Numerical Investigation and Performance Evaluation of A Catalytic Converter

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Abstract*- The catalytic converter is a device which converts harmful exhaust gases from internal combustion engine into harmless gases. Harmful gases like NOX, CO, unburned HC etc. are converted into N2, CO2, H2O respectively. Internal Combustion engines generate undesirable emissions during the combustion process, which include, NOX CO, unburned HC and NOx smoke etc. Apart from these unwanted gases, it produces Particulate Matter (PM) such as lead, soot etc. All these pollutants are harmful to environment and human health. They are the main causes for greenhouse effect, acid rain, global warming. The main materials used in this project is to vary the catalyst materials like palladium rhodium and platinum which are highly used as a catalyst to control emission.*

Keywords- CFD, Catalytic Converter, Particulate Matter (PM), Wire Mesh

I. INTRODUCTION

Introduction with Catalytic Converter

Exhaust gases from Scooters, Motorcycles, Mopeds and Three Wheelers are contribudes significantly to air pollution, especially in major cities. If, present trends in increased living standards and population migration to cities continue, air quality in major cities is expected to decline because of the increased number of vehicles. To reduce air pollution from motorcycles and scooters, the government since 1996 has enforced emission standards. Most of the motorcycle manufacturers were able to meet the 1996 emission Standards (HC + N02= 3.6 g/km and CO = 4.5 g/km) by making design changes in the transfer ports and tuning the carburettor to a leaner air-fuel mixture. However, to achieve year 2000 emission standards (HC + $N0_2$ = 1.5g/km and CO = 2.0 g/km), the motorcycle manufacturers must either use 4-stroke engines or install catalytic converters on 2-stroke engines Responsiveness and manoeuvrable performance will be lost with a transition to 4-stroke engines.

In Taiwan the catalytic converter approach for reducing HC and CO emissions from 2-stroke motorcycles and scooters has been studied for the last five years on various vehicles. Engine out emissions were measured on European driving cycle R-40 as shown in figure 2.1. These studies have lead to the commercialization of catalytic converters on 2-stroke vehicles. Road tests indicated that the catalytic converters can offer > 15,000 km durability if certain vehicle variables such as fouled spark plug and changes in air/fuel ratio due to worn carburettor jets are properly controlled. The composition of the lubricating oil also plays a major role in determining the durability of the catalytic converter. Therefore, it is necessary to use oils that are low in P, S, Pb and Zn. Another factor that was found to be important in determining the conversion efficiency of the catalytic converter is the amount of free Oxygen in the exhaust gas.

However, the Indian situation is slightly different from the Taiwan situation. The motorcycles in India are tuned lean to improve fuel economy. Also there are significant differences in the driving cycle used to measure emission. The top speed in the driving cycle R-40 is 50 km/h and this speed is maintained for20 seconds. Whereas in the Indian driving cycle as shown in figure-2.2 the top speed is 42 km/h without any hold time at this speed. Because of the difference in top speed in the two driving cycles, the maximum exhaust gas temperature is lower in the Indian Driving Cycle (IDC) compared to the R-40 driving cycle. To meet emission standards in IDC, it is necessary to locate the converter closer to the exhaust port or use a catalyst with a lower light-off temperature. Catalytic Converters have been in use for more than 20 years and at present, these converters offer 1,60,000 km durability in cars. Some of the advantages of catalytic converters include superior h1gh temperature strength. excellent catalyst coating adhesion due to porous cell walls, lower cost, and lower converter sk1n temperature. However, these advantages could not be utilized earlier in motorcycle applications because of the lack of a mounting mat that can withstand the high-temperatures encountered inside the mufflers of 2-stroke engines.

The results indicate that it is possible to reduce emissions· significantly by installing catalytic converters on 2-strokemotorcycles and scooters.

