An Analytical Investigation of Purification and Quantification for Exhaust Gases Emissions

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Abstract- **Nowadays, reducing emissions of the exhaust gases in diesel engines has become a Principal goal for the future. Various norms are implemented all over the world to control the emission of toxic pollutants. A catalytic converter is a device used in automobiles used for the reduction of the toxicity and content of harmful emissions coming from the exhaust system. Instead of carrying out extensive experimentation, a simulation can be carried to find out optimum operating conditions so that exhaust emission can be reduced or the quality of emission gas can be improved. Same models can be taken as base reference for future experimentation. In this investigation, the design of a catalytic converter was proposed for single-cylinder four-stroke engines. The CAD model of the same was created in modeling software. An extensive CFD analysis by considering different standard operating condition was conducted, where back pressure analysis and vorticity analysis were done to get an optimum design which can reduce the pumping work done and also reduces the non-uniformity so that conversion of harmful pollutants to less harmful product can occur at a faster rate. Finally, simulations were performed using Matlab/Simulink which helped us to reduce the time required for the catalytic converter to reach its light off temperature. In Future, we can use the Matlab simulation for different filters (SCR, DPF, DOC, and CPF etc.) in presence of heating element.**

Keywords — Catalytic Converter, CFD analysis, Matlab/Simulink, light off temperature, heating element.

I. INTRODUCTION

With Automobile Industries becoming an ever-growing part of everyday life, air pollution and its major health impacts are becoming a growing concern. This has led to increasingly stringent regulatory laws on exhaust emissions level and composition such as the Indian Automobile Industry which made a transition from BS4 to the stricter BS6 emission norms. Under these emissions regime, NOX levels will go down by 25% petrols engines and a drastic 68% for diesel engines [1].

Catalytic converter is an exhaust emission control device that reduces the amount of harmful gases in the exhaust of IC engines. The most important pollutants from IC engines are CO, HC, NOX, AND PM. It is having the ability to convert these harmful gases to unharmful gases. As the piston moves from BDC to TDC during exhaust stroke the pumping work is done to push the exhaust gas out of engine but if the back pressure is more in that case it increases the pumping work as a result fuel consumption increases. Also, if the vorticity increases it would become difficult for catalyst to perform efficiently. A heating element is introduced to increase the exhaust temperature to withstand the given temperature appropriate material should be selected for substrate and shell of catalytic converter.

II. METHODOLOGY

A single cylinder four stroke engine was selected and from engine specifications design dimensions were calculated. Based on the dimensions obtained from these calculations, a CAD model of shell and substrate of catalytic converter were created [18]. Later, CFD analysis was carried out where appropriate boundary conditions were considered. Based on the engine specifications a Simulink model was developed in Matlab to check the effect of the heating element and to measure the concentration of pollutants [7]. Further the maximum temperature that was obtained in Matlab simulation, thermal and structural analysis was conducted to check the temperature distribution and elastic deformation in order to determine the required design. Steps followed in the methodology are as per Fig.1.

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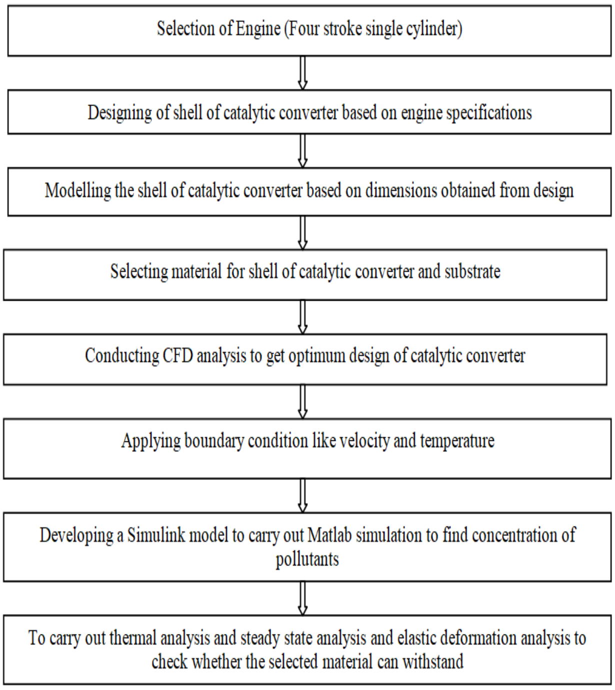

Fig.1. Process Flow Diagram

A. *Design & Modelling Considerations*

a) Single cylinder 4-stroke engine

Table no.1- Design Parameters

Rated engine speed (N)	1000rpm
Stroke length (l)	110mm
Bore diameter (d)	87.5mm

$$\text{Space Velocity} = \frac{\text{Volume Flow Rate}}{\text{Catalyst Volume}} \quad \text{……… (i)}$$

Where, Space Velocity is the space time necessary to process one reactor volume of fluid [2, 3].

