

# Computational Analysis of Three way Monolithic Catalytic Converter using FVM tool ANSYS Fluent

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**Abstract** — Monolithic three way catalysts are wide been used to reduce the emission of combustion engines. Several Factors should be considered while designing the catalytic converter; however, it is a complex process involving the optimization of different physical and chemical parameters. Length, Cell densities, metal coverage, fuel composition is the simple Properties which ready influence the catalytic performance of the converter. In this paper a 3-Dimensional monolith catalytic converter has been modelled by using ANSYS Fluent. Flow and heterogeneous reactions are simulated within the catalytic converters. A surface reaction model is applied to predict the performance of a three-way Pt/Rh catalyst where stoichiometric fuel has been used Mixture. The concentrations of the gas species and the site species are attained. The simulation results are compared with the experimental data of a three-way catalyst and the results are with acceptable limit and shows good agreement with literature.

**Keywords**— Conversion Efficiency, Monolithic, ANSYS.

## I. INTRODUCTION

Catalytic converters have been employed for about thirty-five years to lessen the toxicity of exhaust emissions from the internal combustion engine. The growing concern about the environmental impact of these contaminants have leads to progressively restrictive regulations, which in turn have offered the impetus for the development of increasingly capable exhaust gas after-treatment systems and catalytic converters.

Conventionally, a typical catalytic converter is made of a ceramic “monolith” substrate. It consists of numerous of channels running through the length of the monolith. The channel walls are coated with a thin washcoat (usually made of ceria, alumina, or other metal oxides), which sustain the noble metal catalysts (Pd, Pt and Rh). Generally arrangement of channels in the cross-section is similar to a honeycomb like structure within the monolith. The complete catalytic convertor assembly consists of an inlet manifold – which includes an inlet pipe of uniform cross-section pursued by a diverging section – which directs to the catalytic monolith; the gases exiting the monolith pass through a converging section before exiting passing through an outlet pipe to the atmosphere.

For the design an efficient catalytic converter, several physical and chemical properties of both the catalyst and the exhaust gas must be considered:

- Cell geometry (Diameter and length of the channel, wall thickness),
- Species of promotors,
- Species of noble metal and noble metal loading,
- Exhaust gas Temperature, velocity and chemical composition.

## II. LITERATURE REVIEW

Charles 1985 elaborates the U.S dependence upon the platinum group metals (PGM) and due to the significance of these metals to our way of life and even in their national security, gives are comprehensive report for the pre recovery and recovery system losses of PGM in automotive catalytic converter.

Lai et al. 1992 perform a three-dimensional investigation analytically and experimentally for non-reacting flow field within a conventional dual-monolith automotive catalytic converter. Via analytical approach the monolith brick resistance is formulated by pertaining pressure gradient for fully developed flow (Laminar). [2] It has found that the gas flow intensity mal-distribute in the monolith detains on the inlet flow reynolds number, the brick resistance, along with the pipe length and its bending angle.

Kolrsakis and Stamatelos 1997 gives a review of the catalytic system used in automobiles for emission control. The review covers the catalyst technology appropriate in each case, the working principles and performance uniqueness, durability characteristics and considerations regarding the interactions between catalyst performance and engine management.[4]

Chakarvarthy et al. 2003 studied the impact of flow non-uniformity during cold start transient operation. It has observed inlet region recirculation can lead to noteworthy non-uniformity of the flow in the monolith, and this non-uniformity can lead to significant differences in ignition characteristics among the channels [6]

Kaiser and hobfeld 2003 perform CFD simulation for optimization of flow in order to prevent the converter failure form high thermal and fluid dynamic loads. By means of optimized results, complexities of the flow condition are well understood. [7]

Tsinoglou et al. 2004 propose an alternative flow resistance computation; the proposed model can

predict the convertor efficiency for transient flow field. However, the model has been validated with the CFD results. [8]

Halbei and Jebasinski 2005 conduct Numerical simulation of exhaust gas conversion by employing Eberspächer model and another commercial program wave has also been used and comparative comprehensive report has been given for both the programs. [9]

Liu et al. 2007 perform 3D modelling of methane ignited reverse flow catalytic convertor by means of CFD code .The applied methodology consists of heterogeneous continuum and pseudo-homogeneous model. At last it has been concluded that inlet temperature and condition significantly affects the flow condition.[10]

