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"IMPROVING THE CONVERSION EFFICIENCY OF MONOLITHIC CATALYTIC CONVERTERS THROUGH GEOMETRY CHANGES AND MATRIX LENGTH MODELING IN CFD"

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ABSTRACT

Vehicle population is expected to rise nearly to 1600 million via the year 2036. Because of partial ignition in the engine, there are many inadequate burned products as Carbon monoxide, Nitrous oxides, hydro carbons, harsh substances, etc. The particular toxins have an impact on air properties, atmosphere and human physical conditions that leads in severe norms of pollutant emission. Catalytic converter is a vehicle emissions control device that converts toxic pollutants in exhaust gas to less toxic pollutants by catalyzing a redox reaction (oxidation or reduction). Optimization can no longer be based on traditional approaches, which are intensive in hardware use and laboratory testing. The CFD is in high demand for the analysis and design in order to reduce developing cost and time consuming in experiments. This work describes the conversion efficiency by changing the substrate length of automotive three-way catalytic converters, which are employed to reduce engine exhaust emissions. It is found that the CFD model in simulating the performance of three-way catalytic converter. There is a difference of 2.4% for oxide of nitrogen, 2.1% for propane and 1.8 % for carbon monoxide increase in conversion efficiencies by increasing the substrate length by 10mm while by reducing the substrate length by 10mm conversion efficiency reduced. The result also shows that the increase in substrate length leads to reduce emission concentration.

Keyword: *Catalyst, CFD modeling, chemical reaction, conversion efficiency, simulation, Substrate length.*

I. INTRODUCTION

The internal combustion engine, either rotary or piston cylinder, is the primary power plant of today's world. Although it is used in both an on- and off-road capacity, automobiles are typically their primary customer. Because of their versatility, flexibility and low initial cost, automobiles dominate the market for passenger and transport freight. Furthermore, economic growth in developing countries like India, China, Brazil, and Chile has triggered an increase in the number of automobiles on the road. The combustion of carbonaceous fuel in these engines leads to the formation of various byproducts, released in air as exhaust gases. Since combustion occurs at a high temperature and pressure in fractions of a second, dissociation and incomplete combustion lead to partial and complete products of combustion. Exhaust species like carbon monoxide (CO), carbon dioxide (CO2), particulate matter (PM), water (H2O), oxides of nitrogen (NOx), oxides of sulfur (SOx) and hydrocarbons (HC) resulting from combustion pollutes the air and has drastic effects on human life and nature. When these pollutants are near the earth surface, they cause various health issues like asthma, respiratory problems, and irritation to the eyes and damage to the lungs. Away from the surface, they are directly responsible for acid rain and global warming. For example, Figure 1 and Figure 2 illustrate how the

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increasing number of automobiles around the globe has increased the total carbon dioxide footprint in the atmosphere. As a result, before irreparable damage is done to nature and mother earth, pollution must be controlled. Most of the cities have a large number of automobiles; as a consequence they suffer from problems of air pollution. People of all ages can be affected from air pollution and particularly from sources, such as vehicle exhausts and residential heating, but mainly those with existing heart and respiratory problems are in an extra risk. Considering all the above, it can be concluded that transport has a great impact on the atmospheric environment and therefore it is necessary to reduce emissions from the road traffic.

CATALYTIC CONVERTOR

A catalytic converter is an air pollution abatement device that removes pollutants from motor vehicle exhaust, either by oxidizing them into carbon dioxide and water or reducing them into nitrogen and oxygen. The catalytic converter device uses a catalyst to convert three harmful compounds in the car exhaust into harmless compounds. The three compounds are:

- Hydrocarbons (HC)
- Carbon monoxide (CO)
- Nitrogen oxides (NOX)

In a catalytic converter, the catalyst (in the form of platinum and palladium) is coated onto a ceramic honeycomb or ceramic beads that are housed in a muffler-like package attached to the exhaust pipe. The catalyst helps to convert carbon monoxide into carbon dioxide. It converts the hydrocarbons into carbon dioxide and water. It also converts the nitrogen oxides back into nitrogen and oxygen

CONSTRUCTION

The catalytic converter's construction is as follows:

- Substrate: For automotive catalytic converters, the core is usually a ceramic monolith that has a honeycomb structure (commonly square, not hexagonal). The substrate is structured to produce a large surface area.
- Wash coat: A wash coat is a carrier for the catalytic materials and is used to disperse the materials over a large surface area. Aluminum oxide, titanium dioxide, silicon dioxide, or a mixture of silica and alumina can be used. The catalytic materials are suspended in the wash coat prior to applying to the core. Wash coat materials are selected to form a rough, irregular surface, which greatly increases the surface area compared to the smooth surface of the bare substrate. This in turn maximizes the catalytically active surface available to react with the engine exhaust. The coat must retain its surface area and prevent sintering of the catalytic metal particles even at high temperatures (1000 °C) [12]
- Ceria or ceria-zirconia: These oxides are mainly added as oxygen storage promoters.