For Single Cylinder, from table no.1

Space Velocity = 20,000 hr^{-1}

Volume Flow Rate = Swept Volume x No. of Intake strokes per hr……… (ii)

$$= \frac{\pi}{4} \times d^2 \times l \times \frac{N}{2} \times 60$$

$$= \frac{\pi}{4} \times 0.0875^2 \times 0.11 \times 500 \times 60$$

$$= 19.84 \ m^3/hr.$$

$$\text{Catalyst Volume } \frac{19.84}{20000} = 0.000851 m^3$$

Shell Dimensions:

Here, D – Diameter of the catalyst

L – Length of the catalyst

For L=2D

Volume = Area x Length……… (iii)

$$0.000851 = \frac{\pi}{4} \times D^2 \times 2D$$

D=85mm, L =170mm.

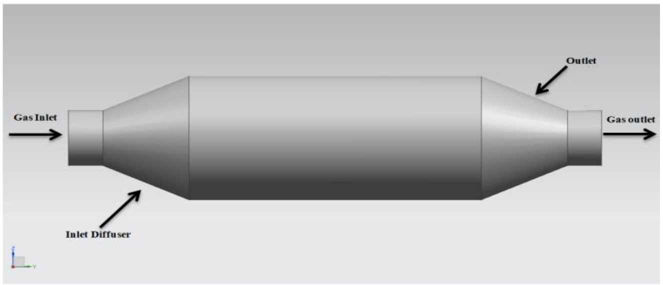

Fig.2 Schematic Structure of the Catalytic converter

b) Design of Catalytic Filter

Table no.2- Filter Parameters

Length of Catalytic Filter	40 mm
Side length of the hexagon	1.25 mm
Type of Mesh	Honeycomb Mesh

There are different types of filter meshes such as corrugated shape, square shape, etc, [2]. In this study, an analysis was performed based on honeycomb mesh type structure. The honeycomb mesh straightens the flow and reduces lateral turbulence and velocity [3]. Honeycomb structure is made up of porous a hole which allows the flow passing through with some pressure drop and can trap particles inside porous holes and can absorb species [6]. As a result, a honeycomb filter was designed by considering the dimensions from table no.2.

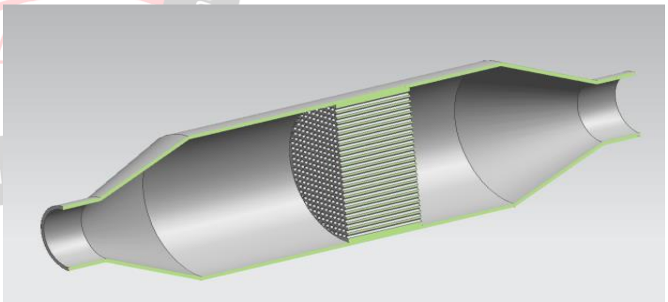

Fig.3 Honeycomb filter in converter

B. *CFD Analysis*

Air is used as fluid media, which was assumed to be steady and compressible. A Transition SST model was used in the CFD model. In transition SST model, it correctly predicts the drop of the skin friction due to the laminar bubble that is why it is preferred over k-ε model [23]. The equations of the mass and momentum are solved using COUPLED algorithm to get velocity and pressure in the fluid domain. Filter media of catalytic converter was modeled as porous media using coefficients. The geometry of the element was considered as tetrahedral mesh, with a refined mesh in this study. In CFD analysis two major flow characteristics (back pressure and vorticity) were studied.

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Case 1: In case 1, the models which had the lesser backpressure were studied for the flow pattern [9].