Santos and costa 2008 evaluate the performance of mass transfer for automotive catalytic converters operating under real conditions. By establishing a new correlation for the mass transfers for 1D two phase model experimentally. The experiments have included measurements of conversion efficiencies for hydrocarbons, CO and NOx from ceramic and metallic three way catalytic converters.[11]

Kumar and Sandip 2010 simulate laboratory-scale catalytic converter using finite volume method. A steady state analysis has been performed in order to analyse the fluid flow, heat and mass transfer and heterogeneous chemical reactions.[12]

Symeon and Mantzaras 2011 perform transient 2D simulation in platinum-coated micro channel made of either ceramic or metallic walls. During simulation inlet pressure, wall thermal conductivity, heat capacity are varied and comparative analysis has been done between 100% CH4 and 90% CH4–10% H2 by volume.[13]

Horneber et al. 2012 perform 3D numerical simulations of structured open-cell foams for the accurate Kelvin cell geometry. The obtained result shows the influence of surface roughness in pressure drop and velocity distribution with the reactor. Moreover, the numerical solutions are compared with dimensionless number such as friction factor, Euler number and Reynolds number. [14]

Yun 2013 present 1-D transient emission analysis using AMESim for LPG fuelled vehicle in order to evaluate optimum operating condition of a Secondary Air Injection (SAI) system. [15] During simulation the effect of SAI flow rate and supply time on CO, HC and NOx emission has been analysed and found that significant reduction in species has been achieved for the desired optimum operating condition.

Ozhan et al. 2014 presents a novel approach for examining the flow features within the automotive catalytic converter. [16] The adopted methodology is a combination of physical and numerical multi-resolution techniques, with the aim of reducing computation cost Adaptive Mesh Refinement techniques has been optimized. It has been conclude that by effective coupling of this technique significant

reduction has been seen in the error of the numerical predictions

Hamed et al. 2014 simulates the flow distribution within the ammonia oxidation reactor at Shiraz Petrochemical Complex (SPC) using CFD.[17] It has found that the flow uniformity inside reactor get distorted because of improper header design and reveals the performance of the reactor significantly affected by an even flow of gas with the reactor.

Francesco et al. 2015 perform comparative analysis between Open-cell foams and Honey combs catalyst substrates using CFD and revealed that the open-cell structures honeycombs, at high flow rates, have higher mass transfer properties by allowing more compact reactors, better conversion efficiency with lower surface along with better porosity. [18]

### III.MATHEMATICAL MODELLING

The **Navier–Stokes equations** can be written in the most useful form for the development of the finite volume method:

$$\rho \frac{Du}{Dt} = -\frac{\partial p}{\partial x} + \text{div}(\mu \text{grad}u) + S_{Mx} \quad (1)$$

$$\rho \frac{Dv}{Dt} = -\frac{\partial p}{\partial y} + \text{div}(\mu \text{grad}v) + S_{My} \quad (2)$$

$$\rho \frac{Dw}{Dt} = -\frac{\partial p}{\partial z} + \text{div}(\mu \text{grad}w) + S_{Mz} \quad (3)$$

Governing equations of the flow of a compressible Newtonian fluid

**Continuity**  $\frac{\partial \rho}{\partial x} + \text{div}(\rho u) = 0$  (

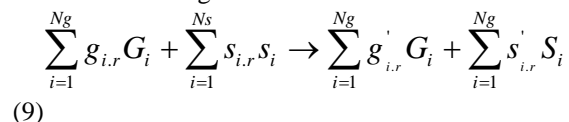
**x-momentum**  $\frac{\partial(\rho u)}{\partial x} + \text{div}(\rho uu) = -\frac{\partial p}{\partial x} + \text{div}(\mu \text{grad}u) + S_{Mx}$  (4)

**y-momentum**  $\frac{\partial(\rho v)}{\partial y} + \text{div}(\rho vu) = -\frac{\partial p}{\partial y} + \text{div}(\mu \text{grad}v) + S_{My}$  (5)

**z-momentum**  $\frac{\partial(\rho w)}{\partial z} + \text{div}(\rho wu) = -\frac{\partial p}{\partial z} + \text{div}(\mu \text{grad}w) + S_{Mz}$  (6)

**Energy**  $\frac{\partial(\rho i)}{\partial t} + \text{div}(\rho iu) = -p \text{div}u + \text{div}(k \text{grad}T) + \Phi + S_i$  (7)

