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Design and Analysis of Catalytic Converter Using Computational Fluid Dynamics (CFD)

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Abstract

Now a days the global warming and air pollution are big issues 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 a 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 rare earth metals now used as catalyst to reduce NOX are costly and rarely available. The scarcity and high demand of present catalyst materials necessitate the need for finding out the alternatives. Among all other particulate filter materials, knitted steel wire mesh material is Change and selected platinum, palladium, and rhodium coated on the surface of ceramic honeycomb structures as filter materials in this paper. Through CFD analysis, various models with different wire mesh grid shapes rectangular, circular, Diamond combinations were simulated using the appropriate boundary conditions. The comparison of back pressure of different catalytic converter models is made in this paper.

Keywords: Catalytic converter, Mesh materials, Grid shapes, CFD..

Introduction

The fibre was washed thoroughly with water and dried in an air oven at 80°C for 6 h, before being chopped into 6 mm length for fibre treatment and the preparation of the composites. Toluene- 2,4-diisocyanate (TDI) and polypropylene glycol (PPG) of molecular weight 1000 were supplied by the Aldrich Chemical Company, USA. Dibutyl tin dilaurate was obtained from Scientific and Industrial Supplies Corporation, Mumbai. Potassium permanganate, sodium hydroxide and maleic anhydride used in the present study were of chemically pure grade [1]. The chopped fibres were taken in a stainless steel vessel. A 10% solution of NaOH was added into the vessel and stirred well. This was kept for 1 h with subsequent stirring. The fibres were then washed thoroughly with water to remove the excess of NaOH sticking to the fibres. Final washings were carried out with distilled water containing a little acid. The fibres were then air dried [2]. Sugar cane biogases, the fibrous solid residue left over after juice extraction from Sugar cane (*S. Officinarum*) – designated “B” – was supplied by the Montebello distillery (Petit-Bourg, Guadeloupe). Sugar cane bagasse fibers were obtained by milling using a A catalytic converter is a vehicle emissions

control device which converts toxic by-products of combustion in the exhaust of an internal combustion engine to less toxic substances by way of catalyzed chemical reactions. The specific reactions vary with the type of catalyst installed. Most present-day vehicles that run on gasoline are fitted with a “three-way” converter, so named because it converts the three main pollutants in automobile exhaust: carbon monoxide, unburned hydrocarbon and oxides of nitrogen. The first two undergo catalytic combustion and the last is reduced back to nitrogen. The first widespread introduction of catalytic converters was in the United States market, where 1975 model year gasoline-powered automobiles were equipped to comply with tightening U.S. Environmental Protection Agency regulations on automobile exhaust emissions. These were “two-way” converters which combined carbon monoxide (CO) and unburned hydrocarbons (HC) to produce carbon dioxide (CO₂) and water (H₂O). Two-way catalytic converters of this type are now considered obsolete, having been supplanted except on lean burn engines by “three-way” converters which also reduce oxides of nitrogen (NO_x).

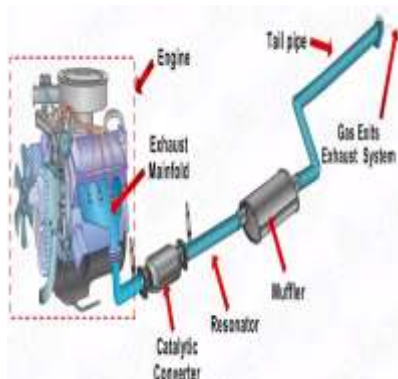


Fig.1 Position of Catalytic Converter

Basic conversion of catalytic converter

3- Way converters working as two catalyst process: 1. Reduction and 2. Oxidation- and a sophisticated oxygen storage/engine control system to convert three harmful gasses- HC, CO and NO_x. This is not an easy task: the catalyst chemistry required to clean up NO_x is most effective with a rich air/ fuel bias. To operate properly, a three- way converter first must convert NO_x (with a rich air/ fuel bias), then HC and CO (with a lean bias).



Fig.2 Basic Conversion of Catalytic Converter

Dangers of pollutants

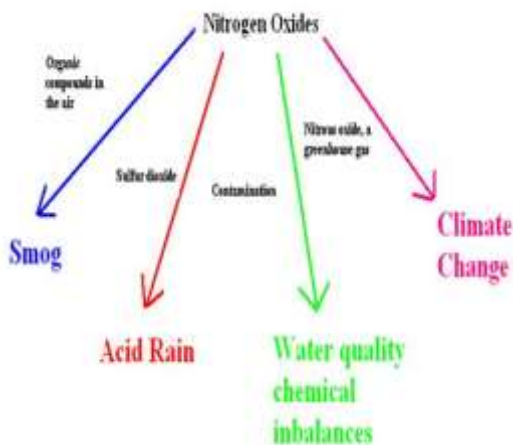


Fig.3 Dangers of Pollutants

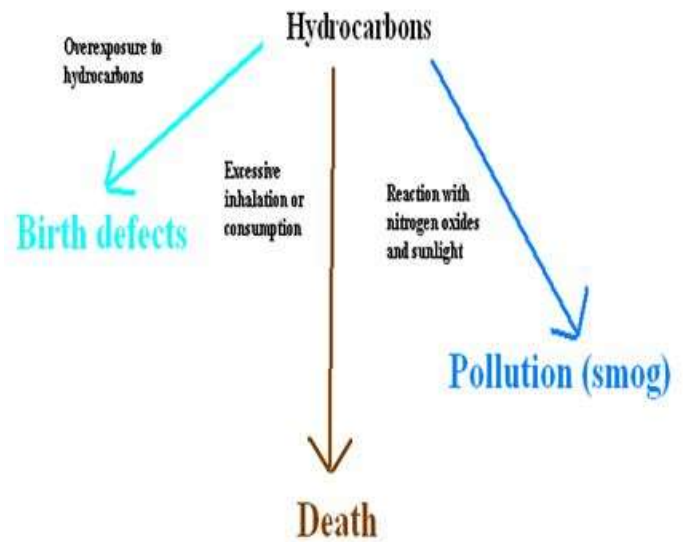


Fig.4 Effect of Pollutants

Without the redox process to filter and change the nitrogen oxides, carbon monoxides, and hydrocarbons into less harmful chemicals, the air quality (especially in large cities) would reach a harmful level to the human being.

Nitrogen oxides- these compounds are in the same family as nitrogen dioxide, nitric acid, nitrous oxide, nitrates, and nitric oxide. When NO_x is released into the air, it reacts with organic compounds in the air and sunlight, the result is smog. Smog is a pollutant and has adverse effects on children's lungs.

Carbon monoxide- this form of CO₂ is a harmful variant of a naturally occurring gas. Odorless and colorless, this gas does not have many useful functions in everyday processes.

Hydrocarbons- inhaling hydrocarbons from gasoline, household cleaners, propellants, kerosene and other fuels can cause death in children. Further complications can be central nervous system impairments and cardiovascular problems.

