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Modeling of Improving Conversion Efficiency for Monolithic catalytic Converter by Geometrical Changes in Substrate Length Using CFD

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***Abstract*- In an engine transient condition, effects of different exhaust mass flows, inlet signal amplitudes and periods on dynamic responses of the three-way catalytic converter were investigated experimentally. Experimental results show that exhaust mass flows, inlet signal amplitudes and periods have important influence on engine emissions and oxygen storage capacity of Ceria for the three-way catalytic converter with CO2 catalyst in the wash coat. 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 catalysing a redox reaction (oxidation or reduction). The CFD simulation of catalytic convertor has been done by using Ansys 14.5. 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*- Catalyst, CFD modelling, chemical reaction, conversion efficiency, simulation.**

I. INTRODUCTION

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
- Carbon monoxide
- Nitrogen oxides

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.

Types of 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: $2 CO + O_2 \rightarrow 2 CO_2$

2. Oxidation of hydrocarbons (unburnt and partially burned fuel) to carbon dioxide and water: $C_xH_{2x+2} + [(3x+1)/2]\ O_2 \rightarrow x\ CO_2 + (x+1)\ H_2O$ (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 (NO_2) (both together abbreviated with $NO_x$and not to be confused with nitrous oxide (N_2O)), which are precursors to acid rain and smog.

A three-way catalytic converter has three simultaneous tasks:

Reduction of nitrogen oxides to nitrogen (N_2)

- $2\ CO + 2\ NO \rightarrow 2\ CO_2 + N_2$
- hydrocarbon + $NO \rightarrow CO_2 + H_2O + N_2$
- $2\ H_2 + 2\ NO \rightarrow 2\ H_2O + N_2$

Oxidation of carbon monoxide to carbon dioxide

- $2\ CO + O_2 \rightarrow 2\ CO_2$

Oxidation of unburnt hydrocarbons (HC) to carbon dioxide and water, in addition to the above NO reaction

- hydrocarbon + $O_2 \rightarrow H_2O + CO_2$

II.LITERATURE REVIEW

Many researchers are focusing on modification of fuels, and engine design, but very few researchers are concentrating on engine out emission reduction. 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, C_3H_6 are the function of temperature. On increasing temperature the rate of surface reaction with the catalyst first increases and then become stable.[1]

S.P. Venkatesan et al. (2017) have 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. [2]

A.K. Sharma et al. (2016) A catalytic monolith converter usually comprises several hundred or thousands of channels. Mathematical modeling that seeks to resolve the coupled transport phenomena mass, momentum, species and heat on a discrete-channel scale is a computationally challenging task. The computational penalty for reduced model is much less as compared to the full model, making it a possible candidate for detailed monolith simulations.[4]

Young-Deuk Kim et al. (2009) in this case, the active metal distribution along the length of the converter may influence its performance. The optimal design of a longitudinal noble metal distribution of a fixed amount of catalyst is investigated to obtain the best performance of a dual monolithic catalytic converter. The optimal design for the optimal axial distribution of the catalyst was determined by solving multi-objective optimization problems to minimize both the CO cumulative emissions during the FTP-75 cycle, and the difference between the integral value of a catalyst distribution function over the monolith volume and total catalytic surface area over the total monolith volume. [5]

Thundil Karuppa Raj.R et al. (2008) analysed that the design of catalytic converter has become critical which requires a thorough understanding of fluid flow inside the catalytic converter. In this paper, an attempt has been made to study the effect of fluid flow due to geometry changes using commercial CFD tool. The study has been conducted assuming the fluid to be air. The numerical results were used determine the optimum geometry required to have a uniform velocity profile at the inlet to the substrate. [6]

Chen et al. (2017) utilized a 3D CFD flow modelling and a heterogeneous reaction model of the catalytic converter. They calculated the pressure and the velocity field with incorporating the flow resistance within the monolith substrate. They concluded that the flow field is influenced by the monolith substrate resistance for a specific geometry and Reynolds number. Moreover, the flow uniformity at the front face increased with increasing cell density of the monolith and decreased when increasing the flow Reynolds number.[11]

