very difficult to visualize inner flow pattern. The study of pressure contours and velocity vectors of exhaust gas are observed using numerical model. the model is created by ANSYS Workbench, domain discretization and analysis was carried out in Fluent. The substrate is modeled as porous media and boundary conditions of mass flow and temperature is applied using analytical calculations. Converter is equipped with air box for further increase in turbulence thereby decreasing the emissions rapidly. The results showed that the converter with air box performed better that converter without air box.*

**Keywords—** CFD, Catalytic Converter, Spark Ignition, Flow, Fluent,

## I. INTRODUCTION

The spark ignition engine exhaust gases contains oxides of nitrogen (NO<sub>x</sub>) 20g/kg of fuel, carbon monoxide (CO) 200g/kg of fuel, and organic compounds which are unburned or partially burned hydrocarbons (UHC) 25g/kg of fuel [2]. Catalytic converter is a stainless steel container mounted along the exhaust pipe of engine and inside the container is a porous ceramic structure through which the exhaust gas flows [3]. In most of the converters, the ceramic is a single honey comb structure with many flow passages. The passages comprises of many shapes, including square, triangular, hexagonal and sinusoidal. Early converters used loose granular ceramic with the gas passing between the packed spheres. Since it is difficult to keep the sphere in place, many converter developers opted for ceramic monolith which offers various advantages. Among these advantages are smaller volumes, lower mass and greater ease of packaging (Heck & Farrauto, 1995), [4]. The active catalyst layer is applied on the monolith walls. The coating, called washcoat, is composed of porous, high surface area inorganic oxides such as  $\gamma$ Al<sub>2</sub>O<sub>3</sub>(gamma alumina), CeO<sub>2</sub> (Ceria) and ZrO<sub>2</sub> (Zirconia). Noble metal catalyst, such as Platinum (Pt), Palladium (Pd) and Rhodium (Rh), are deposited on the surface and within the pores of the washcoat (Pontikakis, 2003) . Exhaust gas flowing in a catalytic converter diffuses through the washcoat pore structure to the catalytic sites where heterogeneous catalytic reactions occur. The specific reactions vary with the type of catalyst installed. Most present-day vehicles that run on gasoline are fitted with a “three way” converter, so named because it converts the

three main pollutants in automobile exhaust: carbon monoxide, unburned hydrocarbon and oxides of nitrogen. The first two undergo catalytic combustion and the last is reduced back to nitrogen [5]. The nature of the exhaust gas flow is very important factor in determining the performance of catalytic converter. The pressure gradient and velocity distribution through the substrate are important in particular. Therefore CFD analysis is used to design efficient catalytic converters by modeling the exhaust gas flow, the pressure drop and the uniformity of flow through the substrate can be determined. In this paper ANSYS FLUENT (ANSYS Work Bench 14.5, Fluid Flow-Fluent) is used to model the flow of exhaust gas through catalytic converter, so that the flow field may be analyzed. Catalyst substrates coated with the active catalyst washcoat are packaged in steel housings to form catalytic converters. Emission performance durability and mechanical durability are the two key aspects of the overall durability of an emission control system. The emission durability depends on the quality of the catalyst coating and on the operating conditions such as temperature or levels of catalyst poisons in the exhaust gas. In CFD, the system consumes less memory space and less response time, if the rectangular cross section is assumed. However, in actual practice, the rectangular corners are suitably rounded off which ensures the smooth flow of exhaust gas with less turbulence near the wall sides [6]. On other hand the flow characteristics of emissions such as velocity, pressure and temperature play an important role for conversion rate and light-off behaviour of converter [8]. Jamuna Rani.G et.al performed flow analysis on diesel engine and found back pressure and emissions using catalytic converter with air box. The emissions and the back pressures are identified at different speeds. The Back pressure exerted by the catalytic converter during the working condition causes the decrease in the volumetric efficiency and it leads to increase in fuel consumption [9]

## II. EMISSION CONTROL USING CATALYTIC CONVERTER

Besides the efficiency, emissions of an engine are also an important parameter as it directly affects the environment. The primary constituents of the exhaust gas from an engine are unburnt hydrocarbons and oxides of carbon and nitrogen, which can be controlled by varying the engine design and operating parameters. CO/ UBHC emissions in engine exhaust of different versions of the combustion chamber of engine were measured with Netel Chromatograph analyzer at full load operation of the engine. The accuracy of measurement of emission is  $\pm 1\%$  at full load operation.