Literature survey

A.K.M.Mohiuddin [1] et al, said that the purpose of this paper is to present the results of an experimental study of the performance and conversion efficiencies of ceramic monolith three-way catalytic converters (TWCC) employed in automotive exhaust lines for the reduction of gasoline emissions. Two ceramic converters of different cell density, substrate length, and hydraulic channel diameter and wall thickness were studied to investigate the effect of varying

key parameters on conversion efficiencies and pressure drop. The conversion efficiencies from both converters were calculated and evaluated.

Thundil Karuppa Raj.R [2] et al, analyzed 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 to determine the optimum geometry required to have a uniform velocity profile at the inlet to the substrate.

MingChen [3] et al, Analyzed that a modeling approach to the design optimization of catalytic converters is presented. The first step of the optimization is the model-assisted sizing of catalysts. The second step deals with the flow optimization of the catalyst converter under the given geometric restraints. The substrate is modeled as porous media, where viscous and in it all resistances are specified via empirical formula. With the help of the CFD tool, the flow in the converter can be optimized using appropriate boundary layer control methods.

Problem finding

Once the catalytic converter reaches its operating temperature (known as "light off temperature" and usually between 400 and 600 degrees Fahrenheit) the catalyst compound coating the inner ceramics start to convert the three regulated harmful emissions into less harmful emissions. The three harmful emissions regulated by the EPA are Carbon monoxide (CO), Hydrocarbons (or VOCs for Volatile Organic Compounds), and Nitrogen compounds (NOx).

Carbon monoxide: Most of the used air leaving your engine is Carbon dioxide or CO₂. But since combustion isn't always perfect or complete, some of the Carbon molecules only pick up one oxygen molecule to create carbon monoxide, a deadly, odorless gas. The catalytic converter creates a reaction between the CO and its surrounding air particles to create CO₂ and H₂O (water).

Hydrocarbons: A Hydrocarbon is any compound made of Carbon and Hydrogen that can be burned. Hydrocarbon emissions cover a range of harmful emissions, but they are all made up of unburned Carbon and Hydrogen. Hydrocarbons are harmful when breathed and contribute greatly to smog build up in urban areas.

NOx: Nitrogen compounds referred to as NOx have caused many an emissions test failure. NOx emissions are basically Nitrogen molecules that have combined with Oxygen and escape the engine unburned. NOx emissions cause smog and acid rain.

The compounds coating the inner structure of the catalytic converter strip, ram together, and otherwise muscle these emissions into less harmful gases and water, leaving the stuff that comes out of your tailpipe in much better shape.

Overview of this project

They are extruded from dense, high strength ceramic substrate without sacrificing mechanical strength, total surface area remains same, back pressure reduces, conversion efficiency increases and thermal expansion reduces.

1. Circular structure
2. Triangular Structure
3. Diamond type structure

Methodology

Fig.5 shows the methodology which is used in this analysis.

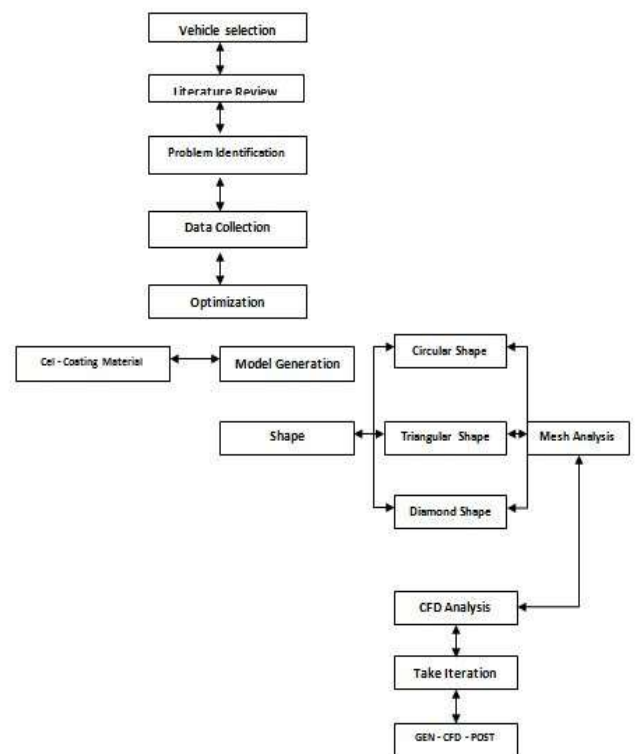


Fig.5 Methodology

Modeling

The flow distribution across the monolith frontal area depends on the geometry of a specific design of inlet

diffuser of drawings create modeling at done the models were done. At first we are doing numerical analysis of models being used in using experiments. The data's collected include,

- ❖ Dimensions for flow full setup.
- ❖ Scaling measure at reengineering.
- ❖ Conversion data analysis in Inches in to metric.

Dimensions for full assembly model

The details of the parameters are given in the following

Table.1 Design parameters of catalytic converter

DESCRIPTION	DETAILS	UNITS
Monolith diameter	72	mm
Monolith length	120	mm
Channel density	200-400	channel/cm ²
Monolith type	TWC -metallic	---
Precious metals	Pt/Rh	---
Surface area	2.41	m ²
Wash coat	45	Gr/m ²

The data's regarding design parameters like width of the flow channel, catalyst thickness etc. are collected from the assembly.