Chakravarthy et al. (2003) Utilizing multi-dimensional channel model. It was recorded that the ignition behaviour can be dramatically affected by flow recirculation at the inlet of the substrate which lead to high flow misdistribution especially at lower exhaust temperatures. The study concluded that flow non-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.[8]

III. METHODOLOGY

In this study the CFD simulations of 3 way catalytic convertor have been done. The model designing of catalytic convertor have been done in Ansys 14.5 design modular. By using various design operations. Then the meshing of this model has been done in icem CFD 14.5. The meshing have been done in this analysis are tetrahedral and quardcore. The number of nodes and the elements are uses in the meshing of this model are 93298 and 87650 respectively. For result simulations have been done in CFD post processing. The methods used for it are 3d type Pressure based, steady state, and absolute velocity formulation. The models used are energy on, turbulent K-Epsilon standard wall function is used with species. In this analysis the model material behave like porous media. The solution methods are used coupled scheme, least square cell based gradient, second order pressure, and second order upwind momentum. The model and meshing diagrams are shown below:

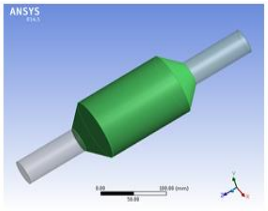

Fig.1 Design model of 3 way catalytic convertor

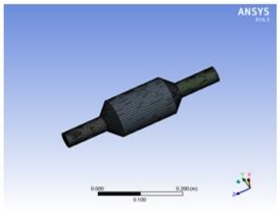

Fig.2 Mesh model of 3 way Catalytic convertor

Boundary conditions:

Table 1 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

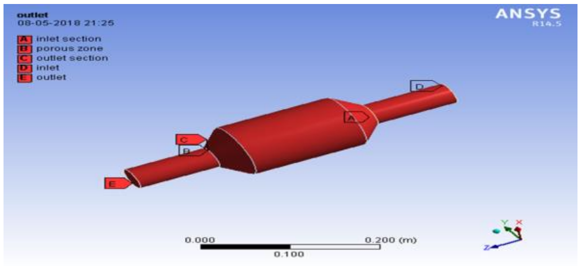

Fig.3 Boundary conditions Catalytic convertor

IV.RESULTS

Initially the grid independence test was performed to eliminate the errors due to coarseness of the grid; analysis has been carried for different number of cells. The CFD model was assessed using previous measurements under steady state condition. The model's predictions under steady state conditions were compared with the previous measurements. The feed gas conditions used in this case are listed in Table 5.3. The mass fraction of species is plotted as a function of position along the length of the catalytic converter from inlet to outlet. The figure depicts that the CFD model results are in good agreement with the previous measurements.

CONTOURS FOR SUBSTRATE LENGTH OF 190mm

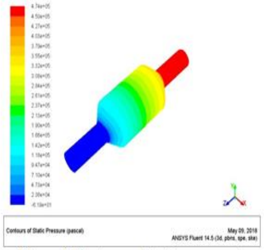

Figure 4 Contours of static pressure for substrate length of 190mm

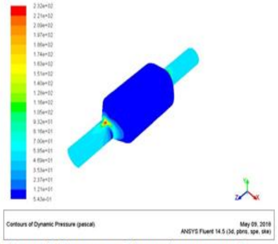

Figure 5 Contours of dynamic pressure for substrate length of 190mm

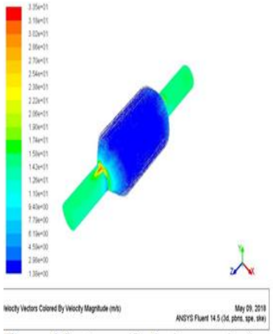

Figure 6 Contours of velocity magnitude for substrate length of 190mm

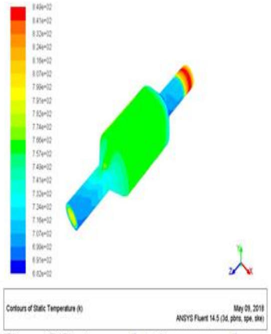

Figure 7 Contours of static pressure for substrate length of 190mm

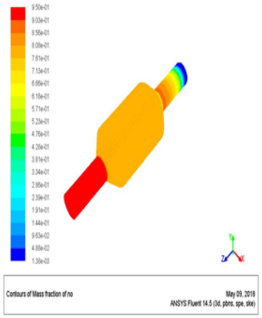

Figure 8 Contours of mass fraction of oxides of nitrogen for substrate length of 190mm