### 2.1 Catalytic Converter

A catalytic converter fitted to exhaust pipe of engine is shown in Fig. 1. A mild steel, hollow cylinders were made and chemically cleaned with a solution of 10% sodium hydroxide and then with 5% nitric acid and finally dried. For the preparation of catalytically active coating, aluminium oxide was used as the oxidizing catalyst. Kaolinite is clay mineral with the composition of  $Al_2SiO_5(OH)_4$ , high temperature RTV silicone, bentonite clay and gel solutions consisting of tetra ethyl orthosilane and ethanol were used as the binders. The finely powdered catalyst and chosen binder were intimately mixed and slurry was made by mixing with a suitable solvent. The hollow cylinders are coated by dipping in the slurry solution and then dried. After drying, the adhesion of the catalytic coating was tested by manual abrasion of the coatings. Aluminium oxide of thickness 500 microns was coated on inside portion of catalytic converter. Discharge of the engine was calculated from diameter of the opening through which exhaust gases enter into the catalytic chamber by assuming the velocity of exhaust gases (2–4 m/s). The length of the chamber was determined calculating the pressure drop. Provision was also made to inject a definite

quantity of air (60 l/m) into catalytic converter. Air quantity drawn from compressor and injected into converter was kept constant so that backpressure does not increase.

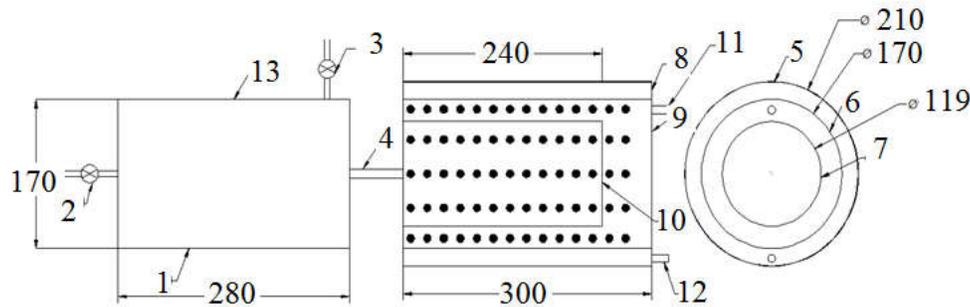


Fig. 1 Details of catalytic converter. (All dimensions are in mm)

1. Air chamber 2. Inlet for air chamber from the engine 3. Inlet for air chamber from the compressor 4. Outlet for air chamber 5. Catalytic chamber 6. Intermediate-cylinder 7. Inner-cylinder 8. Outer sheet 9. Intermediate sheet 10. Inner sheet 11. Outlet for exhaust gases 12. Provision to deposit the catalyst and 13. Insulation.

### III COMPUTATIONAL FLUID DYNAMICS (CFD)

Computational fluid dynamics usually abbreviated as CFD, is a fluid mechanics branch that uses numerical methods and algorithms to analyze problems that involve complex fluid flows. It gives insight into flow regime that are very difficult, expensive or sometimes impossible to study using traditional methods. A commercial tool of FLUENT simulation is used in this work to determine the flow patterns and pressure drop across the catalytic converter. Catalytic Converter consist of substrate where emission conversion reaction takes place.

#### 3.1 Objective of CFD Study

The main objective of CFD study is to simulate fluid flow and heat transfer in a Catalytic Converter in order to determine internal flow pattern and its impact on flow distribution, flow distribution over inlet of substrate, velocity and pressure flow across the catalytic converter.

#### Governing Equations:

The governing equations are the equations of conservation of mass \_both overall and individual species\_, momentum and energy, and are written as

$$\text{Mass: } \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho V) = 0$$

$$\text{Momentum: } \frac{\partial (\rho u)}{\partial t} + \nabla \cdot (\rho u V) = -\frac{\partial p}{\partial x} + \frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{yx}}{\partial y} + \frac{\partial \tau_{zx}}{\partial z} + \rho f_x$$

$$\text{Energy: } \frac{\partial (\rho h)}{\partial t} + \nabla \cdot (\rho U h) = -\nabla q + S_h$$

$$\text{Species mass: } \frac{\partial(\rho Y_k)}{\partial t} + \nabla \cdot (\rho U Y_k) = -\nabla \cdot \mathbf{J}_k + S_k$$

Where  $\rho$  is the mixture density;  $p$  is the pressure;  $\tau$  is the shear stress tensor; and  $\mathbf{f}_x$  is the body force vector.,  $Y_k$  is the mass fraction of the  $k^{\text{th}}$  species,  $\mathbf{J}_k$  is the mass diffusion flux of the  $k^{\text{th}}$  species, and  $S_k$  is the production rate of the  $k^{\text{th}}$  species due to homogeneous chemical reactions. The total number of gas-phase species in the system is denoted by  $N$ .