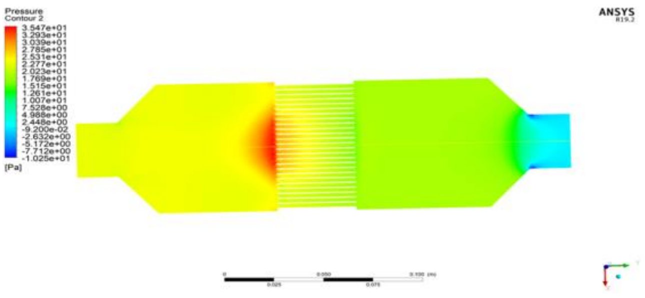

Fig.4 Pressure Drop for Diffuser Length 20 mm

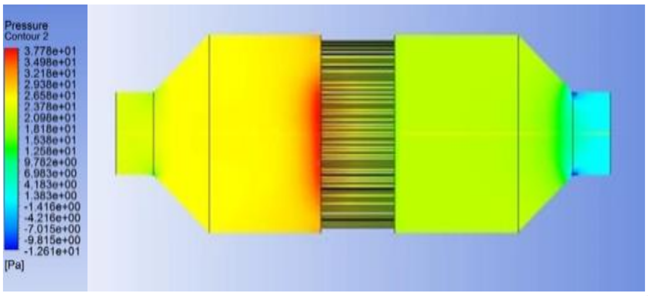

Fig.5 Pressure Drop for Diffuser Length 30 mm

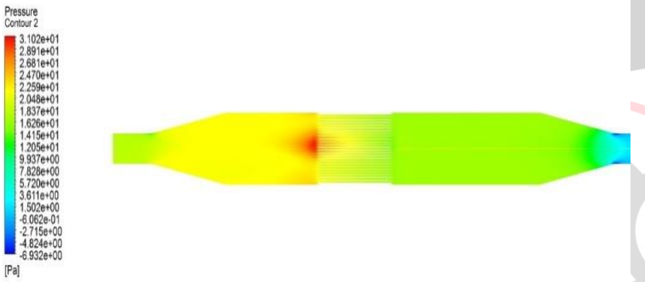

Fig.6 Pressure Drop for Diffuser Length 40 mm

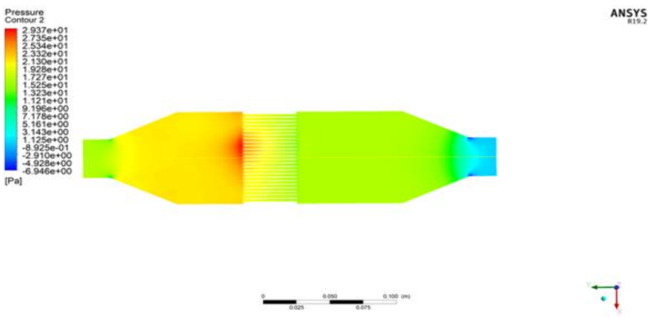

Fig.7 Pressure Drop for Diffuser Length 50 mm

It can be observed from Fig. 4, Fig.5, Fig.6, Fig.7 that the backpressure in model of diffuser length 20mm, 30mm, 40mm and 50mm are found to be 25.31 Pa, 23.78 Pa, 18.37 Pa, 15.25 Pa respectively.

Case 2: In case 2, the vorticity of the structures were studied. This study offered to find the recirculation zone which causes the in-active zones [8].

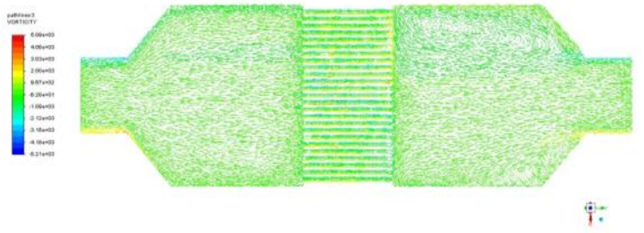

Fig.8 Vorticity for Diffuser Length 20 mm

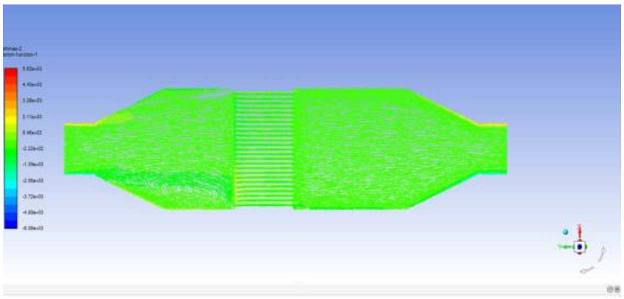

Fig.9 Vorticity for Diffuser Length 50 mm

The vorticity analysis was carried out which can be seen in Fig.8 & Fig 9 for two extreme cases of diffuser lengths 20 & 50 mm, out of which the vorticity incase of 20 mm, was found to be higher**.** Extreme cases were considered to check and validate about the results that were obtained from back pressure. In back pressure, model with diffuser length of 50 mm was found to be the optimum design so to check whether it was suitable with less vorticity we followed the analysis on two extreme cases.

