Emission Reduction by Design Optimization in Catalytic Converter Using CFD

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***Abstract*- Internal Combustion engines generate undesirable emissions during the combustion process, which include, NOX, CO, unburned HC, smoke etc. Apart from these unwanted gases, it produces Particulate Matter (PM) such as lead, soot. All these pollutants are harmful to environment and human health. They are the main causes for greenhouse effect, acid rain, global warming etc. The simplest and the most effective way to reduce NOX and PM, is to go for the after treatment of exhaust. Devices developed for after treatment of exhaust emissions includes thermal converters or reactors, traps or filters for particulate matters and catalytic converters. The most effective after treatment for reducing engine emission is the catalytic converter found on most automobiles and other modern engines of medium or large size. Now a days the global warming and air pollution are big issue in the world. The 70% of air pollution is due to emissions from an internal combustion engine. The harmful gases like , NOX CO, unburned HC and particulate matter increases the global warming, so catalytic converter plays an vital role in reducing harmful gases, but the presence of catalytic converter increases the exhaust back pressure due to this the volumetric efficiency will decrease and fuel consumption is higher. So analysis of catalytic converter is very important.**

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.

Index Terms- Catalytic converter, CFD modeling, chemical reaction, conversion efficiency, simulation, Substrate length.

I. INTRODUCTION

Nowadays, automobiles are one of life essentials. This need encouraged the industry to increase the production of automobiles. Most automobiles produced are operated with fuel for which combustion is necessary. This combustion process is associated with releasing harmful emissions including carbon monoxide (CO), unburnt hydrocarbons (HC) and nitrogen oxides (NOx) which have negative effects on humans and the environment. This has led to the development of emission control units to treat exhaust gases and convert them to less harmful products. These units are called catalytic converters (Kummer, 1980 and Taylor, 1984).

1.1 Construction

Catalytic converters consist of honeycomb-like structures often referred to as "the monolith substrate" as shown in Figure 1, the catalyst which primary consists of one or more noble metals that facilitate the oxidation and reduction chemical reactions and a padding mat surrounding the substrate that helps in maintaining higher temperatures necessary for the continued operation of the converter.

The monolith substrate is typically constructed of a ceramic material namely cordierite and is shaped into a honeycomb structure to maximize the surface area to promote the chemical reaction (Heck et al. 2001, Heck and Farrauto 2001 and Shuai and Wang 2004). This honeycomb structure is loaded with the wash coat. The wash coat consists of aluminum oxide, silicon dioxide, titanium dioxide or a mixture of alumina and silica (Kummer 1980 and Ramanathan et al. 2004). The wash coat increases the surface roughness of the substrate to increase the overall surface area and act as a catalyst carrier due to its high porosity (Richardson et al. 2003).

The catalysts used are noble metals mostly palladium, rhodium and platinum.

1.2 Types of catalytic converter

The first type is “two-way catalytic” converters in which two chemical reactions take place; oxidation of CO to CO2 and oxidation of unburnt HCs to CO2 and water vapor. Two-way catalytic converters were widely used for diesel and gasoline engines and are no longer used since 1981 as they don’t treat NOx emissions.

The second type is “three-way catalytic” converters (TWCC). TWCC incorporate three chemical reactions; two oxidation reactions (similar to “two-way catalytic converters “) and a reduction reaction in which NOx are converted to O2 and N2 (Diesel Net 2004; Kummer 1980; Pontikakis et al. 2004).

Figure 1 Typical catalytic converter

(i)Two-way catalytic converter:

A 2-way (or "oxidation", sometimes called an "oxi-cat") catalytic converter has two simultaneous tasks:

1. Oxidation of carbon monoxide to carbon dioxide: 2 CO + O2 → 2 CO
2. Oxidation of hydrocarbons (unburnt and partially burned fuel) to carbon dioxide and water: CxH2x+2 + [(3x+1)/2] O2 → x CO2 + (x+1) H2O (a combustion reaction).