Catalyst: Platinum is the most active catalyst and is widely used, but is not suitable for all applications because of unwanted additional reactions and high cost. Palladium and rhodium are two other precious metals used. Rhodium is used as a reduction catalyst, palladium is used as an oxidation catalyst, and platinum is used both for reduction and oxidation. Cerium, iron, manganese, and nickel are also used, although each has limitations. Nickel is not legal for use in the European Union because of its reaction with carbon monoxide into toxic nickel tetra carbonyl. Copper can be used everywhere except Japan [17].

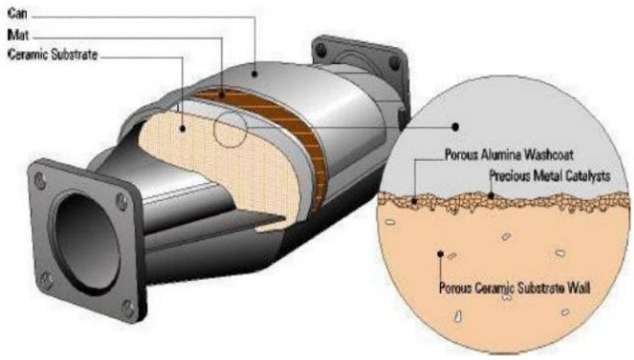

Figure 1 Construction of a catalytic converter

II. METHODOLOGY

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The present study i.e. "Modeling Of Thermal Behavior Of The Monolithic CATALYTIC Converter By Geometrical Changes In Substrate Length Using CFD" is a simulation study on pre-defined system which is similar to the one in the previous study i.e. "CFD Analysis OF Three Way Monolithic Catalytic Converter Using ANSYS 14.5R" with similar boundary conditions and material, selection also dimension of catalytic converter remains same. The geometry creation and meshing operation is done in simulation software Ansys fluent 14.5

III. GEOMETRY SETUP AND MODELLING

POROUS MEDIA

The Catalytic Converter is a vehicle emission control device which converts toxic byproducts of combustion in the exhaust of an internal combustion engine to less toxic substances by way of catalyzed chemical reactions. In catalytic converters, the design of inlet cone is of utmost importance, since it determines the gas flow distribution over the substrate (a structure located inside the converter where the emission conversion reaction takes place.) The substrate includes the active catalyst material such as Palladium, Rhodium and Platinum which initiates chemical reactions to convert exhaust pollutants into less harmful materials. This substrate may be either metallic or ceramic substrate and is modeled as porous media in CFD. Porous media can be used for modeling a wide variety of engineering applications, including flows through packed beds, filters, perforated plates, flow distributors, and tube banks. It is generally desirable to determine the pressure drop across the porous medium and to predict the flow field in order to optimize a given design. Characteristics of the porous medium are generally defined in solver in terms of following properties:

- Porosity
- Viscous resistance
- Inertial resistance.