### 3.2 FLUENT steps

Geometry, mesh model, physics setup / Solution and Post processor are the steps involved in simulation.

#### 3.2.1 Geometry

A 2D converter model is created in design modeler the main benefits of this 2D figure is reducing the computing time as number of elements are less the most accurate mesh can be generated and convergence error is reduced therefore very accurate results will be obtained. But in case of 3D analysis too many elements too much of care required while meshing takes more computing time chances of errors will be more therefore whenever the problem meets the 2D approximation criteria it is best to go with as shown in Fig. 2 and 3.

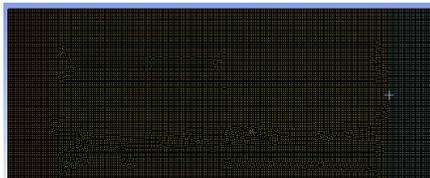


Fig. 2 Geometric modeling of catalytic converter without air box

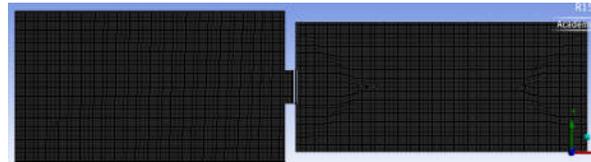


Fig. 3 Geometric modeling of catalytic converter with air box

#### 3.2.2 Mesh model

A mapped face meshing is created using ICEM CFD with 37549 nodes and 35795 elements for without air box and 68517 nodes and 67725 elements for converter with air box. The domain names velocity inlet at entrance of converter where exhaust gases flow in and out of manifold, pressure outlet at exhaust to atmosphere and porous substrate to surface for catalytic activity takes place have been assigned as shown in Fig. 4 and 5.

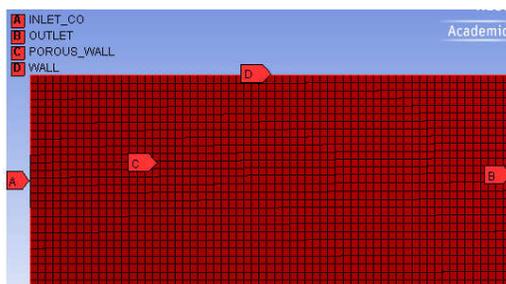


Fig.4 Mesh model with boundary names without air box

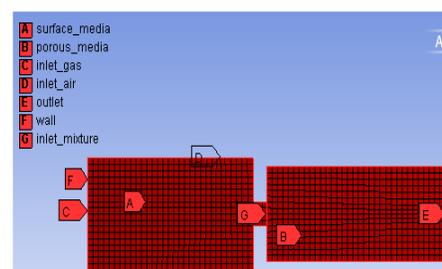


Fig.5 Mesh model boundary names with air box

### 3.2.3 Boundary Conditions

The boundary conditions for CFD analysis has been calculated analytically using fundamental formulas of internal combustion engine and given mass flow as 0.816 kg/s, velocity 2m/s, temperature 723 <sup>0</sup>K and pressure 1.35bar. External air properties are assigned as atmospheric conditions.

## IV RESULTS AND DISCUSSION

### 4.1 Velocity in catalytic converter

The flow velocity is shown in Fig. 6 and 8 for Set-B-catalytic converter without air box and Set-C-catalytic converter with air box.