(ii)Three-way catalytic converter:

Three-way catalytic converters (TWC) have the additional advantage of controlling the emission of nitric oxide (NO) and nitrogen dioxide (NO2) (both together abbreviated with NOx and not to be confused with nitrous oxide (N2O)), which are precursors to acid rain and smog.

Reduction of nitrogen oxides to nitrogen (N2)

- 2 CO + 2 NO → 2 CO2 + N2
- hydrocarbon + NO → CO2 + H2O(vapor) + N2
- 2 H2 + 2 NO → 2 H2O(vapor) + N2
- Oxidation of carbon monoxide to carbon dioxide
- 2 CO + O2 → 2 CO2
- Oxidation of unburnt hydrocarbons (HC) to carbon dioxide and water, in addition to the above NO reaction
- hydrocarbon + O2 → H2O(vapor) + CO2

Emission control is one of the biggest challenges in today's automotive industry. Emission control can be achieved either by controlling combustion or by treating the exhaust gas. The latter is comparatively easier since there is less or no need to modify the engine itself. One such after treatment method is the use of catalytic converter. But, the 3-way converter is expensive due to use of both platinum and palladium/rhodium. One of the alternatives is the use of selective catalytic reduction, i.e., reduction of a particular mission based on the type of the engine used. The flow distribution across the monolith frontal area depends on the geometry of a specific design of inlet diffuser Mainly, NOx, CO, and unburned hydrocarbons (HC). Significant effort has been invested into the design of a converter that will lead to maximum use of the catalyst volume. It is known that this maximum utilization of the catalyst volume would be achieved by having a uniform flow distribution through the monolith substrate. Therefore, most modern catalytic converters have long, tapered inlet and outlet headers to smooth the flow between sections of different cross-sectional areas. This tapered header provides a uniform flow distribution across the monolith inlet face. A no uniform flow across the substrate leads to uneven residence time distribution and non-uniform poison accumulation during the catalyst aging.

II. LITERATURE REVIEW

For analyzing the catalytic convertor the various researches have been study some of these are explained here.

Yugal Kishore et.al.2017 carried out a 3D CFD analysis on three way monolithic converter on the basis of it various conclusions have been drawn. The rates of conversion of NO, CO, C3H6 are the function of temperature. On increasing temperature the rate of surface reaction with the catalyst first increases and then become stable.

S.P. Venkatesan et.al 2017 has study on emission control of catalytic convertor by using copper oxide. The main aim of this work is to fabricate system, where the level of intensity of toxic gases is controlled through chemical reaction to more agreeable level. This system acts itself as an exhaust system; hence there is no needs to fit separate the silencer. The whole assembly is fitted in the exhaust pipe from engine. In this work, catalytic converter with copper oxide as a catalyst, by replacing noble catalysts such as platinum, palladium and rhodium is fabricated and fitted in the engine exhaust.

Shamim et al. 2015 developed a numerical simulation to predict the performance of the three-way catalytic converter. The model incorporates heat conservation and chemical reaction sub model with oxygen storage mechanism and it showed that the conversion efficiency was improved when operating under rich oxygen content.

Groppi & Tronconi, 2014 investigated the heat and mass transfer for a monolith with equilateral triangular channels. They implemented 3-D modeling to approach the analysis in which they assumed a fully developed laminar flow and equal thermal and mass diffusivity. Their analysis concluded lower heat and mass transfer for the triangular channels due to the acute corners of the triangles compared to square and circular channels which resulted in reaching operating temperatures and lower gas heating rates for the coefficients of heat and mass transfer.

Chakravarty et al., 2013 utilizing multi-dimensional channel model. It was recorded that the ignition behavior can be dramatically affected by flow recirculation at the inlet of the substrate which lead to high flow maldistribution especially at lower exhaust temperatures. The study concluded that flow no uniformity effects were more significant with increasing flow temperature. In addition, the pressure drop distribution remained constant and was dependent on the recirculation pattern at the front face of the monolith.