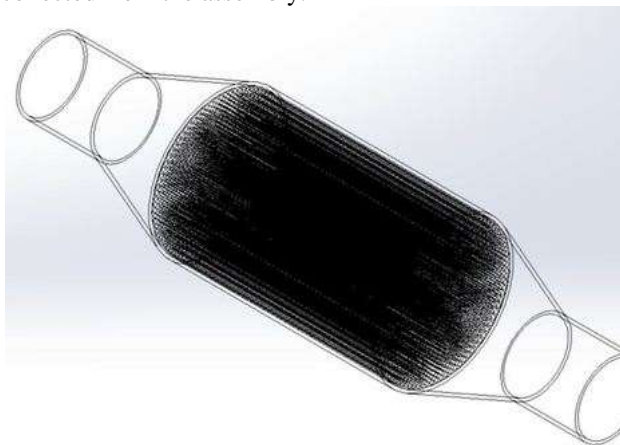


Fig.6 Wire frame model of catalytic converter

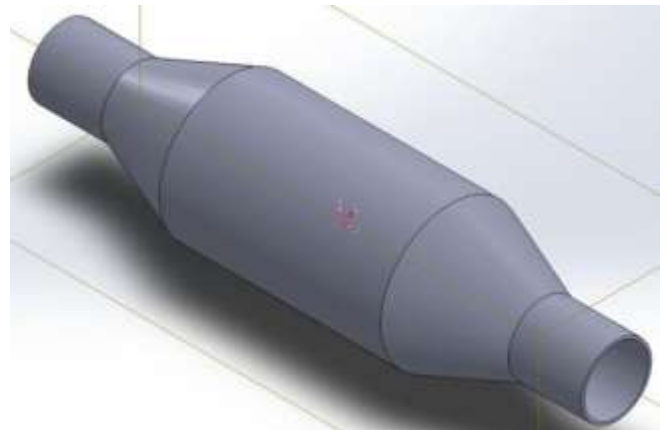


Fig.7 Isometric model of catalytic converter

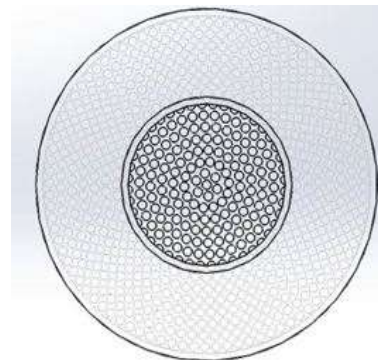


Fig.8 Full assembly front view – pentagon type cross section



Fig.9 Full assembly front view – circular type cross section

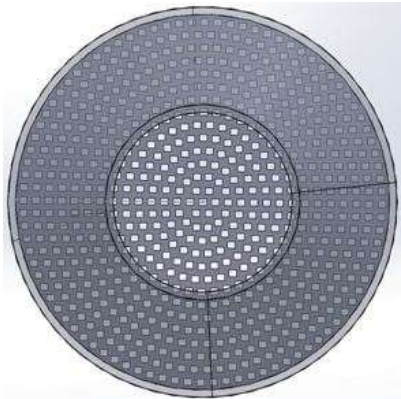


Fig.10 Full assembly front view – diamond type cross section

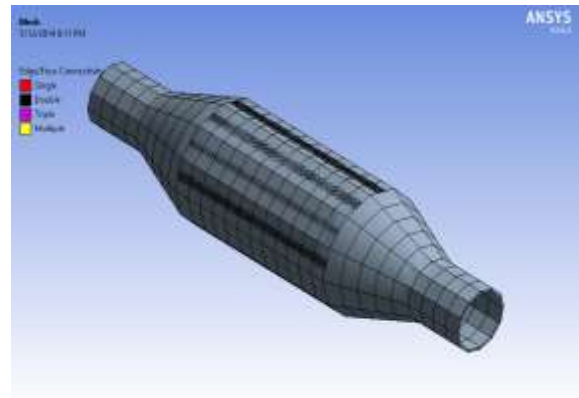


Fig.13 Boundary conditions

Meshing

The following mesh model has been created by using ANSYS 14.5 software.

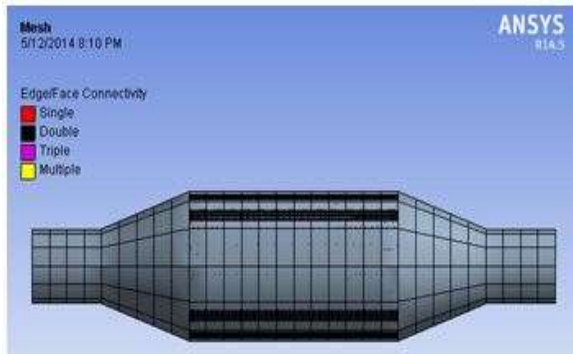


Fig.11 Mesh model of catalytic converter

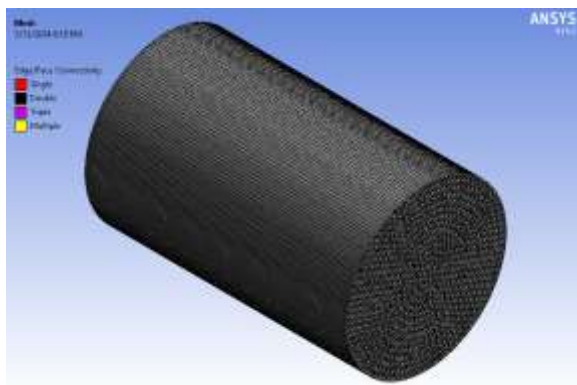


Fig.12 Mesh model of inner structure

Boundary conditions

The following boundary conditions have been given to that catalytic converter.

Analysis

In our project how to model porous media in FLUENT. Workshop models a catalytic converter. Nitrogen flows in through inlet with a uniform velocity 22.6 m/s, passes through steel with paladium with rothiem coating is monolith substrate with square shaped channels, and then exits through the outlet. Substrate is impermeable in Y and Z directions, which is modeled by specifying loss coefficients 3 order higher than in X direction.

Results and discussions

Numerical results of circular cross section for CO₂

Fig.14 shows the dynamic pressure distribution inside the catalytic converter with circular cross section for CO₂ fluid flow. Maximum and minimum values of dynamic pressure distribution is 1.08 Pa and 1.26×e⁴ Pa respectively

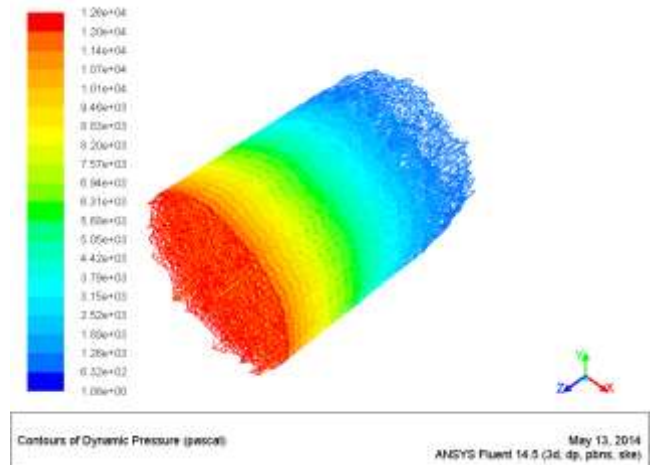


Fig.14 Dynamic pressure

Fig.15 shows the wall temperature distributions inside the catalytic converter with circular cross section for CO₂ fluid flow. Maximum and minimum

values of wall temperature distributions is 0 K and 300 K respectively.

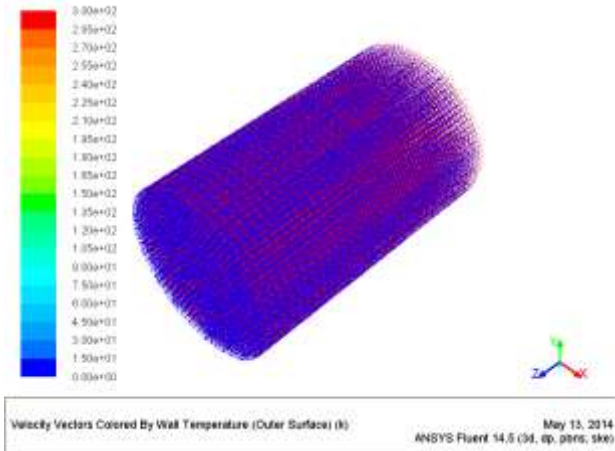


Fig.15 Wall temperature

Fig.16 shows the velocity distributions inside the catalytic converter with circular cross section for CO₂ fluid flow. A maximum and minimum value of velocity distributions is 0 m/s and 1.20 m/s respectively.