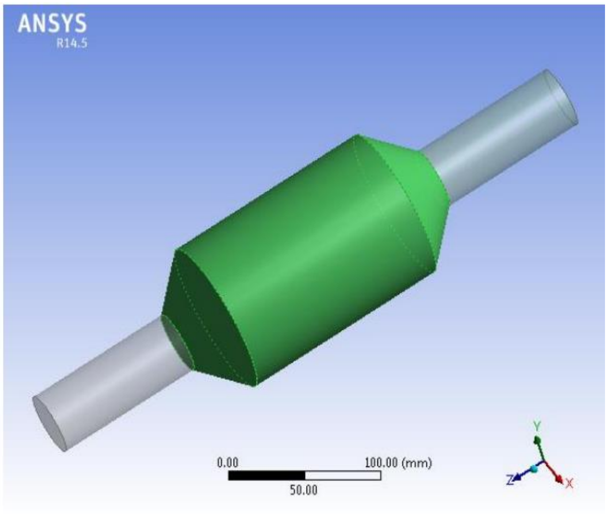

Figure 2 Geometry for substrate length of 190mm

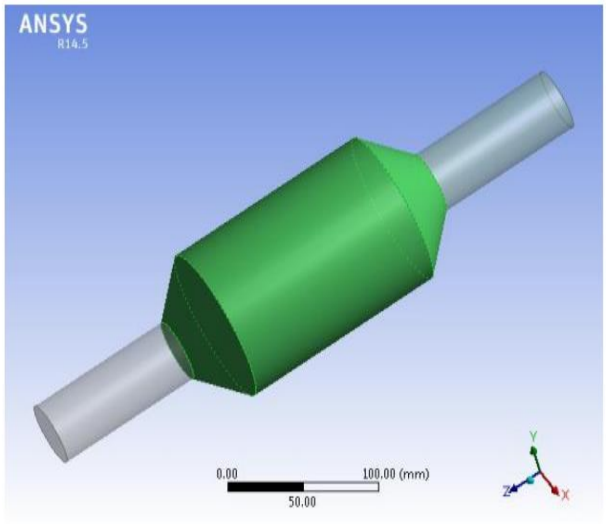

Figure 3 Geometry for substrate length of 200mm

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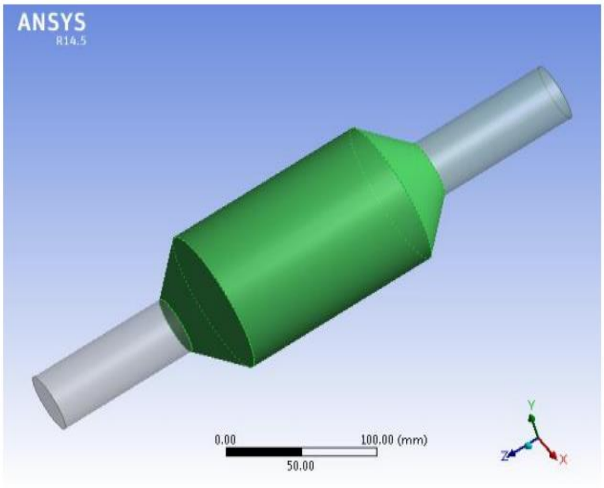

