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Evaluation of Emission Parameters in 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 NO_X, CO, unburned HC and particulate matter increases the global warming, so catalytic converter plays an vital role in reducing harmful gases, but the presence of catalytic converter increases the exhaust back pressure due to this the volumetric efficiency will decrease and fuel consumption is higher. So analysis of catalytic converter is very important. The rare earth metals now used as catalyst to reduce NO_X 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, Emission Parameters,CFD.

1. Introduction

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 (CO_2) and water (H_2O). 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 (NOx).

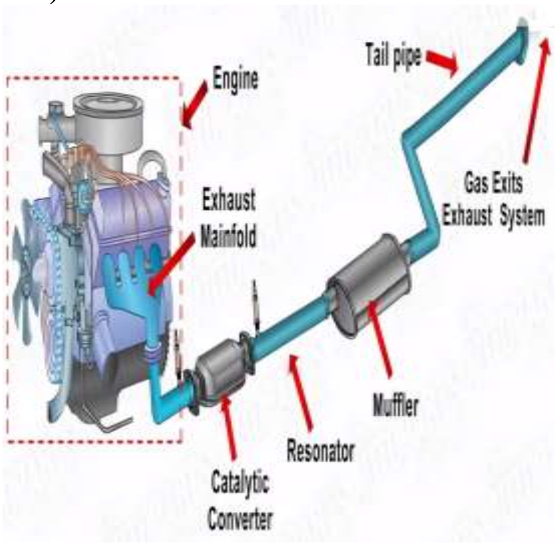

Figure 1 Position of Catalytic Converter

1.1 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 NOX. This is not an easy task: the catalyst chemistry required to clean up NOX is most effective with a rich air/ fuel bias. To operate properly, a three- way converter first must convert NOX (with a rich air/ fuel bias), then HC and CO (with a lean bias).

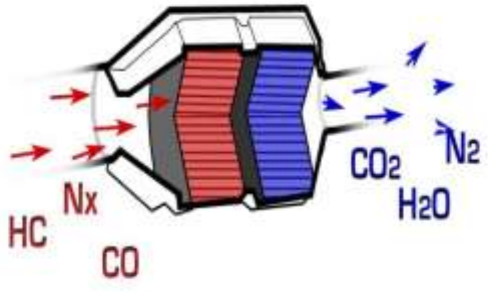

Figure 2 Basic Conversion of Catalytic Converter

1.2 Dangers of Pollutants

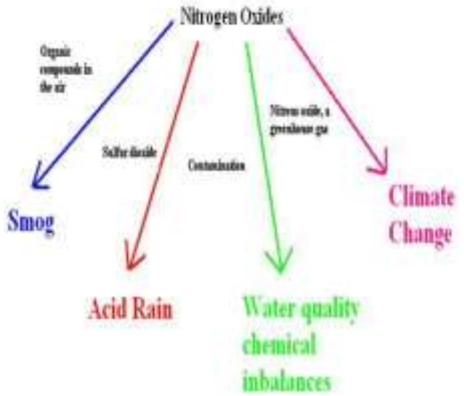

Figure 3 Dangers of Pollutants

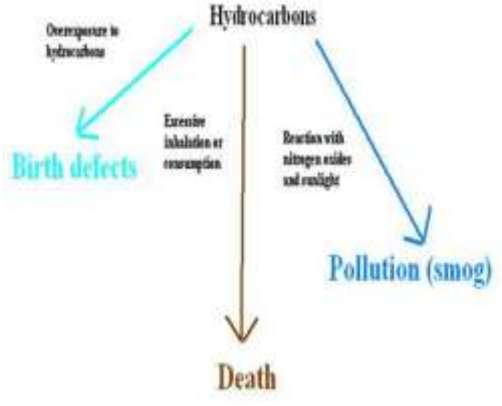

Figure 4 Effect of Pollutants

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 NOx 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 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 modelassisted 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 cat literally 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.