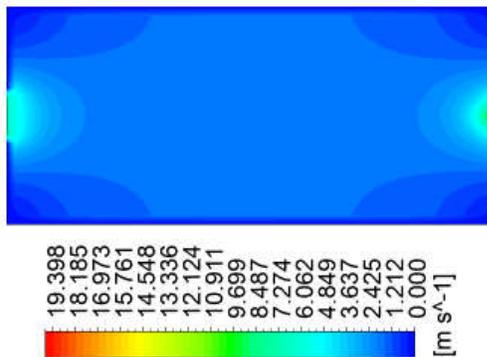


Fig.6 Flow of velocity in catalytic Converter

It is observed that velocity of fluid is maximum during inlet and outlet of catalytic converter with both the sets. The velocity of gases has been rapid in the middle section where the fluid velocity changes as it passes through the porous substrate due to friction developed across the wall of converter but at the substrate region the shear stresses are very less and is negligible resulted in low velocity is in substrate region of 2.42 m/s for Set-B and 2.38 m/s for Set-C . The X-velocity distribution of the fluid flow showed evident how the fluid decelerates rapidly when entering to the porous region and velocity profile becomes more uniform as the fluid passes through the porous media.

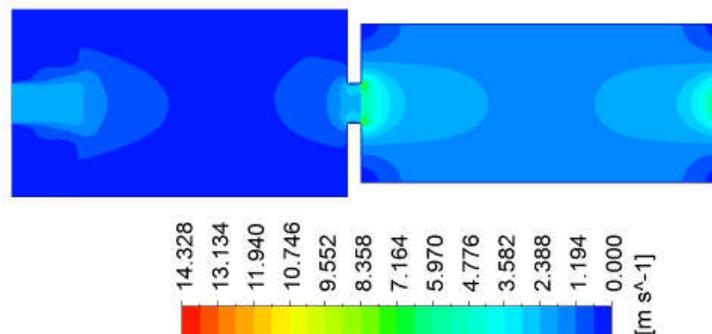


Fig.7 Flow of velocity in air box and catalytic converter

It can also be observed how the fluid recirculates before entering the central region of the catalyst (negative values of X-velocity component in dark blue) due to the resistance exerted by the porous media. This allows the metal catalyst present in the substrate to be more effective. The area in green, which corresponds to a moderate velocity, increases in extent just before the exhaust gases enters the substrate and then decreases as it passes through and

velocity is very high at exits the substrate. The exhaust gases to exit the chamber and speed along at the highest velocity (Set-B-19.398m/s,Set-C-14.328m/s) possible. While it is true that the narrower the pipe, the higher the velocity of the exiting gases, wide enough so that there is as little back pressure as possible while maintaining suitable exhaust gas velocity.

#### 4.2 Pressure flow in catalytic converter

The variation of pressure is shown in Fig.8 and 9 for Set-B-catalytic converter without air box and Set-C-catalytic converter with air box. The contour of total pressure plot explains the efficiency of catalytic converter after changing the inlet geometry by connecting the air box between exhaust pipe and converter. Pressure at inlet is directly proportional to divergence angle. A straight pipe has been used in experiment in place of converging diverging as flow separation is less at low divergence angle is justified. The pressure drop can be high, due to the inertial and viscous resistance of the porous media.

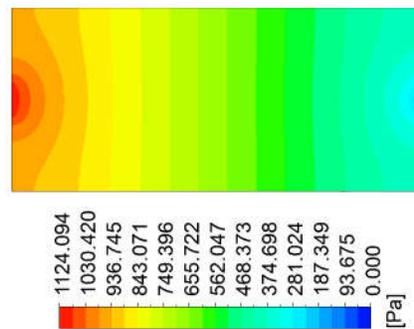


Fig.8 Back pressure in catalytic converter without air box

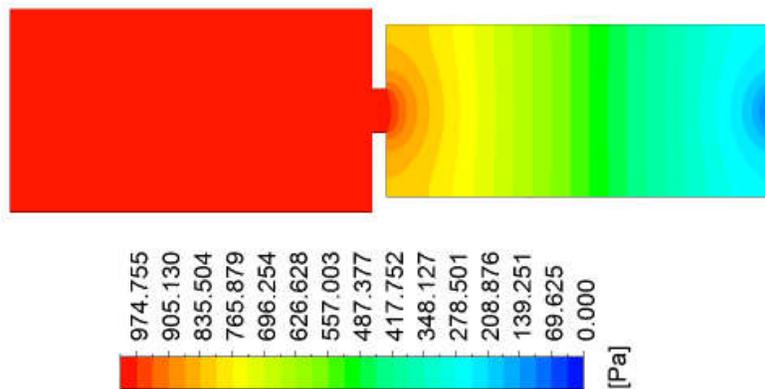


Fig.9 Back pressure in catalytic converter with air box

It is noticed that there is a variation of pressure drop along the distance of catalytic converter. The pressure drop is less at the outlet as the fluid can easily pass through in the inlet and outlet duct because these are not having any obstruction to the fluid. It is spotted that there is a non uniform flow inside the converter due to the flow separation at the inlet section. The Pressure at inlet increases because of the substrate, which is placed at the path of flow. This sudden increase in pressure drop takes place due to presence of catalyst beads and steel wire mesh which resist the motion of the air due to that there is sudden decrease in pressure takes place.