NOx HyCat: A New Catalytic System for Diesel Engines

No catalytic system has yet been commercialized that can eliminate nitrogen oxides (NOx) from the exhaust of vehicles powered by diesel and other lean-burn engines. The problem is temperature: a successful system must operate over the full range of temperatures found in vehicle exhaust: 150°C to more than 500°C, the low temperatures being the most problematic. Our NOx HyCat is the first catalytic system to span that temperature range. The system includes a brand-new iron-containing zeolite catalyst that is augmented with cerium-manganese oxide, an oxidizer that produces a near optimum ratio of NOx components to speed up the catalytic reaction and enable the zeolite to operate efficiently as a low-temperature catalyst. We combine this new low-temperature catalyst with a conventional high· temperature catalyst in a "dual-bed" configuration that provides high rates of NOx conversion over the broadest temperature range ever achieved The NOx Hycat is the first NOx-reduction system for diesel engines that can be used in vehicles:

- Vans.
- SUVs.
- Light and heavy trucks.
- Locomotives.
- Enables "dieselization" of U.S. vehicles to benefit from diesel's
- 25% to 35% mpg advantage over gasoline engines.
- Allows diesel-powered vehicles to meet increasingly stringent
- EPA standards for the reduction of NOx emissions.
- Operates efficiently from 113"C to as high as 600°C.
- Converts from 83% to greater than 98% of NOx, depending on temperature.
- Includes no expensive precious metals and requires no complex engine controls.
- Is compatible with existing manufacturing techniques.

II. OVERVIEW

The thermal efficiency of diesel engines allows diesel-powered vehicles to get 25%-35% more miles per gallon than their gasoline powered counterparts, so in Europe, where the price of fuel is high, diesel-powered cars are common. In the United States, however, diesel-powered vehicles are found mostly in the trucking industry. In fact, essentially all heavy trucks are powered by diesel. If more U.S. vehicles were diesel powered, the increased fuel economy could cut U.S. oil imports by as much as 25%. But diesel has a significant pollution problem-particulates. for which filtersare already available. And nitrogen oxides. Which remain an unresolved issue. Collectively known as NOx. nitrogen oxides are a common by-product of internal combustion engines. Because NOx contributes to smog. ground-level ozone, and ac1d rain. many nations are gradually strengthening their regulations about NOx emissions. In the United States, the Environmental Protection Agency, through Clean Air Act amendments being phased in through 2007, will prohibit cars, SUVs, and light trucks (gasoline and diesel) from emitting more than 0.07 gram of NOx per mile. That amounts to a greater-than-90% tightening of the NOx belt for light diesel engines, which currently release about 1 gram of NOx per mile. Similar NOx reduction will be required of the heavy diesel engines used in the 18-wheelers that carry consumer goods across the country. Unfortunately, there are no catalytic NOx converters for diesel engines in vehicles. The catalytic converters for gasoline-powered vehicles require low-oxygen exhaust and so cannot be used with diesel engines. Gasoline-powered engines use just enough oxygen to burn the fuel (a stoichiometric ratio), resulting in little if any oxygen in the exhaust. Diesel engines are "lean-burn" engines; that is, they use a lean fuel-to-oxygen mixture and so have an oxygen-rich exhaust Lean-burn NOx-abatement systems *do* exist but only for stationary applications-for power-plant emissions and for diesel engines that run equipment such as pipeline compressors or electric generators or that do load levelling for the generation of electricity during peak-use hours. These systems cannot be used in vehicles because their catalysts are not active enough over the full range of vehicular engine temperatures: 150°C during warm-up to more than 500°C during high-load excursions (e.g., high speeds, steep grades, heavy cargo loads). Some catalysts operate efficiently only above 350°C; mothers operate at as low as 290'Cbut because of thermal-stability problems cannot operate near 500'C. NOx HyCat was developed specifically for vehicles with lean burn engines and can fulfil the most stringent NOx-abatement requirements. It links a brand-new hybrid catalyst with another, already-existing catalyst in a "dual-bed" configuration that provides efficient NOx abatement over the broadest temperature range so far: 113oc to more than 500°C.