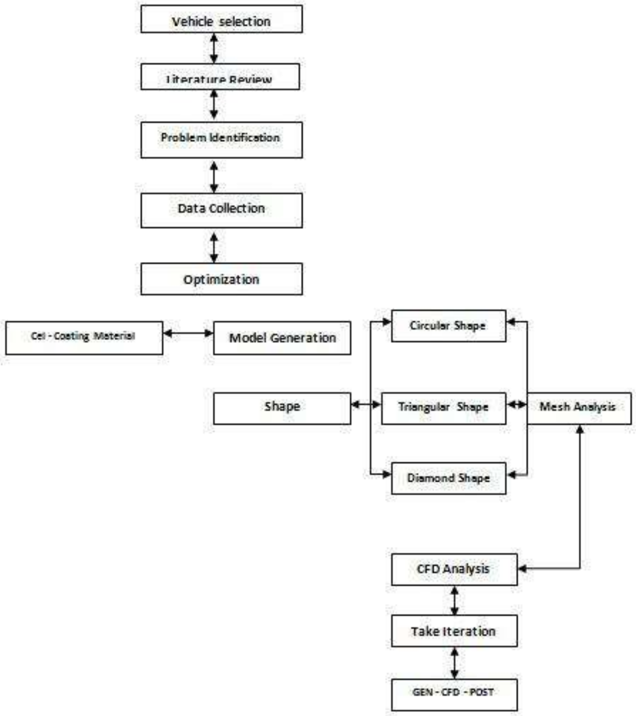

Figure 5 Methodology

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,

1. Dimensions for flow full setup.
2. Scaling measure at reengineering.
3. Conversion data analysis in Inches in to metric.

Dimensions for Full Assembly Model

The details of the parameters are given in the following.

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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.

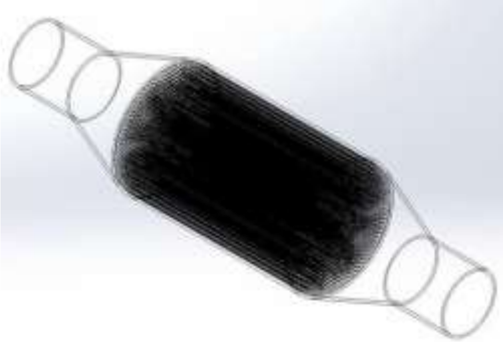

Figure 6 Wire frame model of catalytic converter

Figure 7 Isometric model of catalytic converter

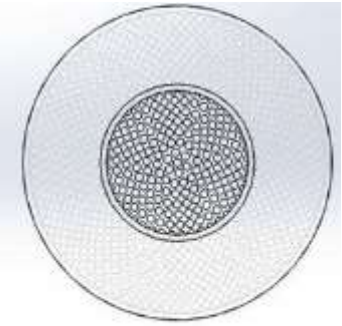

Figure 8 Full assembly front view – pentagon type cross section

Figure 9 Full assembly front view – circular type cross section

Figure 10 Full assembly front view – diamond type cross section

Meshing

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

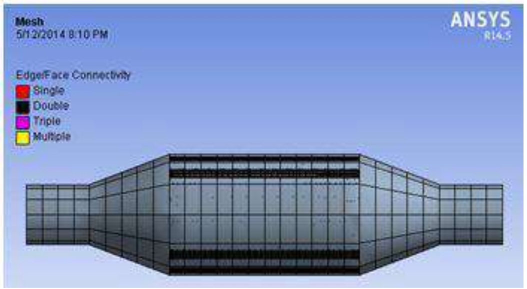

Figure 11 Mesh model of catalytic converter

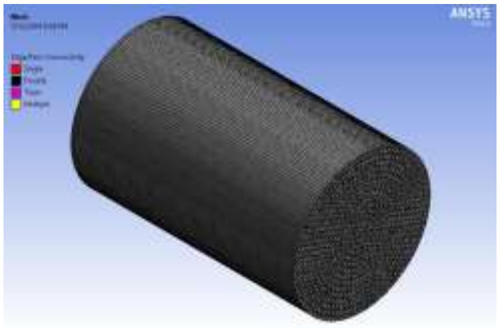

Figure 12 Mesh model of inner structure

Boundary conditions

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

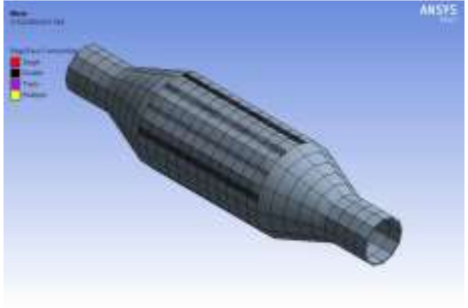

Figure 13 Boundary conditions

Analysis

In our project how to model porous media in FLUENT. Workshop models a catalytic convertor. Nitrogen flows in though inlet with a uniform velocity 22.6 m/s, passes through steel with paladiem 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 H_2O