Surface Reaction Model - The heterogeneous reaction is of the general form



where  $G_i$  and  $S_i$  represent the gas species and the site species (adsorbed species), respectively. The rate of  $r^{th}$  forward reaction reads:

$$R_r = k_{f,r} \prod_{i=1}^{N_g} [G_i]^{g_{i,r}} \prod_{wall} [S_i]^{s_{i,r}} \quad (10)$$

The forward rate constant for  $r^{th}$  reaction,  $k_{f,r}$  is given by

$$k_{f,r}^{ads} = A_s T^{\beta_s} \exp\left(\frac{-E_r}{RT}\right) \quad (11)$$

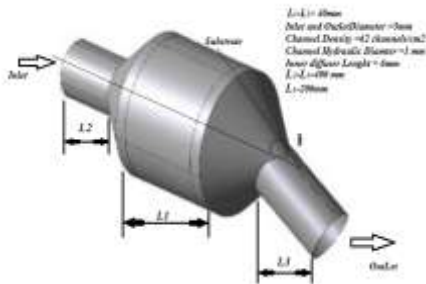
The rate coefficient for adsorption processes is calculated from the initial sticking coefficient  $S_0$ , that is the sticking probability at vanishing coverage:

$$k_{f_i}^{ads} = S_i^0 \frac{1}{\Gamma^\tau} \sqrt{\frac{RT}{2\pi M_i}} \quad (12)$$

Where,  $t$  is the number of occupied adsorption sites of species  $i$

#### IV. METHODOLOGY

The ANSYS 14.5 finite element program was used for simulation of Catalytic Converter. For this purpose, the key points were first created and then line segments were formed. The lines were combined to create an area. Finally, this area was extruded to model the Catalytic Converter. A 8-node three-dimensional structural solid element was selected to model the converter.



The Catalytic Converter was discretized into 2400 elements with 17300 nodes. Catalytic converter boundary conditions can also be modeled by constraining all degrees of freedoms of the nodes located on the left end of the converter. The Pressure velocity coupling extraction method was used to calculate the flow characteristics of Catalytic Converter.

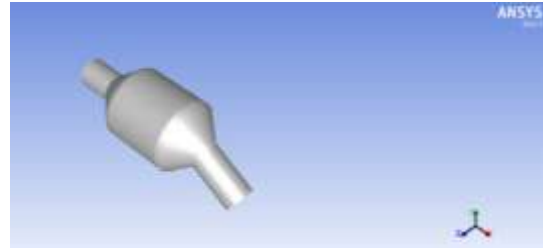


Figure 1 Model Geometry

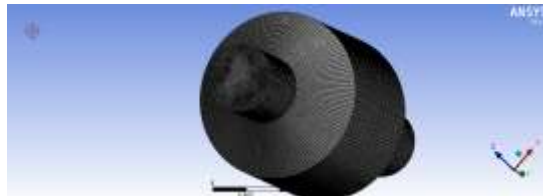


Figure 2 Mesh Model

Table 1 Physical Properties for simulation Ref.[5,19]

Parameter	Value
Cells per square inch, CPSI	400
Substrate volume fraction	0.26
Washcoat volume fraction	0.12
Fluid volume fraction (OFA)	0.62
Hydraulic diameter, Dh, mm	1
Geometric surface area, GSA m <sup>2</sup> /m <sup>3</sup>	2740
Active metal surface	27-28m <sup>2</sup> /g
Ratio of active metal surface	70
Wash coat Material	Ceria Stabilized alumina
Temperature range	100-600°C
Velocity temperature dependent	1.35 m/s at 25°C
Substrate material	cordirite

#### V. RESULT AND DISCUSSION

The governing equations of the problem were solved, numerically, using a Element method, and finite Volume method (FVM) used in order to calculate the Flow characteristics of a three-way catalytic converter. As a result of a grid independence study, a grid size of  $10^6$  was found to model accurately the catalytic converter performance characteristics are described in the corresponding results.

The accuracy of the computational model was verified by comparing results from the present study with those obtained by Siemund [3], Braun [5], Experimental, and FVM results.

In table 3 to table 5 and figure 3-5 shows the validation of FVM result obtained from the ANSYS tool. It has been seen that the obtained result of Threeway monolithic catalytic convertor with diffent

boundary condition shows good agreement with the analytical, Experimental and FVM of available literature.

The small variation in results is due to variation in grid sizing, operating condition, geometrical parameters, etc. but the obtained result shows the same trend so that the results are suitably verified.