C. Matlab/Simulink Simulation

Modelling the catalytic converter dynamics using Simulink and Matlab S-Function. In designing the model several simplifying assumptions were made [5]. Firstly, it was assumed that the catalytic converter could be modeled as a CSTR, so that the temperature of the converter can be treated as uniform rather than accounting for temperature changes along its length [11]. The reaction was assumed to be first order reaction. The conduction between catalyst particles and the body of the convertor were assumed to be faster. Conduction from catalytic converter to other parts of the car was not considered. The total heat transfer in catalytic converter is modeled using total heat transfer coefficient. It was considered that the electric power coming from power supply was completely transferred to the heating element such that the electrical energy was completely converted into thermal energy. Substituting these differential equations into the s-function in Simulink to solve them, using this model the concentration with respect to time was determined [13]. The reaction terms were simplified by assuming that the reaction was first order and in the presence of a platinum catalyst [14].

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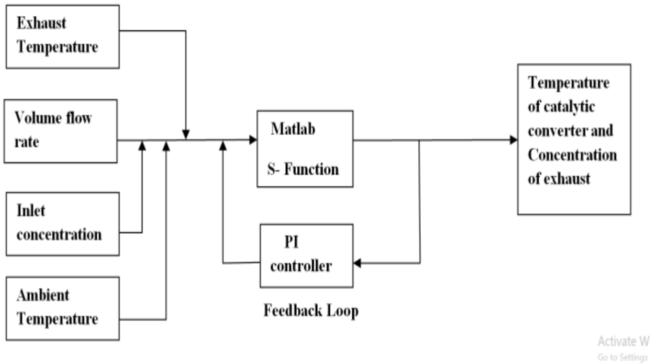


Fig.10 Procedure applied block

The considered equations are given as;

$$\frac{\partial T_C}{\partial t} = \frac{1}{mCp}\,[UA_{inside}(T_E\text{-}T_C)+UA_{outside}(T_A\text{-}T_C)+Q]..(4)$$

$$\frac{\partial C_C}{\partial t} = \frac{q}{V}\,(C\text{-}C_C)\text{-}k_0\, e^{(-Ea/RTc)}\, C_C\,...(5)$$

$$\frac{\partial T_E}{\partial t} = [UA_{inside}(TC\text{-}TE)+\Delta H_{rxn}\, k_0 e^{(-Ea/RTc)}\, CV+\rho\, Cp\, q\,(T_F\text{-}T_E)]....(6)$$

Where,
UA_{inside} - Heat transfer inside the converter body,
$UA_{outside}$ - Heat transfer outside the converter body,
Q- Heat source,
Tc - Changed in temp of catalytic converter,
Te-Exiting exhaust temperature,
q- Exhaust flow rate,
Ea - Activation energy,
Cc- Concentration of exhaust,
Cp- Specific heat at constant pressure,
m- Mass flow rate,
ρ- Density of exhaust.

With these simplifications, the transient energy and balanced species were determined to describe the changes in catalytic converter temperature, TC, concentration of exhaust gases in the exiting exhaust, C_C, and exiting exhaust temperature T_E. The balances are shown in Equations 4, 5, and 6, where q is the exhaust flow rate and V is the volume of the catalytic converter [5]. Substituting these balances into an S-Function in Simulink to solve the differential equations which can be seen in Fig 10.

D. Steady State Thermal Analysis

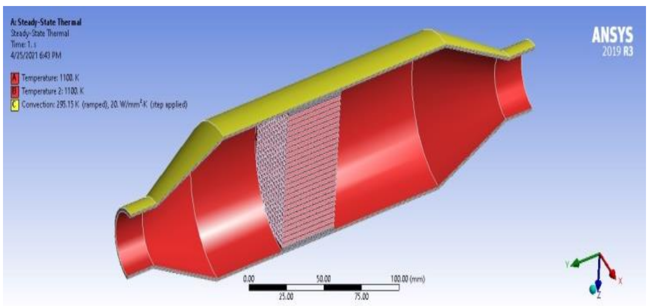


Fig.11 Convection Heat Transfer Analysis

At first the CAD model was imported in design modeller after which a mesh was generated, followed by applying boundary conditions and the shell properties of the catalytic converter along with its substrate were defined.