NOx HyCat uses the same chemical process that is used for NOx abatement in stationary diesel engines-selective catalytic reduction (SCR). SCR mixes NOx with an ammonia source (most likely, urea) and passes the mixture through a catalyst, where an ammonia-NOx reaction converts the NOx to nitrogen and water. Thehighest rates of SCR occur with a 1:1 ratio of nitric oxide and nitrogen dioxide, but NOx from vehicles has approximately a 9:1 ratio of those oxides. Lowering the ratio requires oxidizing some of the nitric oxide to nitrogen dioxide, which is particularly difficult to do at low temperatures. We achieve ratios close to the optimum

1:1, even at low temperatures, with a new catalyst design-an iron-containing zeolitethat is augmented with a cerium-manganese oxide. The iron converts the NOx during the SCR process; the cerium-manganese oxide oxidizes about 50% of the nitric oxide to nitrogen dioxide, enabling a faster rate of SCR. (The exact oxidation percentage depends on engine exhaust temperature.) It is this dual functionality, NOx conversion and oxidation, which make the new design a hybrid SCR

Our new hybrid converts from 80% to more than 98% of the NOx at engine temperatures ranging from 113°C to 350°C. Above 350°C, however, it becomes so active that it oxidizes the urea produced ammonia along with the nitric oxide, thus eliminating the reductant needed for NOx conversion. To counter this effect, the NOx HyCat has a "dual-bed" configuration in which the new hybrid catalyst works in tandem with a second catalyst that we position just upstream (shown in Figure 2.4). The upstream catalyst is a conventional iron-containing zeolite SCR catalyst, that is, one without the cerium manganese oxide. It operates efficiently above 350°C but is fairly inactive below that temperature, for example, when the engine is warming up or running under low-load conditions. In the dual bed configuration. the NOx-containing exhaust gas and ammonia pass relatively unchanged through theupstream catalyst at low temperatures to be converted efficiently by the hybrid catalyst. As the engine's temperature rises above 350°C, the upstream catalyst becomes active, converting nearly all of the NOx before the exhaust reaches the hybrid. In both· cases, the resultant nitrogen and water (in the form of steam) are released as exhaust. This tandem system, the NOx HyCat, provides unprecedented NOx reduction-a maximum of more than 98%-spanning a temperature range never before possible. An artist's rendition of the NOx HyCat dual-bed configuration in a car's undercarriage interacting with the rest of the emissions-control system has been shown in fig 24. The blue l;ne represents the path taken by engine exhaust. NOx in the exhaust. mixed with ammonia from an onboard urea supply (between the back wheels). f1rst contacts the portion of the NOx HyCat that is a conventional SCR catalyst (right. upstream) When the exhaust is at 350°C and above. The conventional catalyst- a high-temperature catalyst-converts the NOx before it reaches the NOx HyCat's downstream section occupied by our new hybrid catalyst, a low-temperature catalyst. At exhaust temperatures below 350°C, the conventional SCR catalyst is relatively inactive, so the exhaust passes through it relatively unchanged and is converted by the hybrid. The diesel oxidation catalyst-upstream from the catalytic system, just behind the engine-oxidizes unburned and partly burned hydrocarbons to carbon dioxide. The filter downstream from the NOx HyCat captures particulates.

III. LITERATURE REVIEW

Muraki et al. (1990) have studied the effects of palladium catalyst in a three way catalytic converter in SI engine. Increasing the palladium and rhodium loading from 0.5 g/1 and 0.1 g/1, respectively, to 1.0 g/1 and 0.2 g/1, respectively, resulted in improved catalyst light-off and conversion performances. The light-off performance under the dynamic conditions improved with the increasing A/F perturbation until the optimum value, and its behaviour was different from platinum/rhodium catalyst. The effect of palladium on the durability performance of the palladium/rhodium catalyst was compared with that of the platinum/palladium/rhodium catalyst. Further studies were done in the characterization of catalysts and the surface enrichment of palladium-rhodium and platinum-rhodium alloy systems heated in air and hydrogen. They reported that the light-off performance of NO_x reduction efficiency has been improved with the addition of lanthanum to the palladium catalyst.