III.METHODOLOGY

Model description

The geometry of catalytic converter performing the simulation study is taken form one of the research scholar's Yugal Kishore et.al 2017 paper with exact dimension excluding substrate length dimensions. The part of model was designed in ANSYS (Fluent) workbench14.5 software. The geometric dimension of the catalytic converter is shown in the Table4.1. For simulating the monolithic catalytic convertor ANSYS 14.5 finite element control volume approach has been used. Where the CAD model of the catalytic convertor is segmented into 105 orders of nodes.

Table 1 Geometric dimension of the catalytic converter [1].

Interior inlet	Porous zone
Interior outlet	Porous zone
Wall	Porous zone
External body	Aluminium
Inlet diameter	40mm
Outlet diameter	40mm
Channel density	62 channels/cm^2
Inner diffuser length	6mm
Channel hydraulic diameter	1mm
Inlet and outlet section length	100mm
Substrate length	190mm,200mm,210mm

3.1 Geometry

Firstly, ANSYS workbench14.5 software was installed on the system. CFD fluent package is required to operate. Select design modular and run then select the dimension in which the model is to be creating and the type of model i.e. either 2D or 3D.

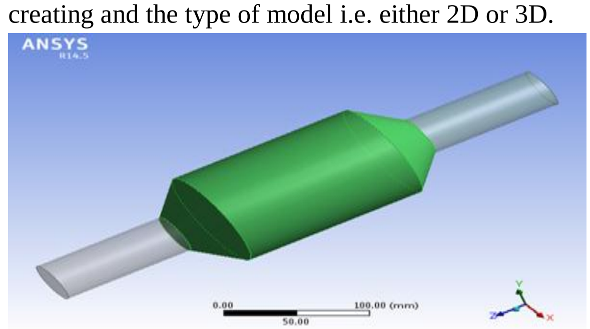

Figure 2 Geometry for substrate length of 190mm Similarly made for 200mm and 210mm

3.2 Meshing

By, default, a coarse mesh is generated by ANSYS software. Mesh contains mixed cells per unit area

(ICEM Tetrahedral cells) having triangular and quadrilateral faces at the boundaries.

For current problem the mesh having 90306 nodes and 84320 elements in generated.

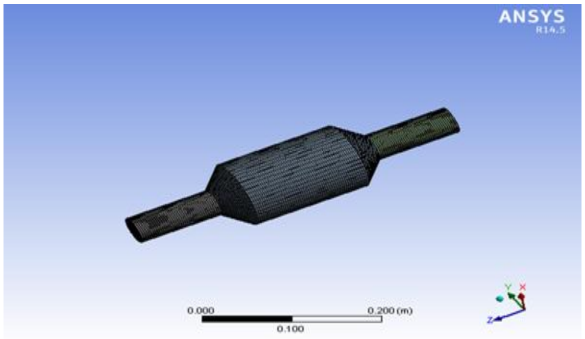

Figure 3 Meshing for substrate length of 190mm

FOR SUBSTRATE LENGTH OF 200MM

For current problem the mesh having 92308 nodes and 86320 elements in generated.

FOR SUBSTRATE LENGTH OF 210MM

For current problem the mesh having 93298 nodes and 87650 elements in generated.

3.3 Fluent Setup

The mesh is properly checked and fine mesh is obtained.. The problem type is 3D and type of solver pressure-based solver. The Velocity is change to absolute velocity and gravity is set y= -9.81 m/s

3.4 Model Selection

In model selection only three parameters are selected. Remaining parameter are remained as default. The three parameters are:-

Species, Energy – on and Viscous -Turbulent k-e standard wall Fn, mixture.