Fig.14 shows the dynamic pressure distribution inside the catalytic converter with circular cross section for H_2O fluid flow. Maximum and minimum values of dynamic pressure distribution are -2.509×10^7 and 1.520×10^7Pa respectively.

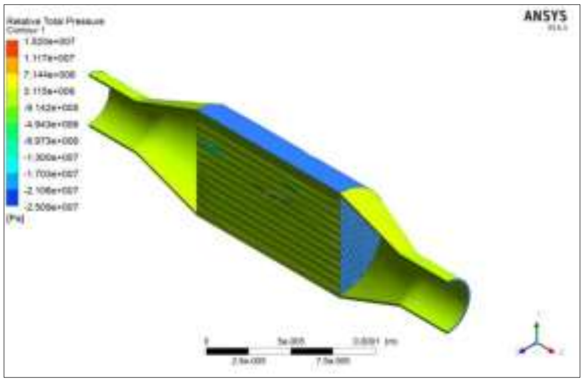

Figure 14 Dynamic pressure

Fig.15 shows the wall temperature distributions inside the catalytic converter with circular cross section for H2O fluid flow. Maximum and minimum values of wall temperature distributions are 1 K and 1.123×10^4K respectively.

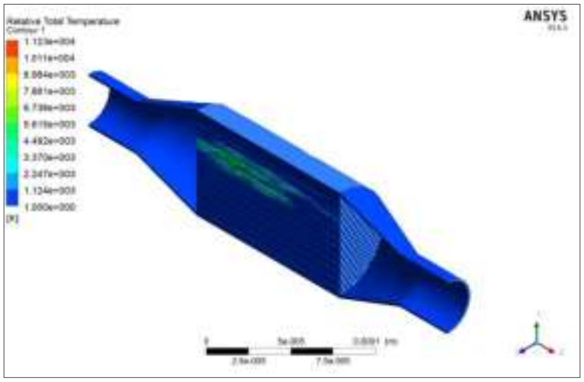

Figure 15 Wall temperature

Fig.16 shows the velocity distributions inside the catalytic converter with circular cross section for H_2O fluid flow. A maximum and minimum value of velocity distributions is 0 m/s and 1.734×10^3 m/s respectively.

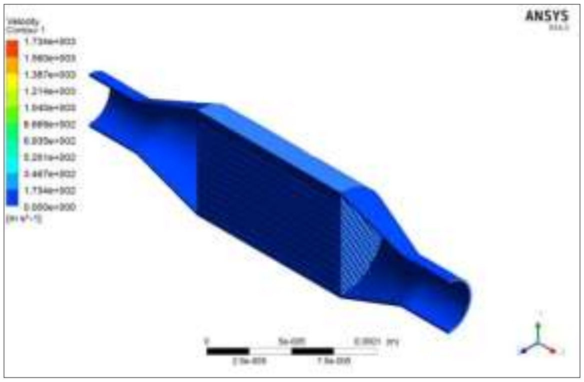

Figure 16 Velocity

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Numerical results of circular cross section for CO_2

Fig.17 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 are -6.41×10^6 Pa and 3.45×10^7 Pa respectively.