Engler et al. (1994) have studied the control of emission in SI engine with tri metal emission control catalysts with a combination of Palladium (Pd) together with Pt/Rh as precious metal components. The performance of high loaded Pd-only catalysts was demonstrated in vehicle tests according to the FTP 75, ECE and Japan-10-mode procedures. It was shown that the advantageous lean HC light-off temperature observed with high loaded Pd-only catalyst can also be reached with similar loaded Pt-only catalysts. Various alternative ways to incorporate Pd in multi-brick converters were evaluated in vehicle tests. It was shown that single brick three metal converters with high Pd-content can have advantages over conventional Pt/Rh-three way catalysts. However, the extent of the improvement depends strongly upon the particular application, and with the present trend of increasing Pd-prices these three metal converters might lead to increased precious metal costs over conventional Pt/Rh-catalysts.

Burch et al. (1995) observed vacuum insulation and phase change thermal storage could be used to enhance the heat retention of a catalytic converter. Storing heat in the converter between trips allows exhaust gases to be converted rapidly thereby reducing the cold start emission. They designed, built and tested catalytic converters with phase change material thermal storage system along with vacuum insulation. Thermal tests demonstrated the ability of vacuum insulation and 2.3 kg of PCM to maintain the converter temperature of 350°C for 17hrs compared to 25minutes with conventional converters. However the FTP test showed the exhaust temperature during the pre-conditioning were not sufficient to melt the phase change material. However, the vacuum insulation performed well, resulting in a converter temperature of 146°C after 23 hours of cold soak at 27°C.Compared to the same converter at ambient temperature overall emissions of CO and HC were reduced by 52% and 29% respectively.

Socha et al. (1998) investigated the impact of different converter substrate cell structures on tailpipe emissions and pressure drop from a total systems perspective. They used a new technology palladium only catalyst in combination with a palladium/rhodium catalyst on a 4.0-liter, 1997 Jeep Cherokee for performing the FTP test. In the study the emissions performance was related to the converter volume for the different cell structures. The results from this study demonstrated that the 93 square cell/cm ^{2} structure has superior performance versus the 62 square cell/cm ^{2} structure and the 46 triangle cell/cm^2 structure when the converter volumes were relatively small. However, as converter volume increases the emissions differences diminish. For this application the results also show that the higher cell density, lower mass substrates have a slight advantage in catalyst light-off. The emphasis of this study was a comparison of different cell structures, however, other factors such as thermal management, catalyst technology and air-fuel ratio control also contributed significantly to the relative performance of these systems. The study demonstrated the advantages of higher cell density structures to help meet future emissions challenges. The authors also suggested that substrate support technology must be integrated with the catalyst technology, the converter packaging, and the engine management control to create a total system, which meets emissions and durability requirements.

Santanam et al. (1998) developed FEA model of air gap manifold to predict inner and outer wall temperature and structural soundness. It was observed that dual wall manifold were durable to meet high exhaust temperature up to 900 $^{\circ}$C while meeting performance ,noise and weight reduction.

Williamson et al. (1999) have investigated the dual-brick catalyst systems containing Pd-only catalysts followed by Pt/Rh metal in three-way catalyst to achieve LEV/ULEV emissions. They reported that the dual-catalyst system allows location of precious metals and optimization of wash coat technologies in attaining ULEV emission compared to single-brick converters. Dual-brick [Pd+Pt/Rh] systems were equivalent to [Pd+Pd/Rh] systems for under floor application using the same wash coat technology, and provide an effective strategy for precious metal management while meeting 100K ULEV emissions. They reported that dual-brick [Pd+Pd/Rh or Pt/Rh] systems can reduce precious metal usage compared to Pd-only systems for ULEV applications. They have also reported that additional HC light-off and vehicle emission benefits can be achieved using thinner-wall substrates and increasing substrate cell densities, especially from 400 to 600cpsi substrates.

Gulati (1999) presents the key advances in ceramic substrates which include lower thermal expansion, lighter weight, higher surface area and improved manufacturing process all of which help meet performance requirements. In addition to above benefits, the compressive and tensile strengths of lightweight substrates, as well as their thermal shock resistance, are found to be adequate following the application of high surface area alumina wash coat. The strength properties are crucial for ensuring safe handling of the substrate during coating and canning and for its long term mechanical durability in service. This work also provides the durability data for thin wall substrates with 600/4 and 400/4 square cell structure and compare them with those of standard substrate with 400/6.5 square cell structure.