#### 4.3 Temperature flow in catalytic converter

Fig. 10 and 11 shows the temperature flow in converter for Set-B & Set-C. In the substrate it is relatively even and symmetrical with steady increase of temperature near the inlet of the monolith due to heat reaction. Behind the reaction zone the temperature decreases steadily. It is observed that there is a temperature decrease in catalytic converter with air box compared to without air box due to compressed air combined with exhaust gases in air box before entering into the converter.

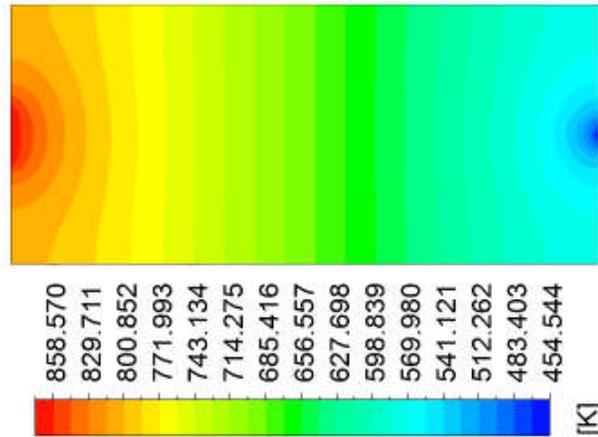


Fig.10 Temperature flow in catalytic converter without air box

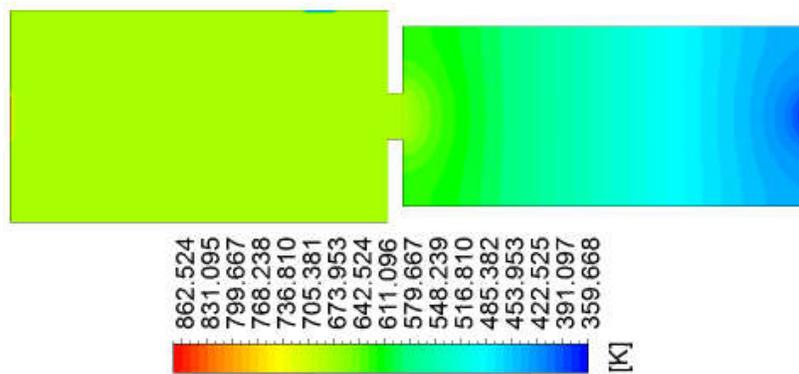


Fig.11 Temperature flow in catalytic converter with air box

Important flow parameters: velocity, pressure and temperature from inlet to outlet showed in Tables 1. Velocity has been reduced in Set-C by 1.5% at inlet and 26.14% at outlet, which helps to improve the catalytic reaction with exhaust gases in converter with air box. Low pressure drop of 974.755 Pa is observed from the below table indicating that Set-C performed 13.28% better than Set-B this is due to air in air box restricts the back flow of gases which reduces the back pressure by 5.25% and temperature reduced by 9.78% in Set-C against Set-B.

Table.1 Inlet & outlet values of converter for Set-B and Set-C

	Velocity(m/S)		Pressure (Pa)		Temperature(°C)	
	inlet	outlet	inlet	outlet	inlet	outlet
Set-B	7.274	19.398	1124.094	0	585.57	181.544
Set-C	7.164	14.328	974.755	0	529.524	86.668

4.4 Flow of CO and UBHC in catalytic converter

The porous media effect on CO and UBHC shown in Fig. 12 and 13 for Set-B: catalytic converter without air box and Set-C: catalytic converter with air box.