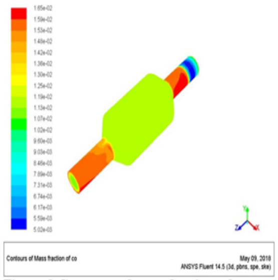

Figure 9 Contours of mass fraction of carbon monoxide for substrate length of 190mm

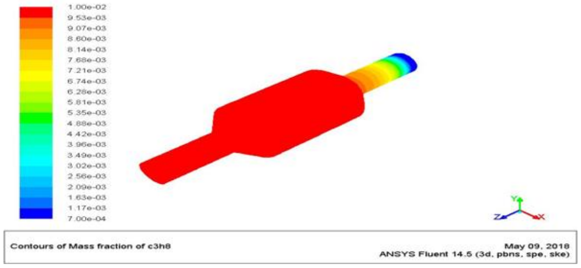

Figure 10 Contours of mass fraction of hydrocarbon for substrate length of 190mm

CONTOURS FOR SUBSTRATE LENGTH OF 200mm

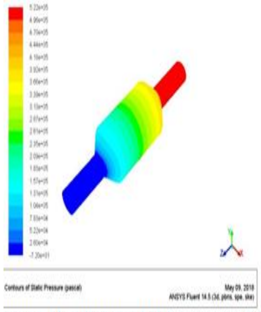

Figure 11 Contours of static pressure for substrate length of 200mm

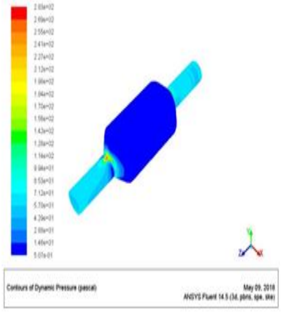

Figure 12 Contours of dynamic pressure for substrate length of 200mm

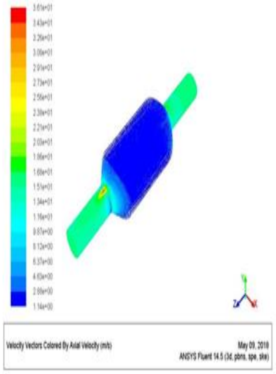

Figure 13 Contours of velocity vector for substrate length of 200mm

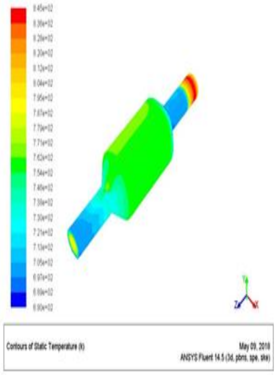

Figure 14 Contours of static temperature for substrate length of 200mm

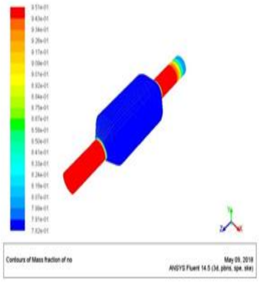

Figure 15 Contours of mass fraction of oxides of nitrogen for substrate length of 200mm

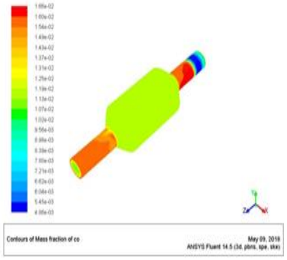

Figure 16 Contours of mass fraction of carbon monoxide for substrate length of 200mm