IV. STEPS INVOLVED IN ANSYS:

In general, a finite element solution can be broken into the following these categories.

1. ***Pre-processing module:*** Defining the problem

The major steps in pre-processing are given below

- defining key points /lines/areas/volumes
- define element type and material /geometric /properties
- mesh lines/areas/volumes/are required

The amount of detail required will depend on the dimensionality of the analysis (i.e. 1D, 2D, axis, symmetric)

2. ***Solution processor module:*** assigning the loads ,constraints and solving

Here we specify the loads (point or pressure), constraints (translation, rotational) and finally solve the resulting set of equations.

3. ***Post processing module:*** further processing and viewing of results

In this stage we can see:

- List of nodal displacement

- Elements forces and moments
- Deflection plots
- Stress contour diagrams

V. ANSYS INTERFACE

Graphical Interface vs. Command File Coding

There are two methods to use ANSYS. The first is by means of the graphical user interface or GUI. This method follows the conventions of popular Windows and X-Windows based programs.

The second is by means of command files. The command file approach has a steeper learning curve for many, but it has the advantage that an entire analysis can be described in a small text file, typically in less than 50 lines of commands. This approach enables easy model modifications and minimal file space requirements.

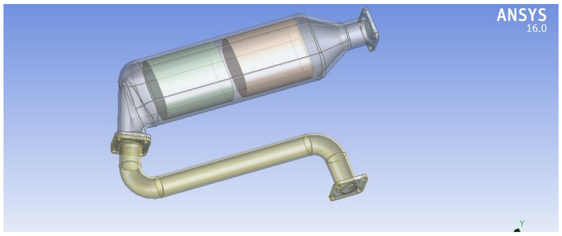


Fig 1 Converted Ansys model

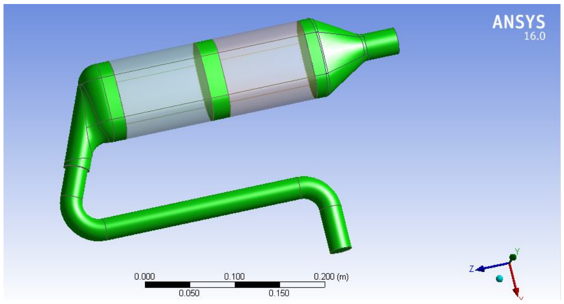
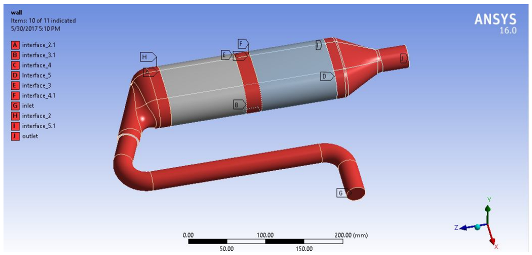


Fig 2 Extracting Fluid volume from the model using Cap Fill option in tools



wall
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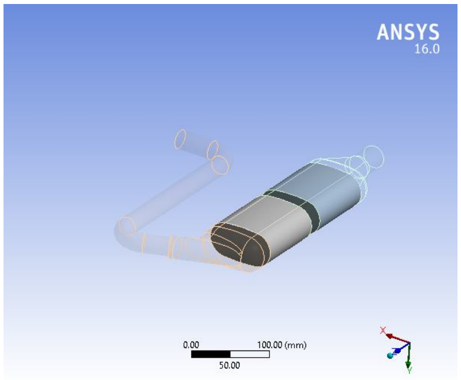
A	interface_2.1
B	interface_3.1
C	interface_4
D	Interface_5
E	interface_3
F	interface_4.1
G	inlet
H	interface_2
I	interface_5.1
J	outlet