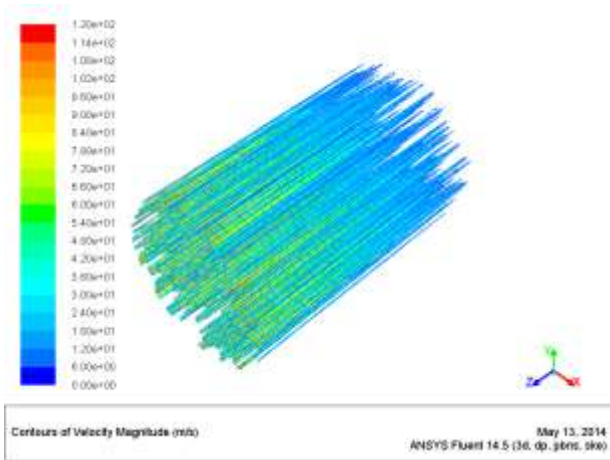


Fig.16 Velocity

Numerical results of circular cross section for CO

Fig.17 shows the dynamic pressure distribution inside the catalytic converter with circular cross section for CO fluid flow. Maximum and minimum values of dynamic pressure distribution is 3.62×10^3 Pa and 8.89×10^3 Pa respectively.

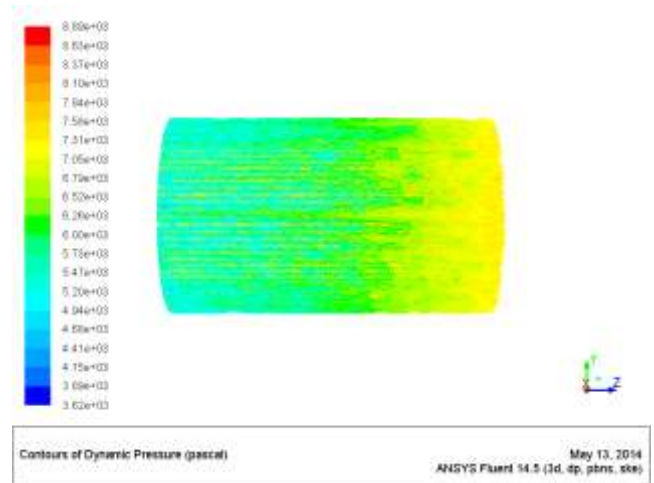


Fig.17 Dynamic pressure

Fig.18 shows the wall temperature distributions inside the catalytic converter with circular cross section for CO fluid flow. Maximum and minimum values of wall temperature distributions is 0 K and 300 K respectively.

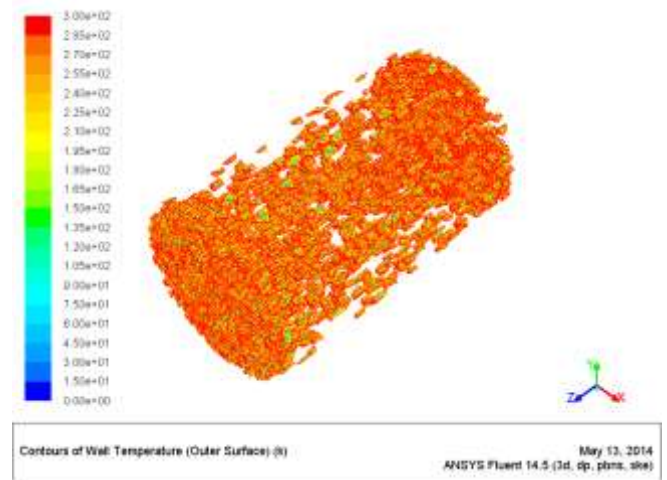


Fig.18 Wall temperature

Fig.19 shows the velocity distributions inside the catalytic converter with circular cross section for CO fluid flow. A maximum and minimum value of velocity distributions is 4.70×10^1 m/s and 1.38×10^2 m/s respectively.

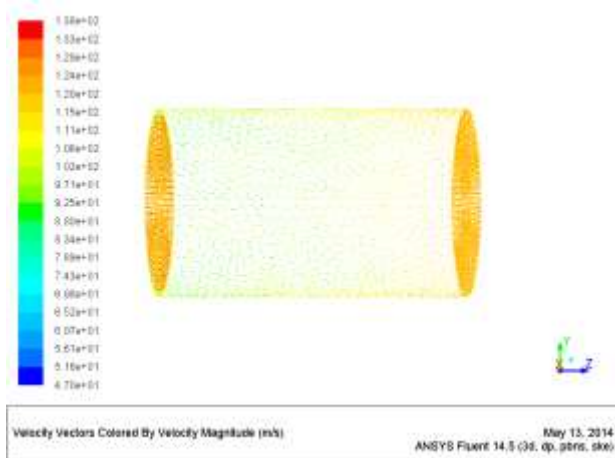


Fig.19 Velocity

Table.1 shows the Numerical result comparison of circular cross section with different fluid flow conditions.

Table.1 Numerical result comparison of circular cross section

Sl.No.	Fluids	Dynamic pressure (P) in Pa	Wall temperature (T) in K	Velocity (V) in m/s
1	CO ₂	1.26×e4	300	1.20×e2
2	CNO ₂	9.84×e5	300	1.02×e3
3	CO	8.89×e3	300	1.38×e2

Numerical results of square cross section for CO₂

Fig.20 shows the dynamic pressure distribution inside the catalytic converter with square cross section for CO₂ fluid flow. Maximum and minimum values of dynamic pressure distribution is 7.17×e³ Pa and 1.26×e⁴ Pa respectively.

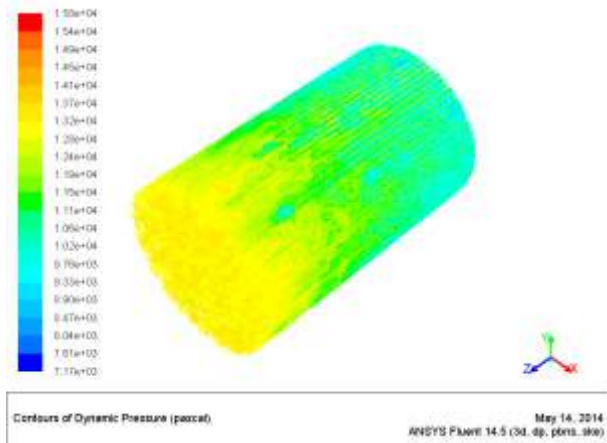


Fig.20 Dynamic pressure

Fig.21 shows the wall temperature distributions inside the catalytic converter with

square cross section for CO₂ fluid flow. Maximum and minimum values of wall temperature distributions is 0 K and 300 K respectively.

Fig.22 shows the velocity distributions inside the catalytic converter with square cross section for CO₂ fluid flow. A maximum and minimum value of velocity distributions is 0 m/s and 1.33×e² m/s respectively.