**Table 3 Validation of CO Conversion at different Temperature**

Temperature	Expt. Ref. [3,5]	Present (FEV)
500	0.00435	0.00441
550	0.03691	0.00912
600	0.28341	0.11597
650	0.62293	0.64619
700	0.85083	0.85549
750	0.87874	0.86014
800	0.87409	0.87882

**Table 4 Validation of NO Conversion at different Temperature**

Temperature	Expt. Ref. [3,5]	Present (FEV)
500	0.00276	0.00282
550	0.00298	0.00302
600	0.29895	0.36079
650	0.67881	0.85994
700	0.95265	0.9659
750	0.96149	0.97916
800	0.96581	0.98936

**Table 5 Validation of C<sub>3</sub>H<sub>6</sub> Conversion at different Temperature**

Temperature	Expt. Ref. [3,5]	Present (FEV)
500	0.00319	0.00325
550	0.0033	0.00335
600	0.04312	0.07848
650	0.56017	0.60436
700	0.86509	0.91812
750	0.96232	0.93581
800	0.96673	0.9137

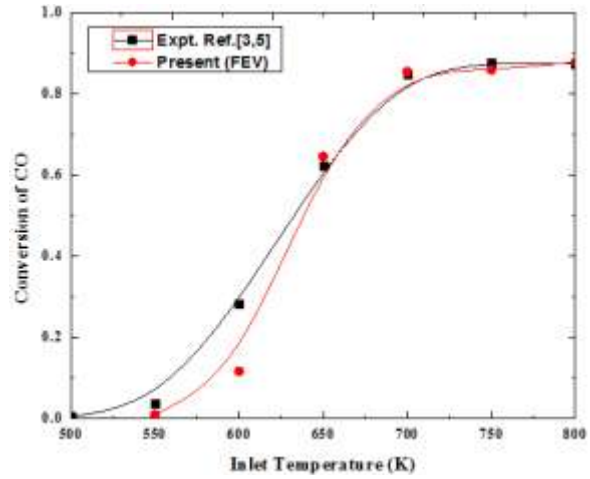


Figure 3 Validation of CO Conversion at different Temperature

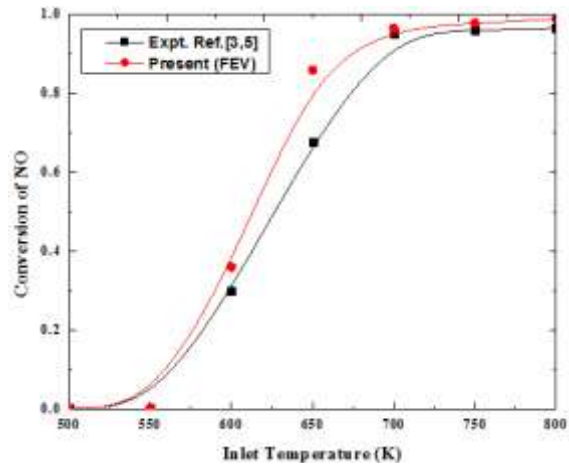


Figure 4 Validation NO Conversion at different Temperature

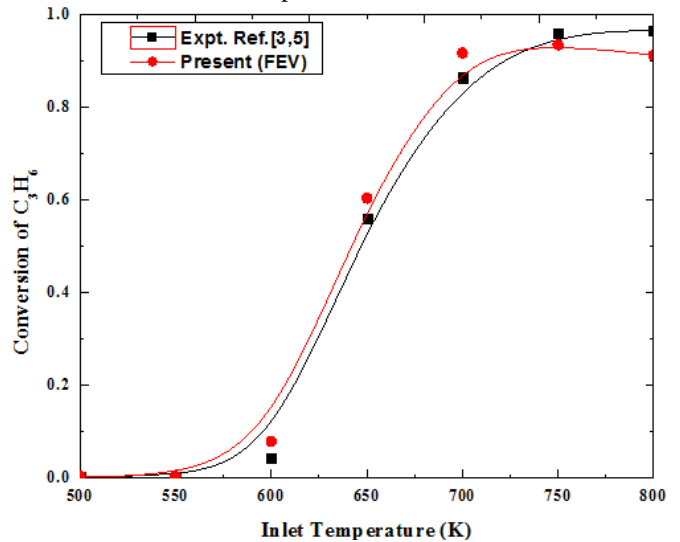


Figure 5 Validation of C<sub>3</sub>H<sub>6</sub> Conversion at different Temperature