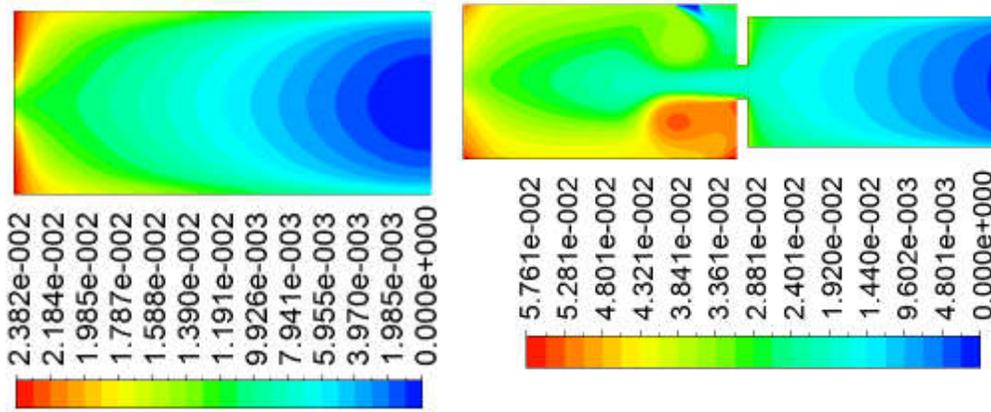


Fig. 12 CO emissions from CE with pure gasoline for Set-B and Set-C

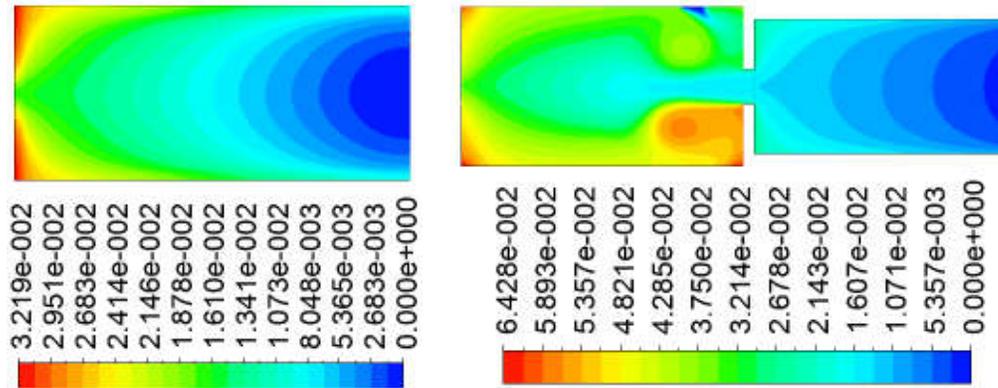


Fig. 13 UBHC emissions from CE with gasoline for Set-B and Set-C

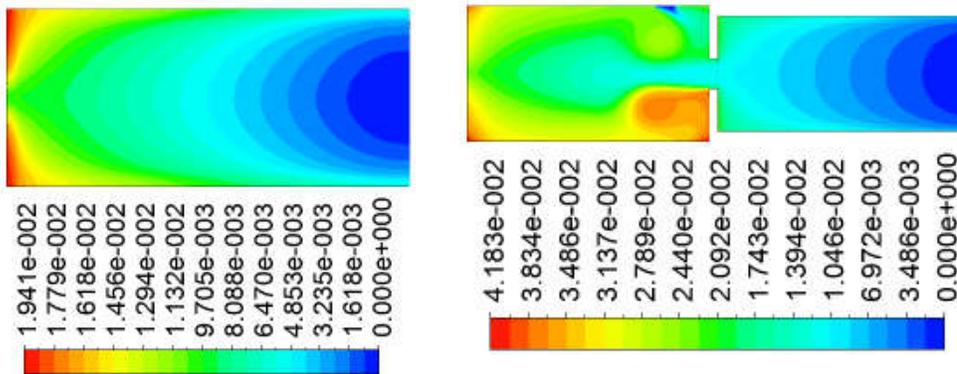


Fig. 14 CO emissions from CCE with gasoline for Set-B and Set-C

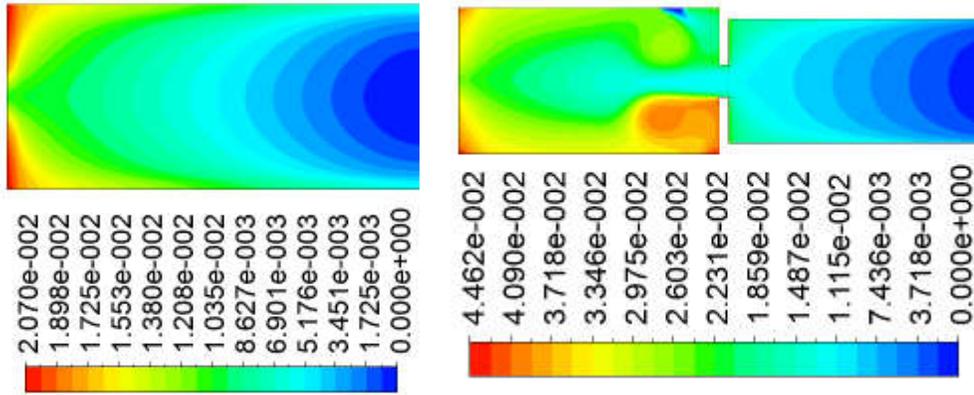


Fig. 15 UBHC emissions from CCE with gasoline for Set-B and Set-C

**4.5 Comparison of simulation with experimental results**

The validation of FVM result obtained from the tool FLUENT with experimental investigations [10] on CO and UBHC is shown in Fig. 16 and 17. It is observed that the obtained result of monolithic catalytic converter with different configurations with air box and without air box and boundary condition shows good agreement, validated in narrow limits of 20% error with the experimental results. The small variation in results is due to variation in mesh sizing, operating condition, geometric parameters and simplification of design