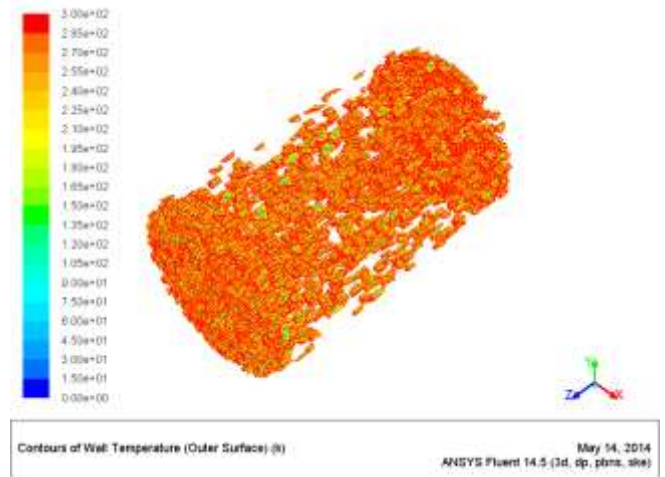


Fig.21 Wall temperature

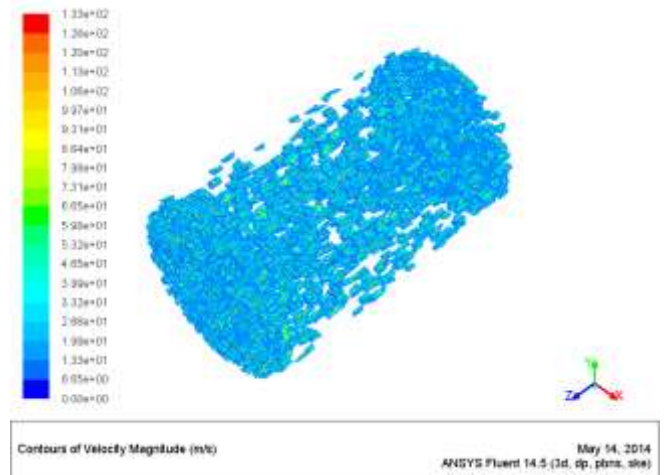


Fig.22 Velocity

Numerical results of square cross section for CNO₂

Fig.23 shows the dynamic pressure distribution inside the catalytic converter with square cross section for CNO₂ fluid flow. Maximum and minimum values of dynamic pressure distribution is 4.19×e³ Pa and 9.95×e³ Pa respectively.

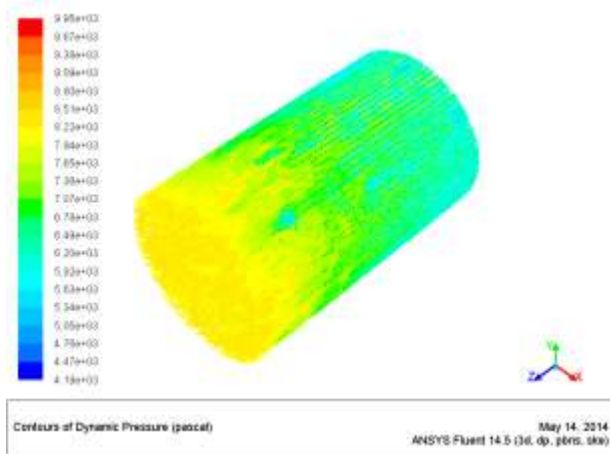


Fig.23 Dynamic pressure

Fig.24 shows the wall temperature distributions inside the catalytic converter with square cross section for CNH₂ fluid flow. Maximum and minimum values of wall temperature distributions is 0 K and 300 K respectively.

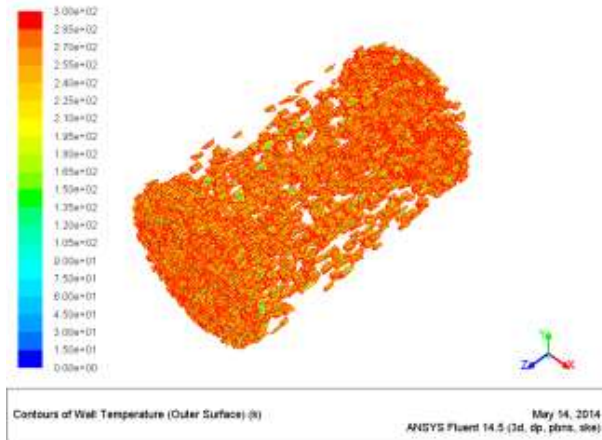


Fig.24 Wall temperature

Fig.25 shows the velocity distributions inside the catalytic converter with square cross section for CNO₂ fluid flow. A maximum and minimum value of velocity distributions is 0 m/s and 1.33×e² m/s respectively.

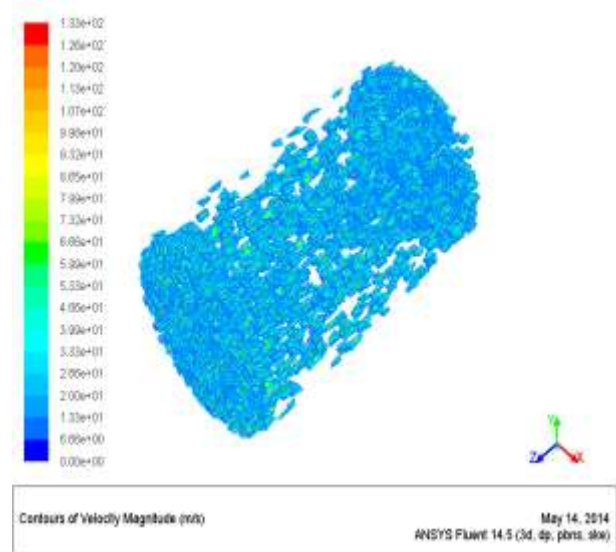


Fig.25 Velocity

Numerical results of square cross section for CO

Fig.26 shows the dynamic pressure distribution inside the catalytic converter with square cross section for CO fluid flow. Maximum and minimum values of dynamic pressure distribution is 3.62×e³ Pa and 8.91×e³ Pa respectively.

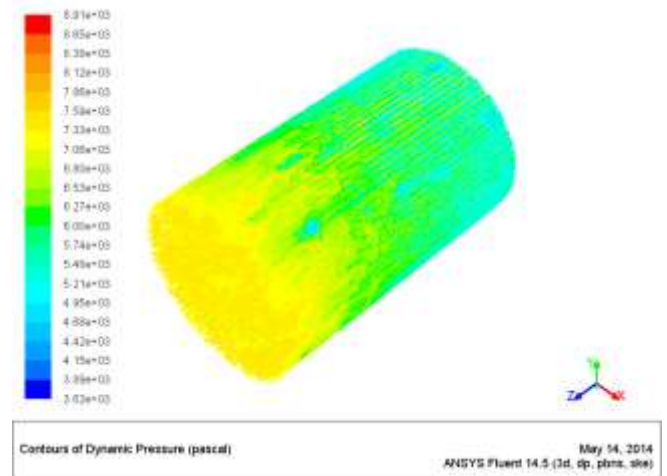


Fig.26 Dynamic pressure

Fig.27 shows the wall temperature distributions inside the catalytic converter with square cross section for CO fluid flow. Maximum and minimum values of wall temperature distributions is 0 K and 300 K respectively.