Fig Fig 3 Boundaries Selection of catalytic converter



VI. RESULTS OF PALLADIUM

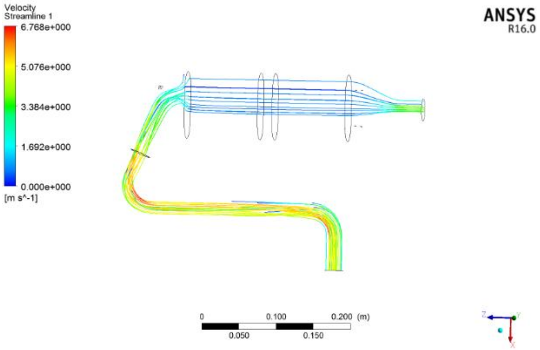


Fig 4 velocity of the Fluid flow in the volume designed for catalytic converter

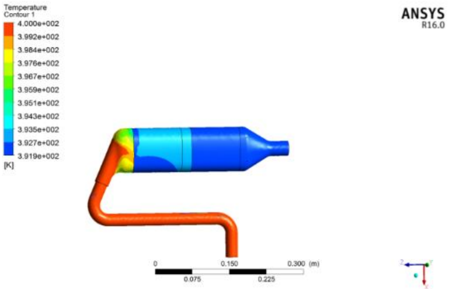


Fig 5 Temperature of the Fluid and the System

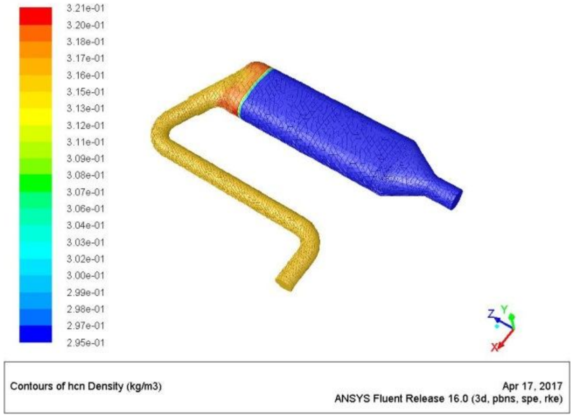


Fig 6 The Above Figure represents the rate of Hydrocarbon density in the Catalytic converter after reacting with the surface catalyst palladium

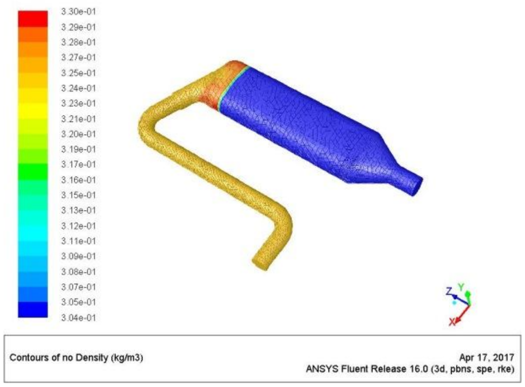


Fig 7 The Above Figure represents the rate of NO density in the Catalytic converter after reacting with the surface catalyst palladium

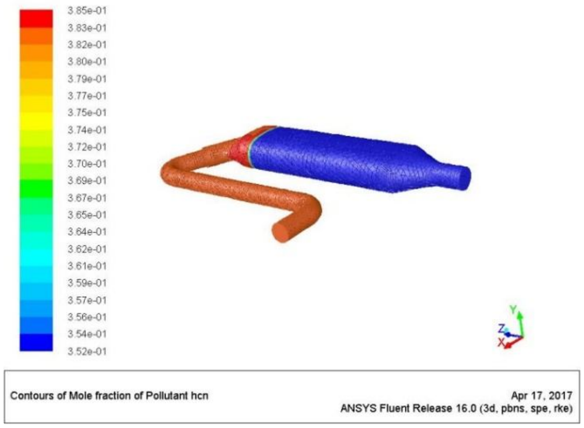


Fig 8 theabove Figure represents the Mole fraction of Hydrocarbon in the Catalytic converter after reacting with the surface catalyst palladium