3.5 Boundary condition

Table 2 Physical Properties for simulation

PARAMETER	VALUE
Cells per square inch, CPSI	400
Substrate volume fraction	0.26
Wash coat volume fraction	0.12
Fluid volume fraction (OFA)	0.62
Hydraulic diameter, Dh, mm	1
Geometric surface area, GSA	2740
Active metal surface	27-28m^2/g
Ratio of active metal surface	70
Wash coat Material	Ceria Stabilized-alumina
Velocity temperature dependent	1.35 m/s at 25°C
Substrate material	cordierite

Table 3 Composition of combustion gases at the inlet

SPECIES	MASS CONCENTRATION
O_2	7470 ppm
N_2	80.026 %
HC	700 ppm
CO_2	17.904 %
CO	1.14 %
NO_2	600 ppm
NO	530 ppm

IV. RESULTS AND DISCUSSIONS

After putting the boundary conditions, the solution is initialized and then iteration is applied so that the values of all parameters can be seen in a curve or line graph. After the iteration gets completed final result could be seen.

4.1 CONTOURS FOR SUBSTRATE LENGTH OF 190mm

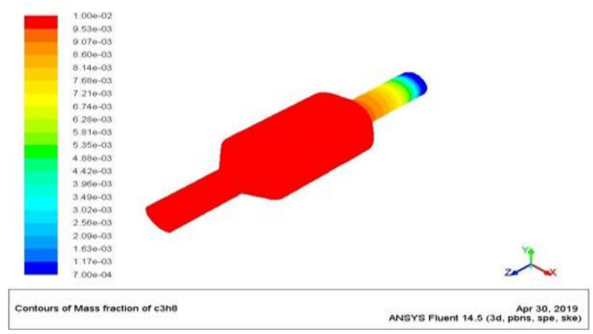

Figure 4 Contours of mass fraction of hydrocarbon for substrate length of 190mm

4.2 CONTOURS FOR SUBSTRATE LENGTH OF 200mm

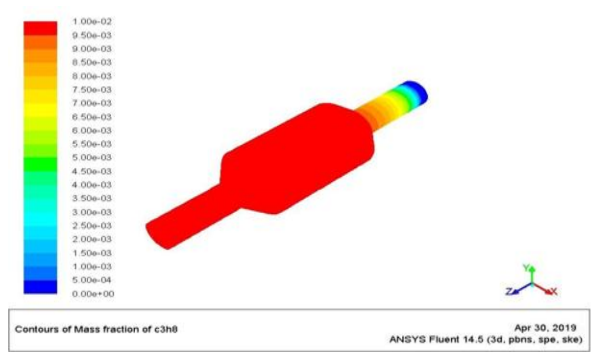

Figure 5 Contours of mass fraction of hydrocarbon for substrate length of 200mm

4.3 CONTOURS FOR SUBSTRATE LENGTH OF 210mm

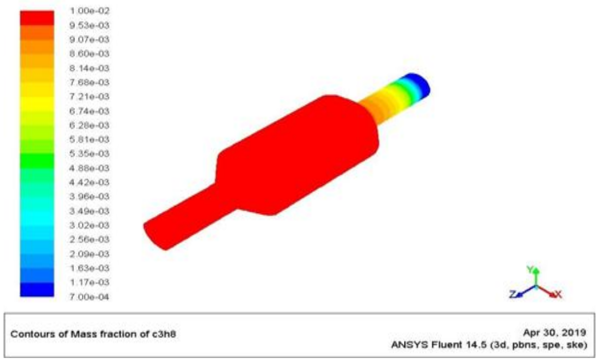

Figure 6 Contours of mass fraction of hydrocarbon for substrate length of 210mm

4.4 Calculation of conversion efficiency

Table 4 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

Table 5 Conversion rate of propane

Inlet temperature (in K)	Conversion rate of propane		
	For substrate length of 190mm	For substrate length of 200mm	For substrate length of 210mm
800	0.889	0.9	0.921

Table 6 Conversion rate of carbon monoxide

Inlet temperature (in K)	Conversion rate of carbon monoxide		
	For substrate length of 190mm	For substrate length of 200mm	For substrate length of 210mm
800	0.839	0.85	0.868

V. 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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