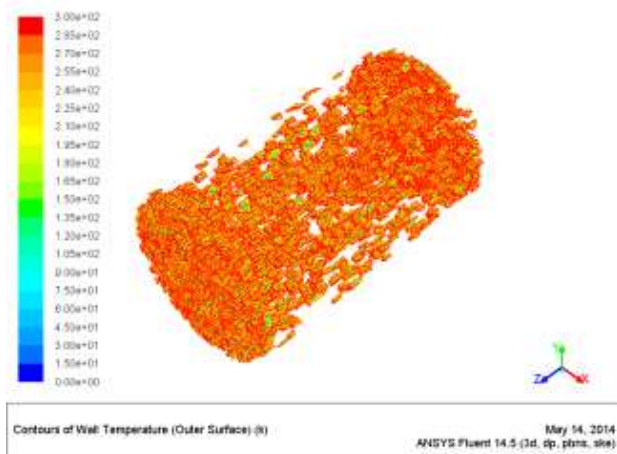


Fig.27 Wall temperature

Fig.28 shows the velocity distributions inside the catalytic converter with square cross section for CO fluid flow. A maximum and minimum value of velocity distributions is 0 m/s and 1.34×10^2 m/s respectively.

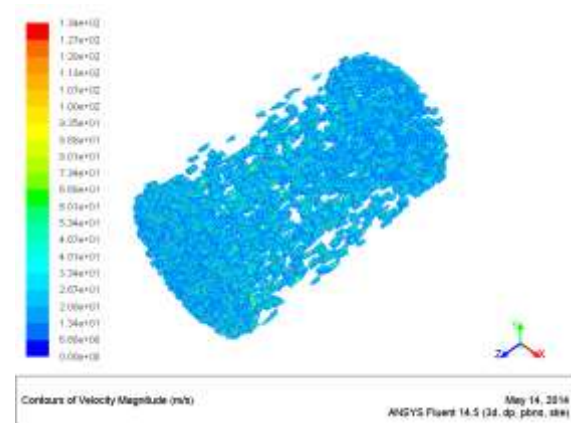


Fig.28 Velocity

Table.2 shows the Numerical result comparison of square cross section with different fluid flow conditions.

Table.2 Numerical result comparison of square cross section

SL.No.	Fluids	Dynamic pressure (P) in Pa	Wall temperature (T) in K	Velocity (V) in m/s
1	CO ₂	1.58×10^4	300	1.33×10^2
2	CNO ₂	9.95×10^3	300	1.33×10^2
3	CO	8.91×10^3	300	1.34×10^2

Numerical results of diamond cross section for CO₂

Fig.29 shows the dynamic pressure distribution inside the catalytic converter with diamond cross section for CO₂ fluid flow. Maximum and minimum values of dynamic pressure distribution is 8.94×10^3 Pa and 1.95×10^4 Pa respectively.

Fig.30 shows the wall temperature distributions inside the catalytic converter with diamond cross section for CO₂ fluid flow. Maximum and minimum values of wall temperature distributions is 0 K and 300 K respectively.

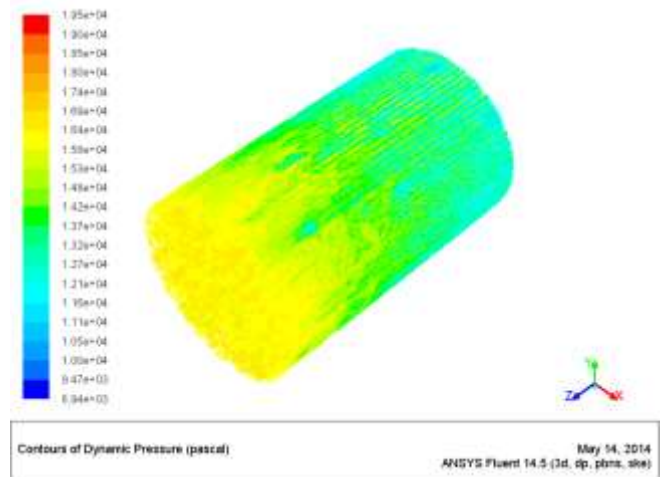


Fig.29 Dynamic pressure

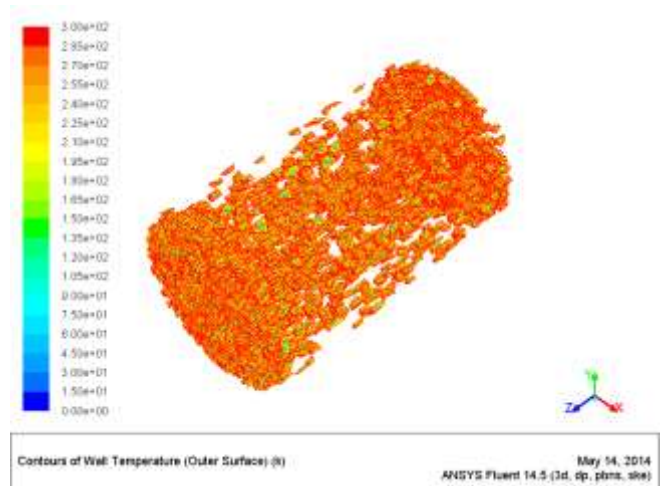


Fig.30 Wall temperature

Fig.31 shows the velocity distributions inside the catalytic converter with diamond cross section for CO₂ fluid flow. A maximum and minimum value of

velocity distributions is 0 m/s and 1.33×10^2 m/s respectively.

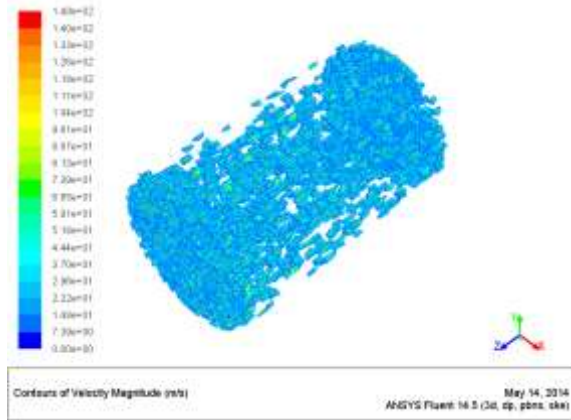


Fig.31 Velocity

Numerical results of diamond cross section for CNO₂

Fig.32 shows the dynamic pressure distribution inside the catalytic converter with diamond cross section for CNO₂ fluid flow. Maximum and minimum values of dynamic pressure distribution is 4.36×10^3 Pa and 1.04×10^4 Pa respectively.

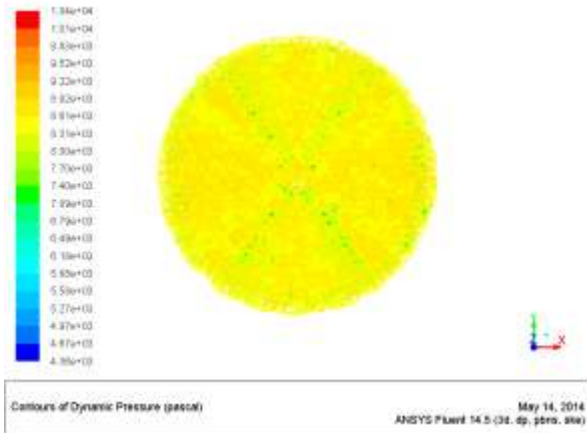


Fig.32 Dynamic pressure

Fig.33 shows the wall temperature distributions inside the catalytic converter with square cross section for CNO₂ fluid flow. Maximum and minimum values of wall temperature distributions is 0 K and 300 K respectively.