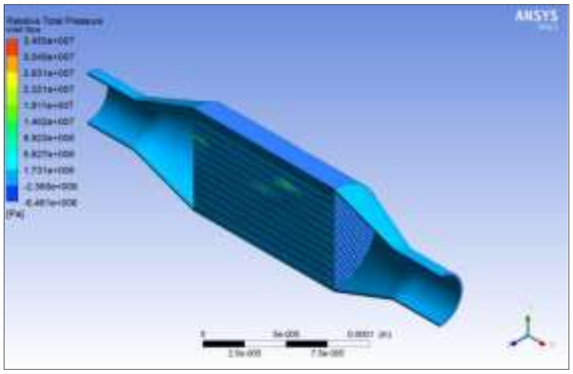


Figure 17 Dynamic pressure

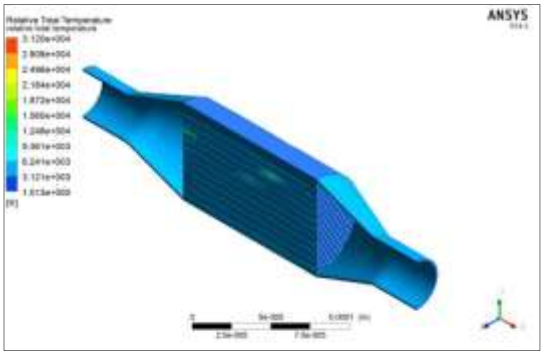


Figure 18 Wall temperature

Fig.18 shows the wall temperature distributions inside the catalytic converter with circular cross section for CO_2 fluid flow. Maximum and minimum values of wall temperature distributions are 1.013 K and 3.12×10^4 K respectively.Fig.19 shows the velocity distributions inside the catalytic converter with circular cross section for CO_2 fluid flow. A maximum and minimum value of velocity distributions is 0 m/s and 5.840×10^2 m/s respectively.

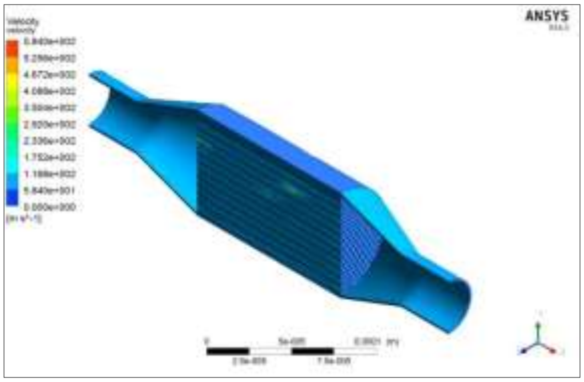


Figure 19 Velocity

Numerical results of circular cross section for N_2

Fig.20 shows the dynamic pressure distribution inside the catalytic converter with circular cross section for N_2 fluid flow. Maximum and minimum values of dynamic pressure distribution are -1.833×106 Pa and 1.534×107 Pa respectively.

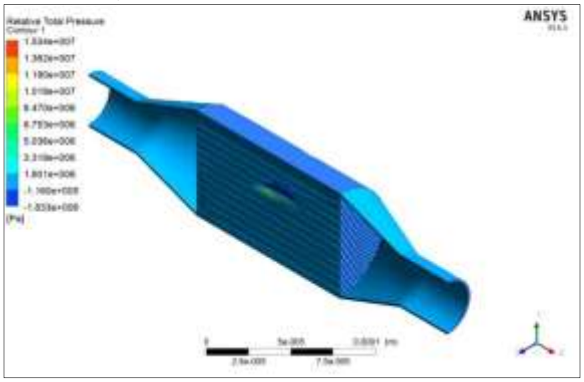


Figure 20 Dynamic pressure

Fig.21shows the wall temperature distributions inside the catalytic converter with circular cross section for N_2 fluid flow. Maximum and minimum values of wall temperature distributions are 1.896 K and 7.971×10^3 K respectively. Fig.22shows the velocity distributions inside the catalytic onverter with circular cross section for N_2 fluid flow. A maximum and minimum value of velocity distributions is 0 m/s and 1.761×10^3 m/s respectively.