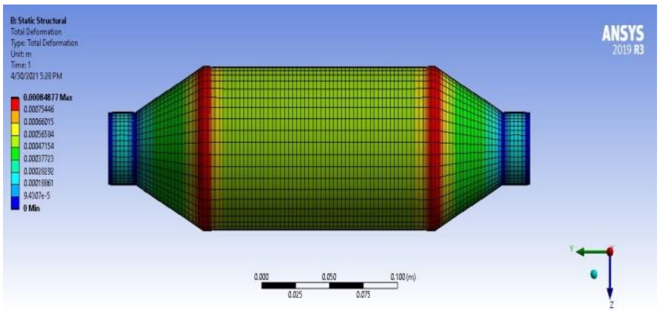
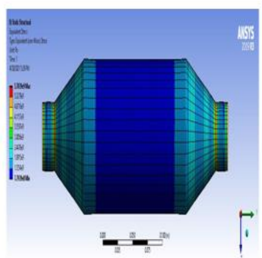
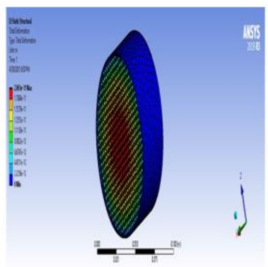


Fig.12 Total Deformation

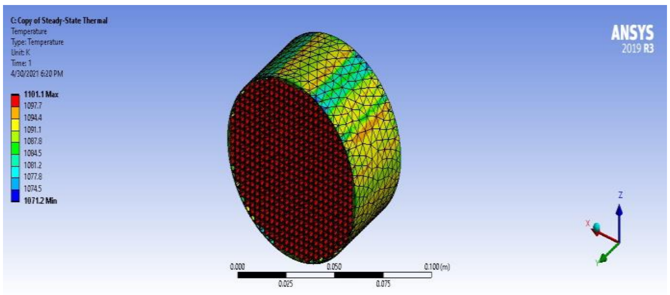
The temperature at the inner surface of the catalytic converter was defined 1100K and the temperature outside the catalytic converter was assumed as 295K and the heat transfer coefficient as 20W/mm^{2}K and the pressure obtained from CFD analysis are applied on the inner surface of catalytic converter as well as on the face of the filter which are mentioned in Fig.11. Here, the temperature distribution shows the heat flux analysis i.e. the total amount of heat transfer through catalytic converter [22]. At the given temperature, thermal stresses are developed in the catalytic converter and because of the thermal stresses, the maximum deformation occurred at the edges of the catalytic converter which is 0.00085m. The average deformation which occurred in the body of the catalytic converter is 0.00047m. The elastic strain which is developed in the body of catalytic converter ranges from 0.0065 to 0.0092 can be seen in Fig.12.



a) Elastic Strain Distribution of Shell



b) Total Deformation of Filter



c) Temperature Distribution of Filter

Fig.13 Results of thermal and Structural Analysis

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The thermal temperature distribution (Fig.13.c) obtained from steady state thermal analysis was imported as a thermal load in static structural analysis. The fixed support at the faces of catalytic converter and the pressure obtained from CFD analysis was applied at the inner surface of catalytic converter pipe and face of the filter and effect of the thermal load on model was observed the Fig.13.a and Fig. 13.b.

III. RESULTS & DISCUSSION

A. CFD ANALYSIS RESULTS

Designed with reference engine as single cylinder four stroke based on the bore diameter and stroke length, dimensions of the shell of the catalytic converter were calculated. Varying the diffuser length while considering four different cases and from the four cases of 20mm, 30mm, 40mm and 50mm. The primary aim of this CFD analysis was to find out the right shape of catalytic converter for the exhaust manifold which can offer minimum back pressure.