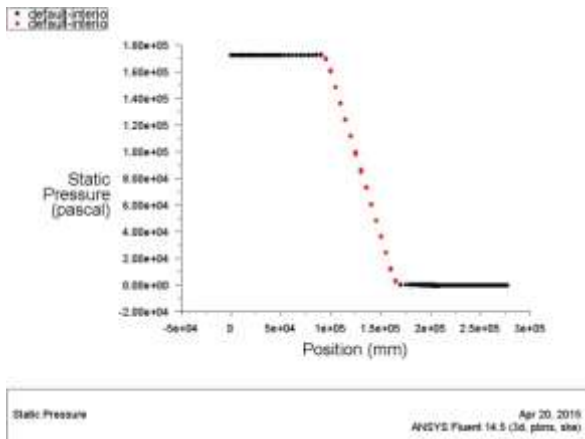


Figure 6 Pressure distribution across the catalytic converter

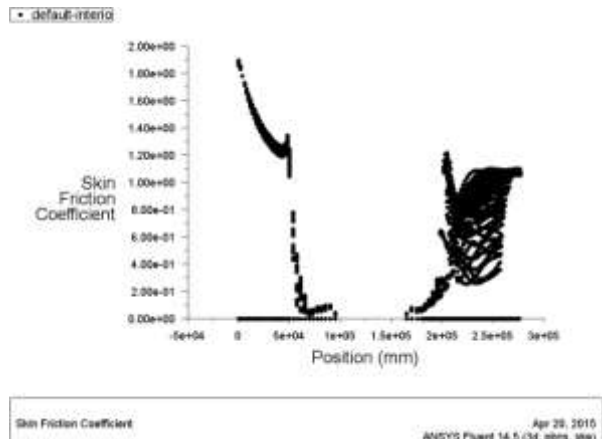


Figure 9 Skin friction coefficient distribution across the catalytic converter

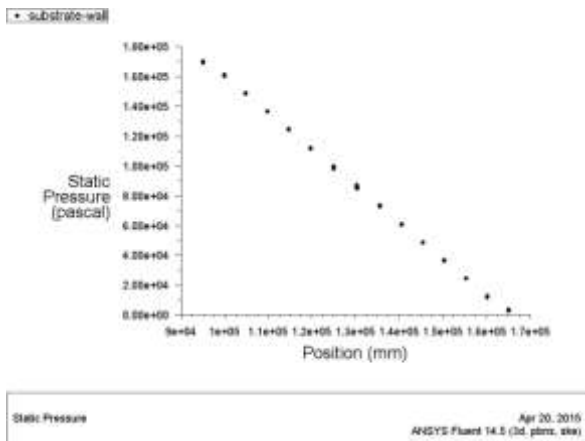


Figure 7 Pressure Drop across substrate

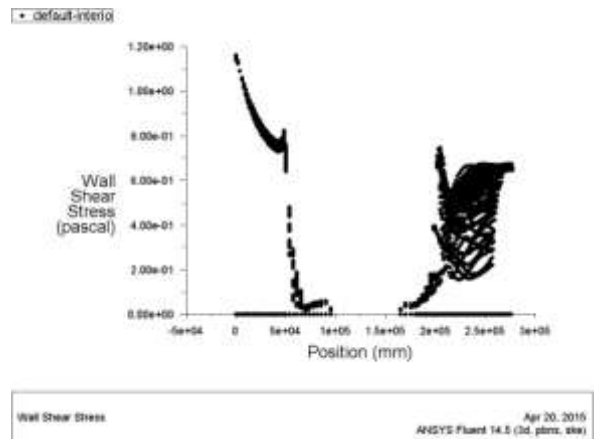


Figure 10 Shear Stress distribution across the catalytic converter

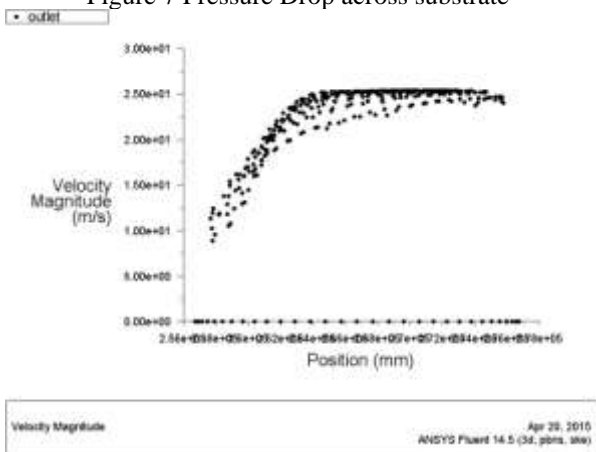


Figure 8 Velocity distribution across the outlet of catalytic converter

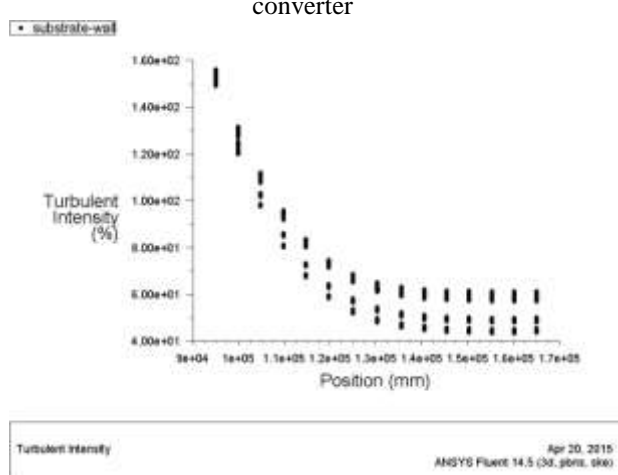


Figure 10 Turbulent intensity across the catalytic converter