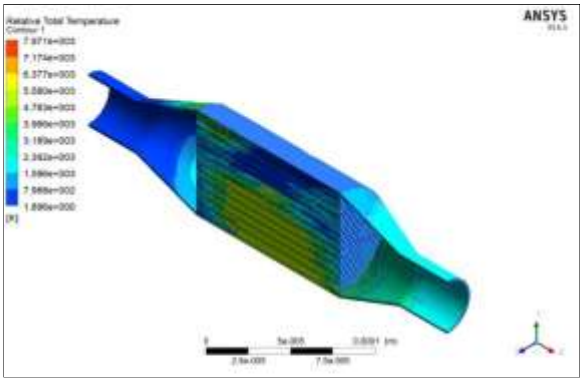


Figure 21 Wall temperature

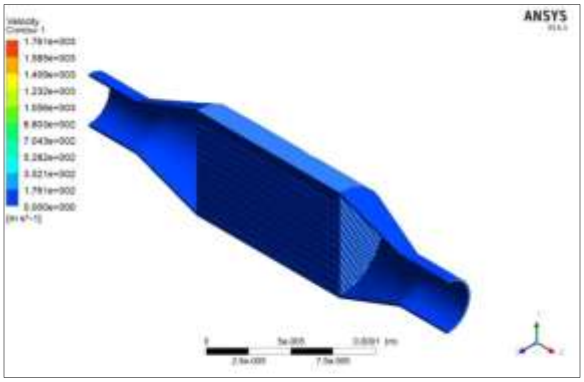
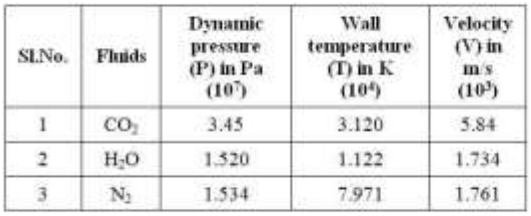


Figure 22 Velocity

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

Table 2 Numerical result comparison of circular cross section



Sl.No.	Fluids	Dynamic pressure (P) in Pa (10^7)	Wall temperature (T) in K (10^4)	Velocity (V) in m/s (10^3)
1	CO_2	3.45	3.120	5.84
2	H_2O	1.520	1.122	1.734
3	N_2	1.534	7.971	1.761

Numerical results of square cross section for H_2O

Fig.23 shows the dynamic pressure distribution inside the catalytic converter with square cross section for H2O fluid flow. Maximum and minimum values of dynamic pressure distribution are -6.655×10^{11} Pa and 7.741×10^{13} Pa respectively. Fig.24 shows the wall temperature distributions inside the catalytic converter with square cross section for H_2O fluid flow. Maximum and minimum values of wall temperature distributions are 1.037 K and 7.454×10^{10} K respectively.

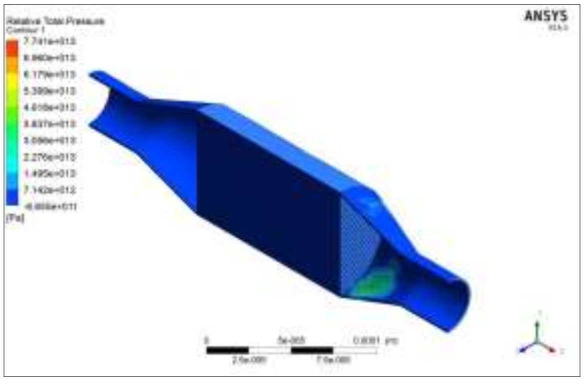


Figure 23 Dynamic pressure

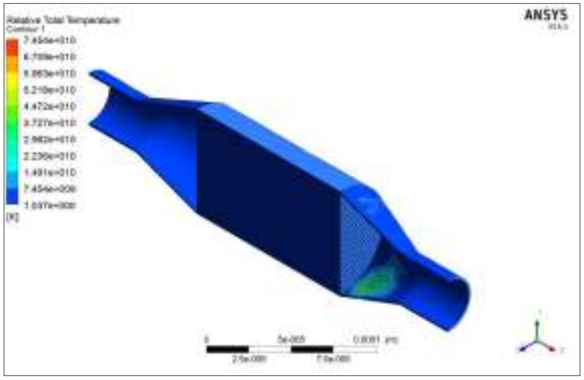


Figure 24 Wall temperature

Fig.25 shows the velocity distributions inside the catalytic converter with square cross section for H_2O fluid flow. A maximum and minimum value of velocity distributions is 0 m/s and 6.267×10^5 m/s respectively.