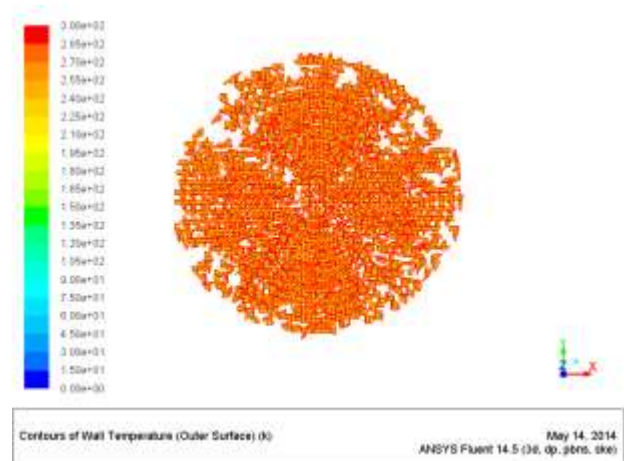


Fig.33 Wall temperature

Fig.34 shows the velocity distributions inside the catalytic converter with diamond cross section for CNO₂ fluid flow. A maximum and minimum value of velocity distributions is 0 m/s and 1.44×10^2 m/s respectively.

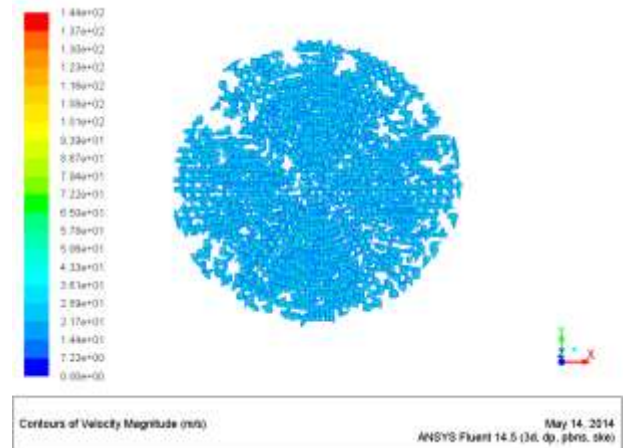


Fig.34 Velocity

Numerical results of diamond cross section for CO

Fig.35 shows the dynamic pressure distribution inside the catalytic converter with diamond cross section for CO fluid flow. Maximum and minimum values of dynamic pressure distribution is 5.46×10^3 Pa and 3.73×10^4 Pa respectively.

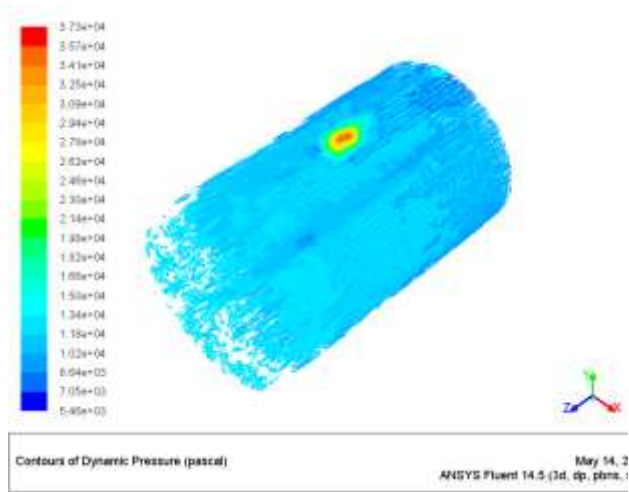


Fig.35 Dynamic pressure

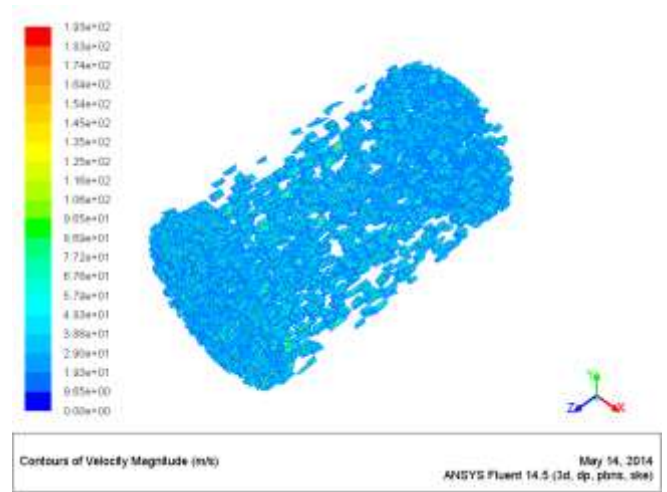


Fig.37 Velocity

Fig.36 shows the wall temperature distributions inside the catalytic converter with diamond cross section for CO fluid flow. Maximum and minimum values of wall temperature distributions is 0 K and 300 K respectively.

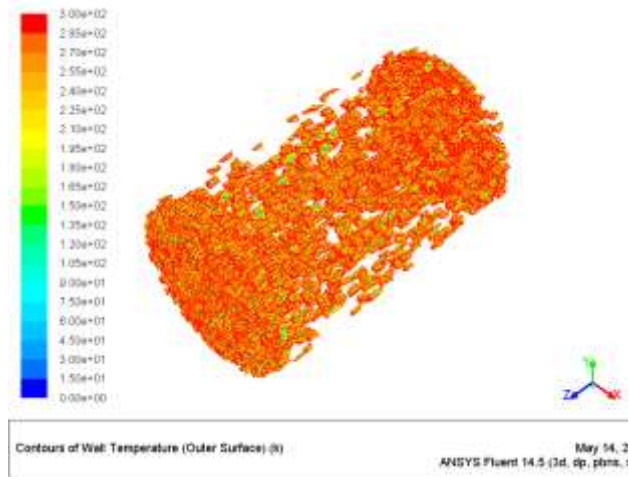


Fig.36 Wall temperature

Fig.37 shows the velocity distributions inside the catalytic converter with diamond cross section for CO fluid flow. A maximum and minimum value of velocity distributions is 0 m/s and 1.93×10^2 m/s respectively.

Table.3 shows the Numerical result comparison of diamond cross section with different fluid flow conditions.

Table.3 Numerical result comparison of diamond cross section

Sl.No.	Fluids	Dynamic pressure (P) in Pa	Wall temperature (T) in K	Velocity (V) in m/s
1	CO ₂	1.95×10^4	300	1.48×10^2
2	CNO ₂	1.04×10^4	300	1.44×10^2
3	CO	3.73×10^4	300	1.93×10^2

Effects of dynamic pressure

Fig.38 to 40 shows the effect of dynamic pressure in different cross section profile of the catalytic converter under the CO₂ fluid flow conditions.