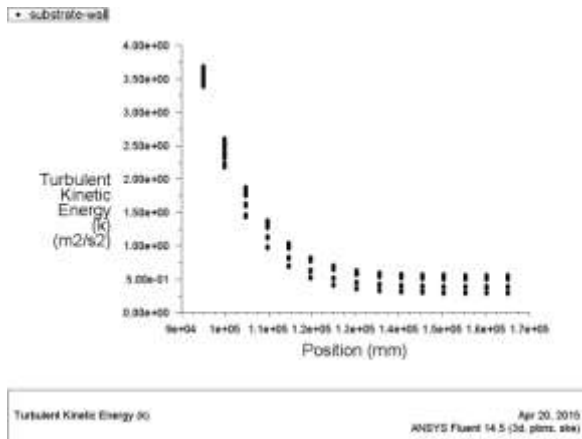


Figure 12 Shear Stress distribution across the catalytic converter

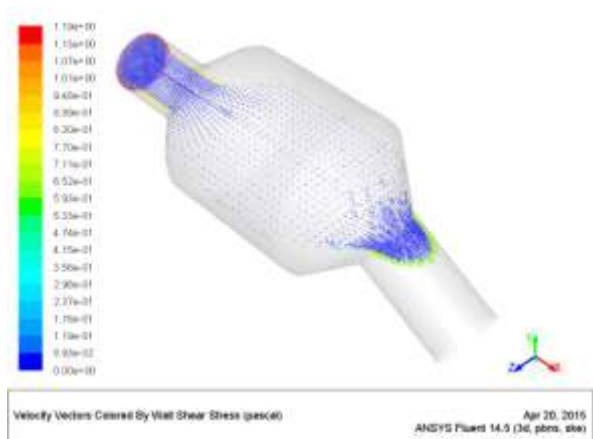


Figure 15 Wall shear stress velocity vectors across the catalytic converter

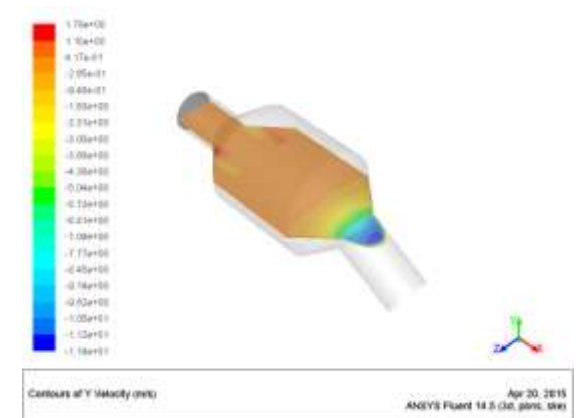


Figure 13 Velocity Contour along Y direction across the catalytic converter

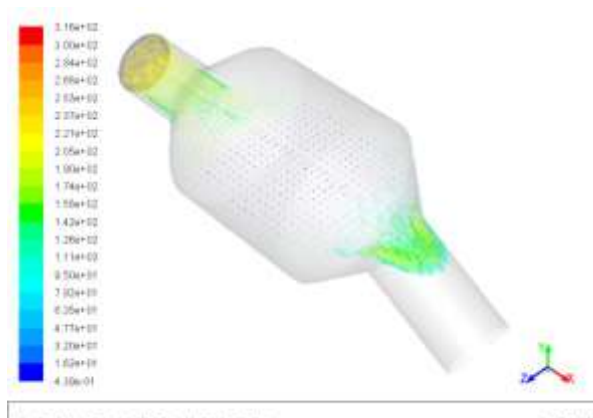


Figure 16 Turbulent Intensity velocity vectors across the catalytic converter

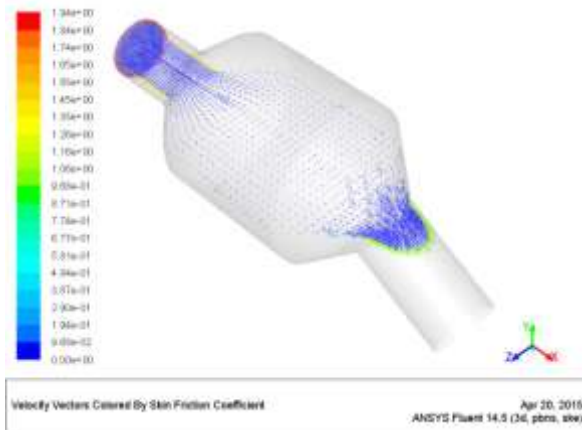


Figure 14 Skin Friction Coefficient velocity vectors across the catalytic converter

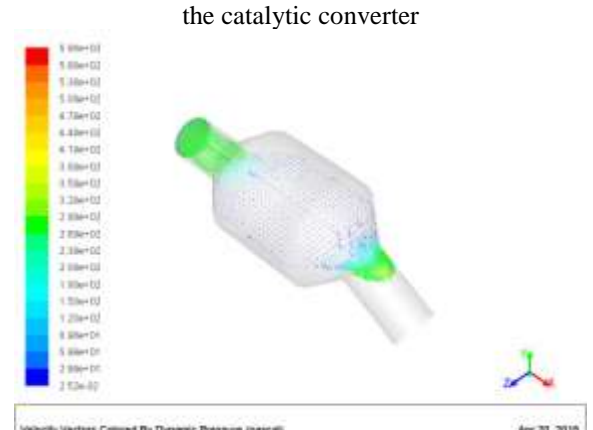