VII. RESULTS FOR THE RHODIUM

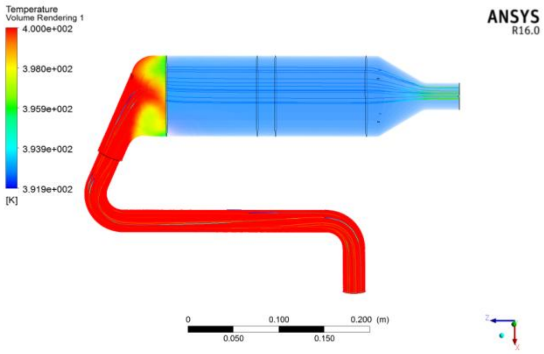


Fig 9 Temperature Of the catalytic Converter

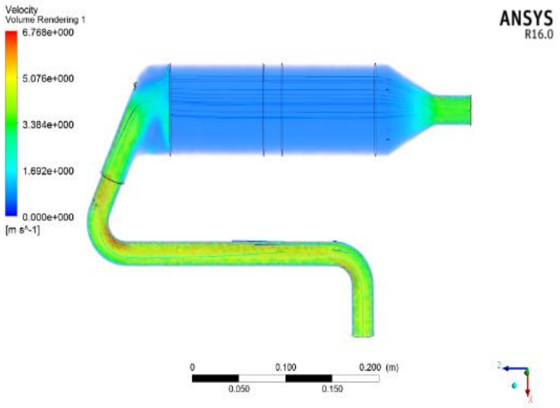


Fig 10 Velocity Contour

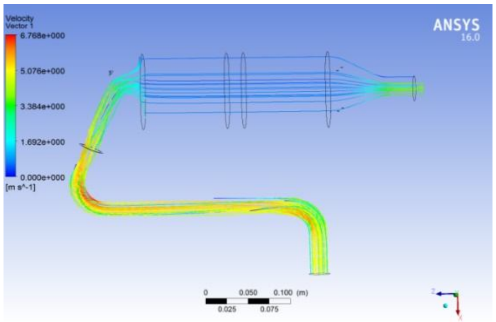


Fig 11 Stream lines of the flow through porous rhodium medium

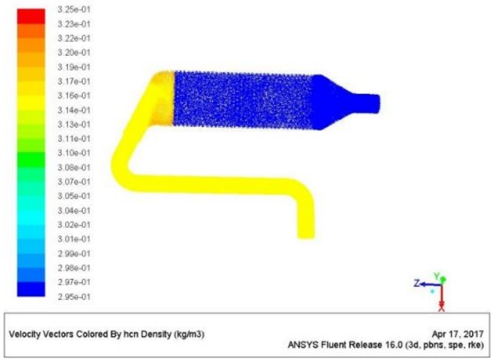


Fig 12 HCN in Catalytic Converter

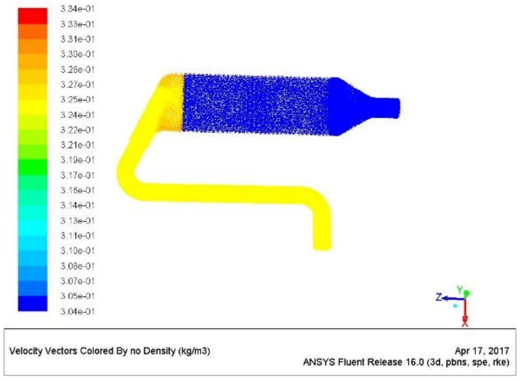


Fig 13 NO in catalytic Converter

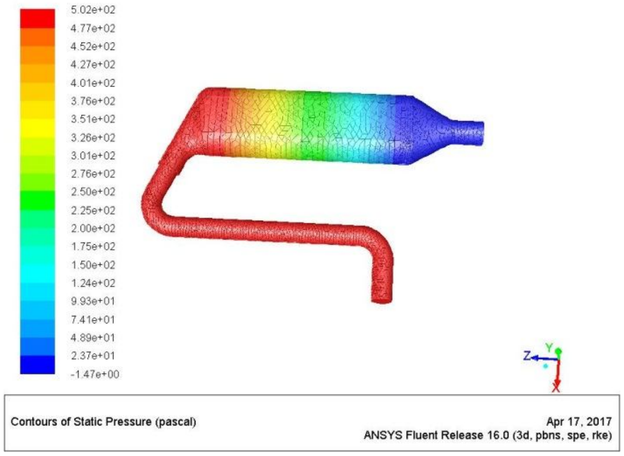


Fig 14 Pressure contour

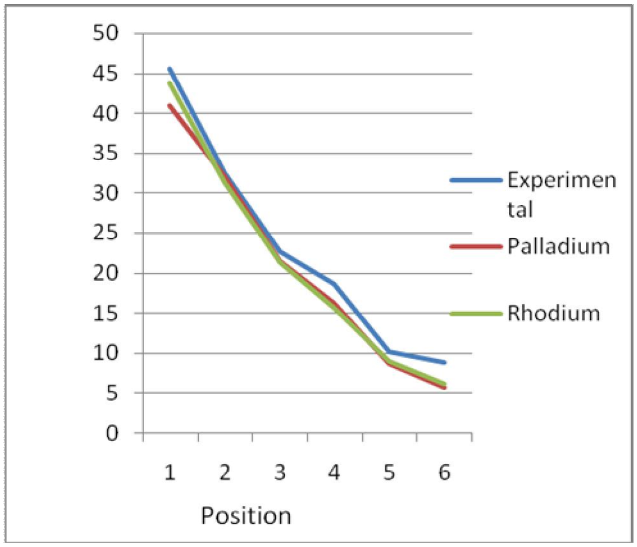


Fig 15 Position Vs HC emissions

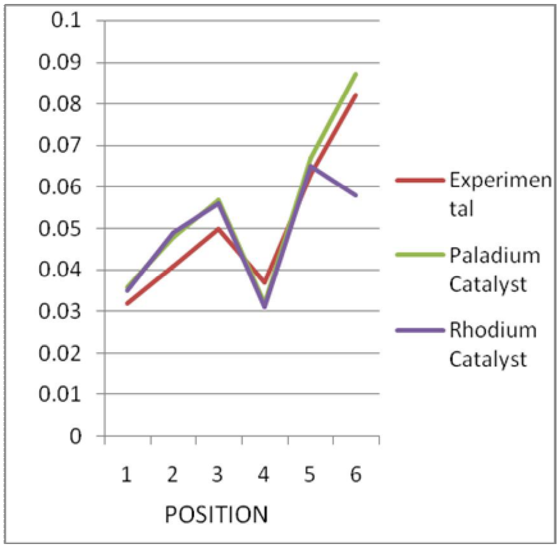


Fig 16 Position VS CO emissions

VIII. CONCLUSIONS

Based upon the work presented in the paper the following conclusions can be drawn. The special catalysts like rhodium allow the exhaust gas to flow freely without making any obstruction or blocking. Since the partial flow technology is used, it helps to limit the back pressure to the minimum level resulting in better engine performance and fuel saving. The process of regeneration of PM through DOC is continuous. Even if the automatic regeneration is saturated with the collected soot over a period of time, the system will not fail as it happens in wall flow filter, rather all the exhaust gases can flow straight to the other end of the neighbouring catalytic bead, similar to flow through substrate. It is estimated that, with the existing volume of catalyst and steel wire meshes, the cleaning may be required for every 10,000 Kilometres of engine run, for efficient fuel consumption. As the catalytic beads are very hard, no wear and tear of catalyst can take place, and hence long life of catalyst is assured. This also ensures no chance of washout catalytic materials coming out along with the exhaust gas adding further pollution to the environment. This after treatment technology for PM reduction is cost effective and robust which needs no interaction with the engine management system and is totally independent.

The robust design of the catalytic converter may vary with the type of catalyst material using therefore from the above analysis the soot or nox emissions with the density and the molar concentration obtained in the result the rhodium as a catalyst substrate is the good and best design that can be proposed for further usage.

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