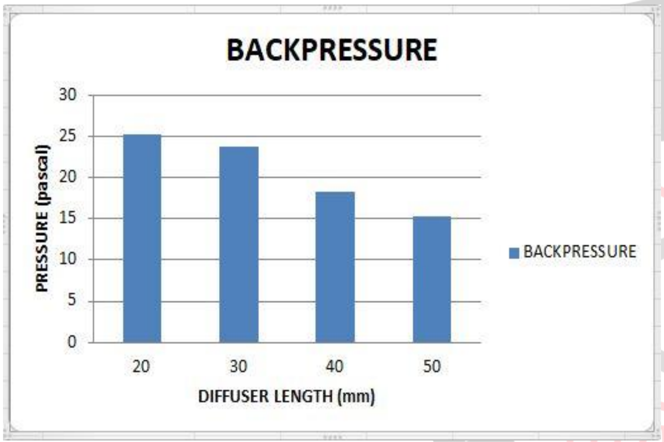

Fig.14 Backpressure plot

From Fig.14, a model was selected which provides minimum back pressure at the inlet the reason for selecting a model From Fig.14, a model was selected which provides minimum back pressure at the inlet the reason for selecting a model with minimum back pressure is that the pumping work is directly proportional to back pressure [10]. In order to reduce the pumping work the back pressure should be as minimum as possible if the pumping work increases the fuel consumption also increases. In back pressure analysis, the catalytic converter of diffuser length 50 mm shows minimum back pressure and hence among the four cases it is the optimum one. Then we conducted vorticity analysis Fig.8 and Fig.9 for extreme cases such as diffuser lengths of 20 & 50 mm and it was found out that catalytic converter of diffuser length 50mm has minimum vorticity that would result in reduced recirculation zone and would also reduce the non-uniformity. Since, lower vorticity results in lesser recirculation zones. This non-uniformity reduces the conversion of the harmful gases.

B. SIMULATION RESULTS

Simulink model was designed, which contains catalytic converter along with heating element [15]. The simulation was performed for initial and obtained parameters where the initial parameters were assumed based on magnitude guesses and research work of the normal model and the obtained parameters were achieved after adjusting the activation energy and the exhaust heating rate [16]. It was concluded that the increase in activation energy and rate of heating the time required for the light off temperature is reduced [21]. When the power supply through heat was constant in that case the light off temperature (the temperature at which the concentration of pollutants starts to decrease) occurred at around 7 minutes and as we increase the activation energy and the rate of heating [20].

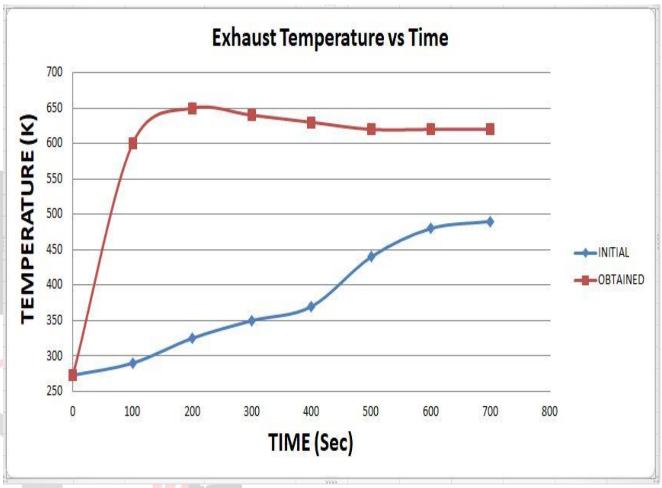

Fig.15 Exhaust Temperature vs. Time

Fig.16 Concentration vs. Time

The light off temperature occurred at around 63 seconds as per the results obtained from Fig.15 and Fig.16. Since, the activation energy and rate of heating increases the temperature rises at a faster rate as a result the efficiency of catalyst increases the maximum temperature achieved was 1100K. Based on the Matlab simulation results in order to withstand given temperature a material was selected for shell of the catalytic converter (Steel grade 409) and the substrate (zeolite) [12]. Then, steady state thermal analysis and heat flux analysis considering the above materials were

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conducted. Steady state thermal analysis in which the maximum temperature of the inner surface of the catalytic converter was 1100 K and the temperature of the surface of the catalytic converter was 653 K. The heat flux analysis that was carried out shows the total amount of heat transfer per unit area. For the steady state thermal analysis the maximum amount of heat flux was 11 W/mm^2 and the substrate material (zeolite) shows the heat flux of 6.9 W/mm^2 which is shown in Fig.13 [19].The total deformation in the filter of catalytic converter was observed to be maximum at the middle portion.

IV. CONCLUSION

It can be concluded from this study that, as the inlet cone length increases there will be reduction in back pressure and vorticity which will allow the flow of the exhaust gas to pass through the catalytic converter effortlessly. It was inferred that the time required for the catalytic converter to reach its light off temperature can be reduced by increasing the activation energy and exhaust heating rate. Thus, lesser harmful pollutants will enter the atmosphere that would prevent several human diseases. As a result, since the model is a simplified version of an important exhaust system it can be developed further to implement more elements and subsystems to replicate the actual physical system even more closely. Currently this model relies on assumed data based on various experimental concepts However, access to real life data and lab test data can assist in improving and fine tuning the model.

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