Figure 17 Dynamic Pressure velocity vectors across the catalytic converter

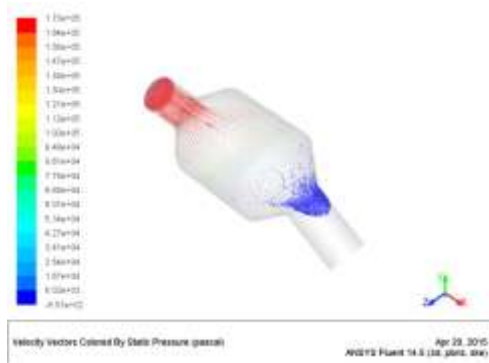


Figure 18 Static Pressure velocity vectors across the catalytic converter

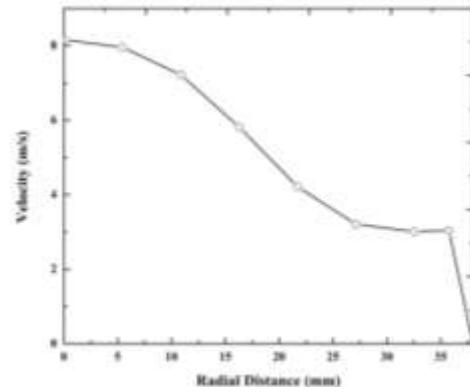


Figure 20 Velocity profile at the radial region

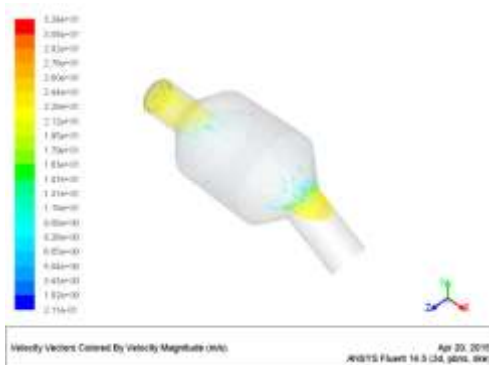


Figure 19 Velocity vectors by velocity magnitude across the catalytic converter

Figure 20 illustrates the Velocity profile at the radial region. There is a large separation region in the diffusers walls, which strongly affects the radial distribution of the longitudinal velocity at monolith inlet phase.