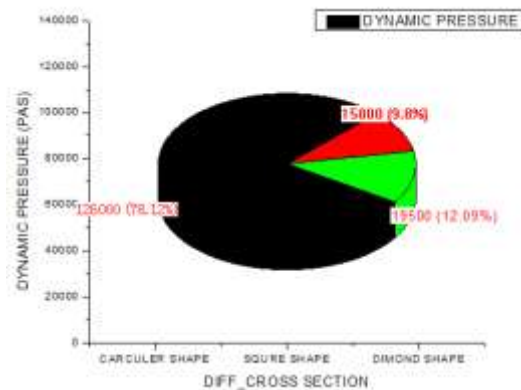


Fig.38 Effects of dynamic pressure in CO₂ fluid flow for different cross section

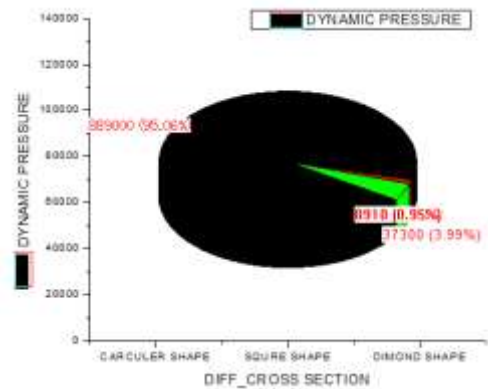


Fig.39 Effects of dynamic pressure in CO fluid flow for different cross section

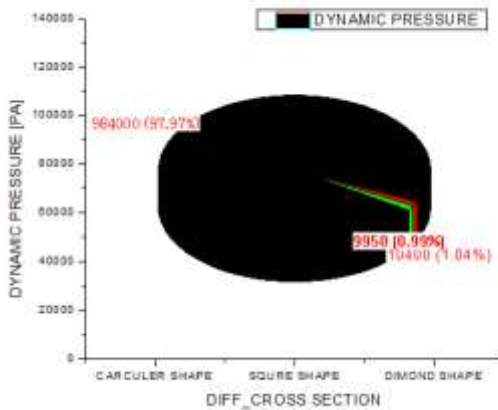


Fig.40 Effects of dynamic pressure in CNO₂ fluid flow for different cross section

Effects of wall temperature

Fig.41 shows the effect of wall temperature in different cross section profile of the catalytic converter under the CO₂, CO & CNO₂ fluid flow conditions.

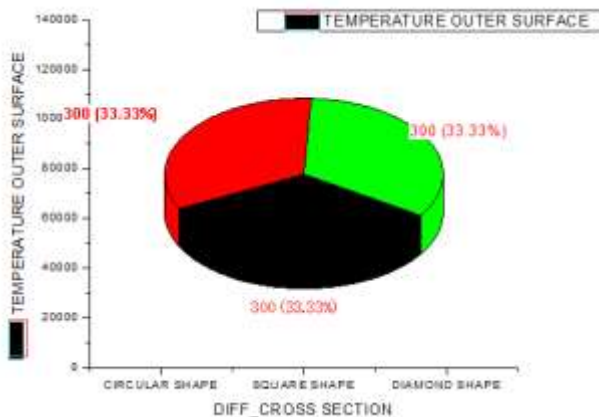


Fig.41 Effects of wall temperature in different cross section

Effects of velocity

Fig.42 to 44 shows the effect of velocity in different cross section profile of the catalytic converter under the CO₂ fluid flow conditions.

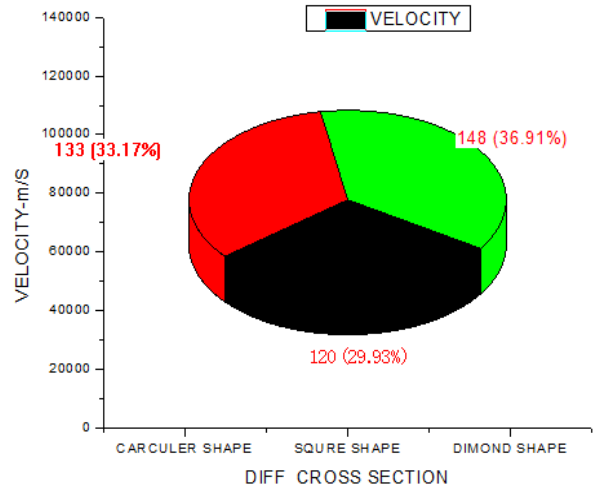


Fig.42 Effects of velocity in CO₂ fluid flow for different cross section

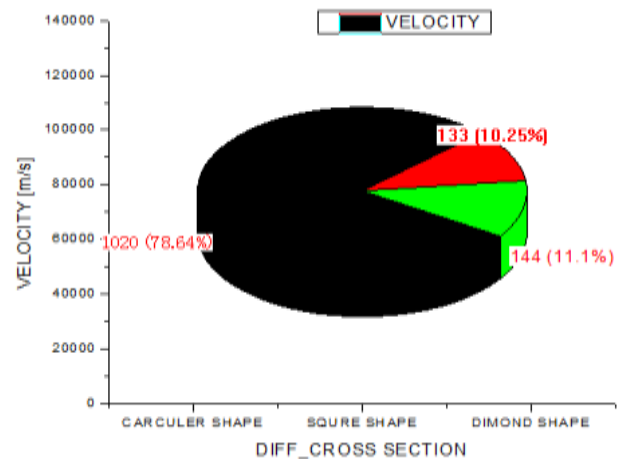


Fig.43 Effects of velocity in CO fluid flow for different cross section

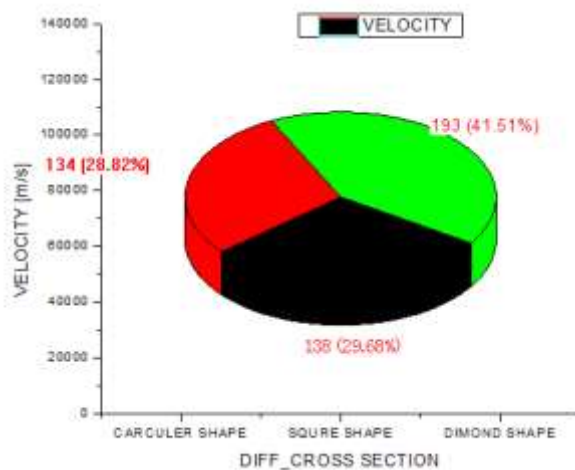


Fig.44 Effects of velocity in CNO_2 fluid flow for different cross section

Conclusions

Dynamic pressure

From the above numerical analysis results and graphs we have concluded that the catalytic converter with square cross section gives the minimum dynamic pressure among the other two cross section models(circular& Diamond).

Relative outer surface temperature

From the above numerical analysis results and graphs we have concluded that the catalytic converter with all cross section posses the same temperature distribution towards the outside.

Velocity magnitude

From the above numerical analysis results and graphs we have concluded that the catalytic converter with square cross section gives the minimum velocity magnitude among the other two cross section models(circular& Diamond).

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