by considering axi-symmetric model to reduce the effort, solution time, burden on PC RAM etc. but the obtained result shows the same trend so that the results are suitably verified.

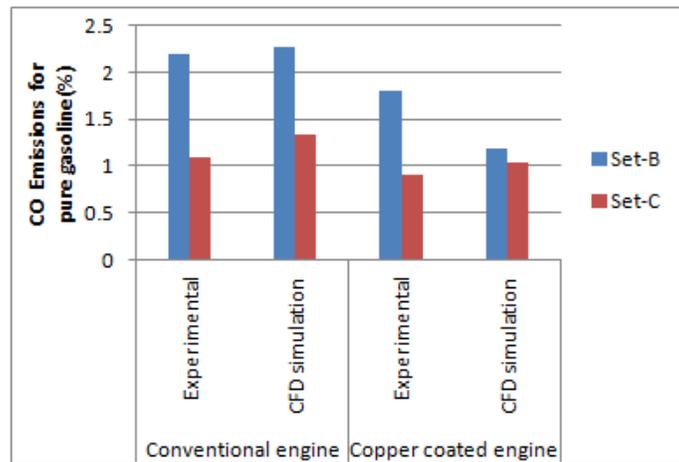


Fig.14 CO emissions from experimental and CFD for Set-B & Set-C with both versions of engine using pure gasoline

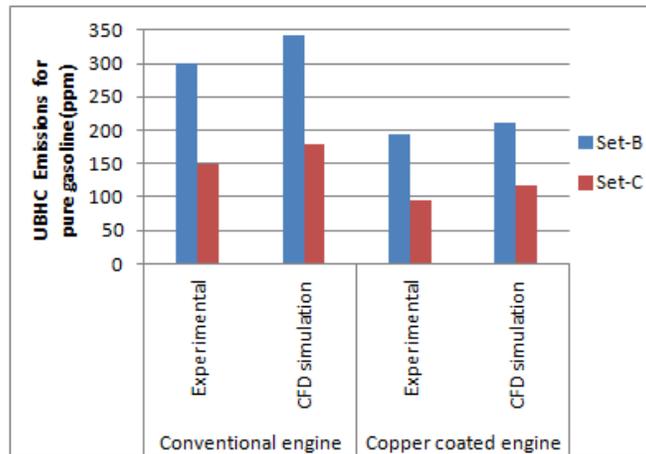


Fig.15 UBHC emissions from experimental and CFD for Set-B & Set-C with both versions of engine using pure gasoline

## V CONCLUSIONS

1. Computational results shown velocity was uniform in porous region resulted in better rate of conversion of pollutants, significantly changed with air box concept.
2. A decreased back pressure shown in Set-C by 13.3% and EGT by 52%.
3. Carbon monoxide and Unburned hydro carbons reduced by 50%-66.6% in CE and 38%-75% in CCE.
4. Flow simulation manifested good agreement and validated in narrow limits of 20% error with the experimental investigations.

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