Figure 6 to 19 shows the contour plot of an catalytic convertor which illustrates the flow pattern across the converter. On the basis of these performance characteristics various graphs has been plotted and discussed there significance in three-way monolithic performance has been stated.

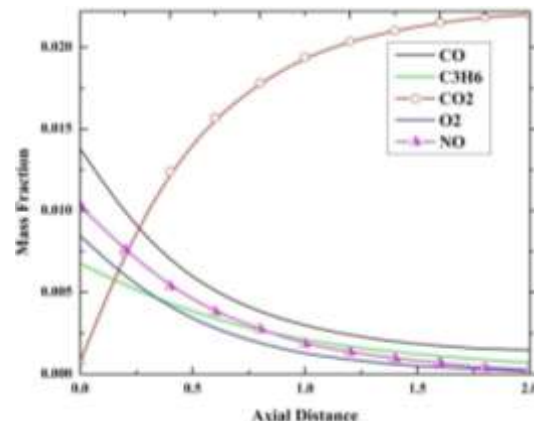


Figure 21 Mass fraction distribution of CO, NO, C<sub>3</sub>H<sub>6</sub>, O<sub>2</sub> and CO<sub>2</sub> along the centre line of the catalyst

It has observed that due to friction shear stress are develop across the wall of catalytic converter but at the substrate region the shear stress are very less and can be negligible. The velocity at the outlet has found to be more because of converging section just before the exhaust outlet increases the velocity at the outlet. During steady state model when throttle is open for maximum power adequate amount of mass flows through the converter at high velocity from engine manifold as rich mixture burn during this process leads to turbulence and the converging and diverging section in the converter also affect the flow uniformity.

Figure 21 shows the mass fraction distribution of CO, NO, C<sub>3</sub>H<sub>6</sub>, O<sub>2</sub> and CO<sub>2</sub> along the centre line of the catalyst. It has observed that CO<sub>2</sub> mass fraction noteworthy goes on increasing where as significant decline has been seen in the mass species of CO, NO, C<sub>3</sub>H<sub>6</sub>, O<sub>2</sub>. This is because of surface reaction takes place across the substrate, i.e. hydrocarbon species and carbon monoxide changes carbon dioxide.

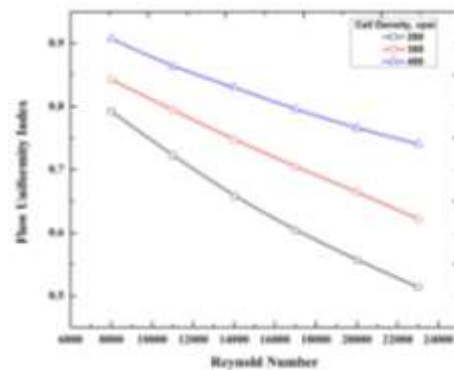


Figure 22 Effect of cell density with respect to Reynolds number on flow uniformity index

Figure 22 illustrate the effect of cell density with respect to Reynolds number on flow uniformity index. On increasing Reynolds number the flow uniformity index significantly decreases and the same trend has also been seen for the low cell density i.e 300 and 400. It can be conclude that for higher cell density higher flow uniformity has been seen.

It can also be revealed and recommended that higher cell density should be adopted for better flow uniformity across the converter for both laminar and turbulent flow.

## VI. CONCLUSION

- 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.
- The present proposed model has higher NOx conversion rate as compared to other species.
- Increasing mass flow rate the pressure drop increases linearly.
- Increasing substrate length improves the performance of converter.
- The order of conversion rate is as follows NO>C3H6>CO.
- On varying the fuel mixture i.e. lean or rich the rate of conversion significantly changes.
- On increasing flow velocity pressure drop across the substrate and converter drastically increases.
- Cell density of substrate plays crucial role in flow uniformity.
- At high Reynolds number due to turbulence flow uniformity affects and the turbulence can be seen across the radial region and the outlet.
- Porosity of substrate extensively gets affected at high temperature and the rate of species conversion decreases.

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