Figure 4 Geometry for substrate length of 210mm

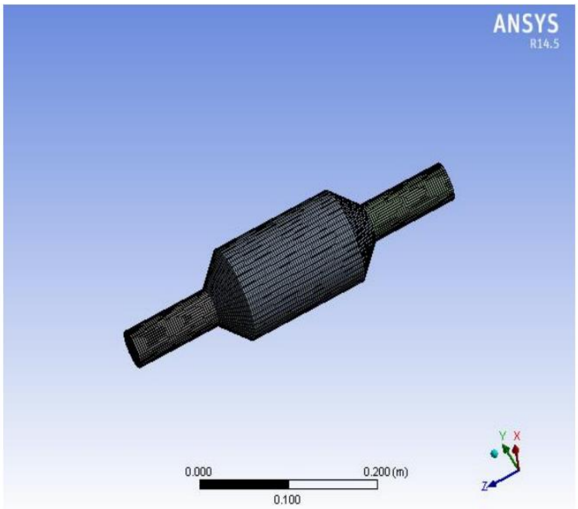

Figure 5 Geometry for substrate length of 190mm

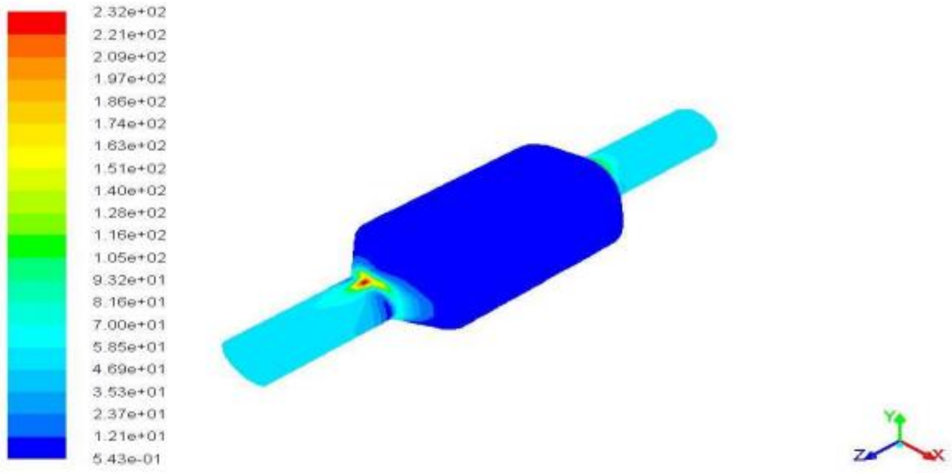

Figure 6 Contours of dynamic pressure for substrate length of 190mm

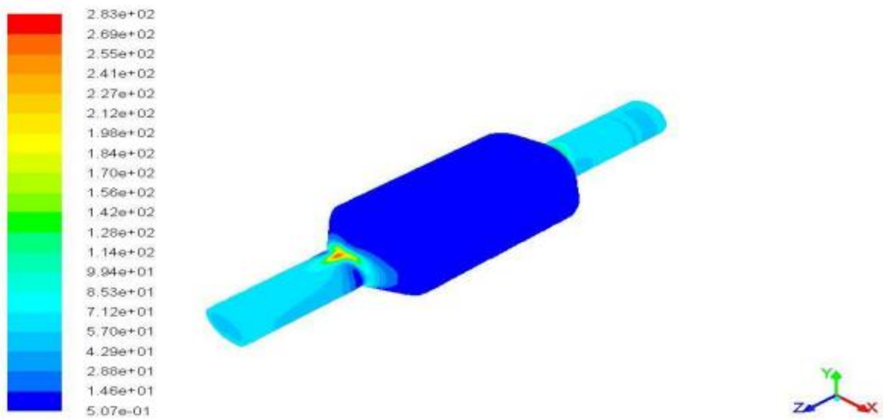

Figure 7 Contours of dynamic pressure for substrate length of 200mm

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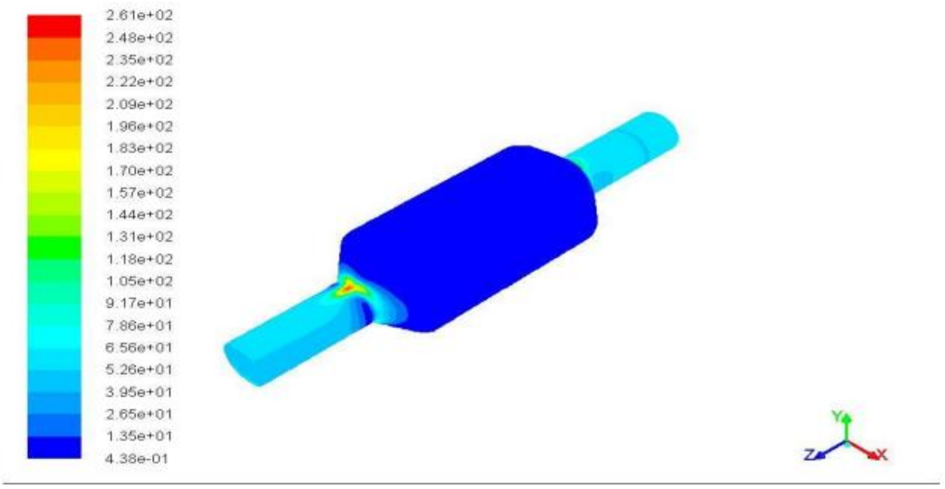

Figure 8 Contours of dynamic pressure for substrate length of 210mm

CALCULATION OF CONVERSION EFFICIENCY

Table 1.1 Conversion rate of oxide of Nitrogen

Inlet temperature(in K)	Conversion rate of oxide of nitrogen		
	For substrate length of 190mm	For substrate length of 200mm	For substrate length of 210mm
800	0.918	0.932	0.952

IV. CONCLUSIONS

From the simulation results it is observed that:

- The flow distribution in a catalytic converter assembly is governed by the geometry configurations of inlet and outlet cone section, the substrate and exhaust gas compositions and therefore a better design of the catalytic converter is very important.
- There is a difference of 2.4% for oxide of nitrogen, 2.1% for propane and 1.8 % for carbon monoxide increase in conversion efficiencies by increasing the substrate length by 10mm
- The present proposed model has 2.4 % higher NOx conversion rate as compared to other species.
- The order of conversion rate is as follows NO>C3H6>CO
- For the current design of 210 mm substrate length configuration, exhaust gas conversion efficiency was found to be optimum.

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V. SCOPE OF FUTURE WORK

It is imperative that the equipment deployed in industries, Automobiles in commercial application should be optimizes and be efficient, while the present research has substrate length to improve the performance of catalytic converter for the research work in following area may be taken up to study the effects of various parameter on conversion efficiency.

- The performance of a catalytic converter is affected by the flow distribution inside the substrate; a uniform flow distribution can increase its efficiency, lower the pressure drop which may optimize engine performance.
- High quality mesh is needed to capture all the geometrical features (substrate) of the 3D CAD model and to get good end results

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