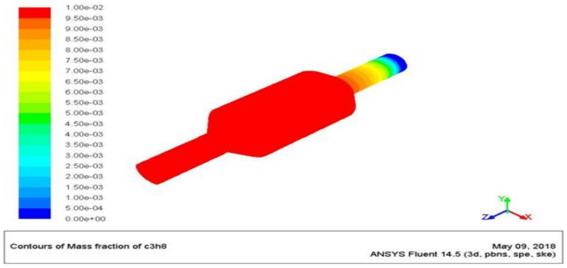

Figure 17 Contours of mass fraction of hydrocarbon for substrate length of 200mm

CONTOURS FOR SUBSTRATE LENGTH OF 210mm

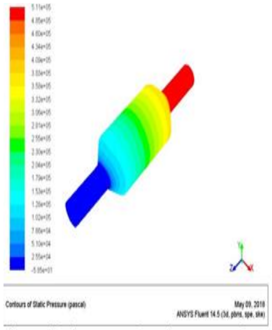

Figure 18 Contours of static pressure for substrate length of 210mm

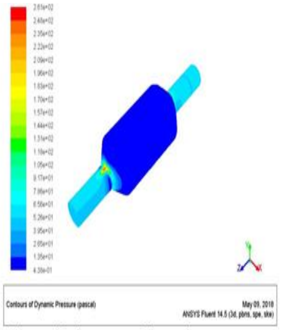

Figure 19 Contours of dynamic pressure for substrate length of 210mm

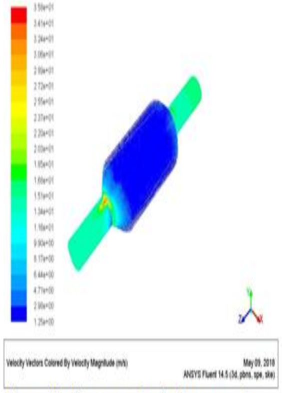

Figure 20 Contours of velocity vector for substrate length of 210mm

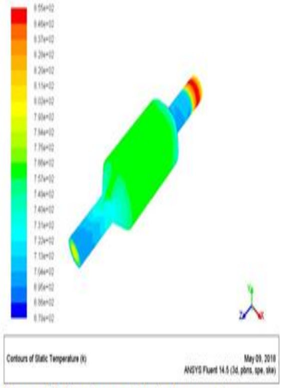

Figure 21 Contours of static temperature for substrate length of 210mm

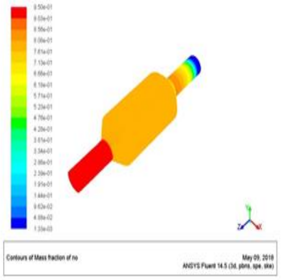

Figure 22 Contours of mass fraction of oxides of nitrogen for substrate length of 210mm

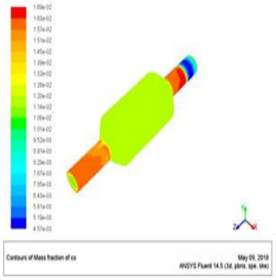

Figure 23 Contours of mass fraction of carbon monoxide for substrate length of 210mm

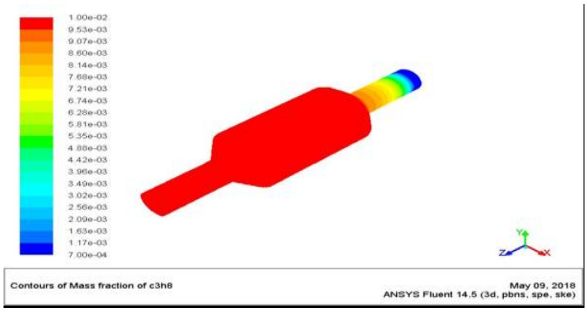

Figure 24 Contours of mass fraction of hydrocarbon for substrate length of 210mm

CALCULATION OF CONVERSION EFFICIENCY

Table 2 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 3 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 4 Conversion rate of carbon monoxide

Inlet Temperature(In K)	Conversion Rate o f 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 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 NO_x 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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