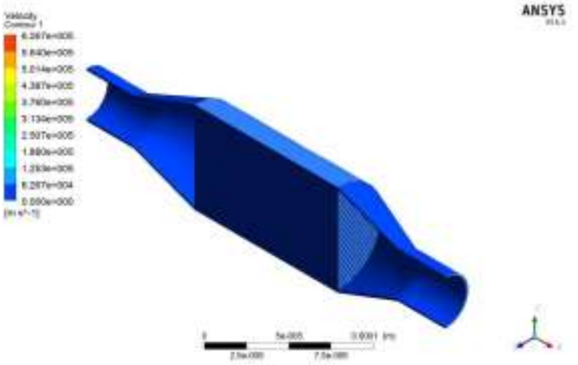


Figure 25 Velocity

Numerical results of square cross section for CO_2

Fig.26 shows the dynamic pressure distribution inside the catalytic converter with square cross section for CO_2 fluid flow. Maximum and minimum values of dynamic pressure distribution are -9.787×10^{11} Pa and 1.203×10^{14} Pa respectively.

Fig.27 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 are 1.691×10^{1} K and 7.525×10^{10} K respectively. Fig.28 shows the velocity distributions inside the catalytic converter with square cross section for CO_2 fluid flow. A maximum and minimum value of velocity distributions is 0 m/s and 8.870×10^{5} m/s respectively.

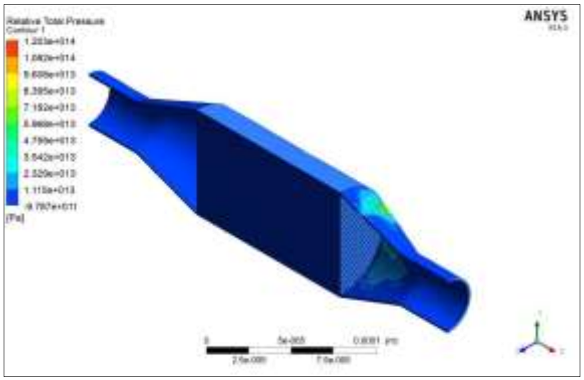


Figure 26 Dynamic pressure

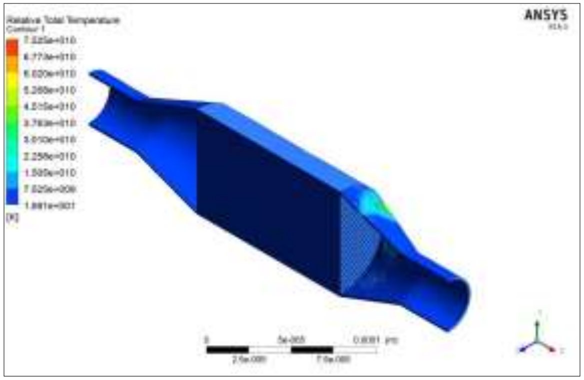


Figure 27 Wall temperature

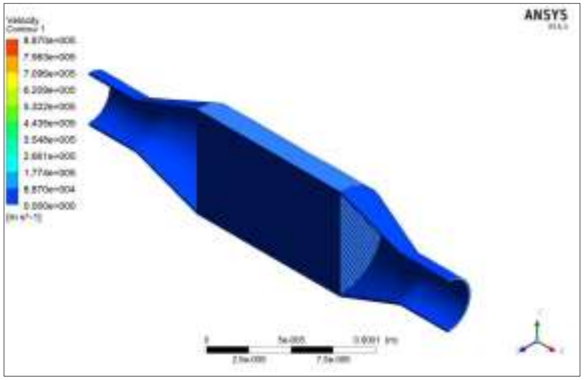


Figure 28 Velocity

Numerical results of square cross section for N_2

Fig.29 shows the dynamic pressure distribution inside the catalytic converter with square cross section for N_2 fluid flow. Maximum and minimum values of dynamic pressure distribution are -4.195×10^{7} Pa and 7.592×10^{8} Pa respectively. Fig.30 shows the wall temperature distributions inside the catalytic converter with square cross section for N_2 fluid flow. Maximum and minimum values of wall temperature distributions are 1.312 K and 6.216×10^{5} K respectively.

Fig.31 shows the velocity distributions inside the catalytic converter with square cross section for N_2 fluid flow. A maximum and minimum value of velocity distributions is 0 m/s and 5.105×10^{3} m/s respectively.

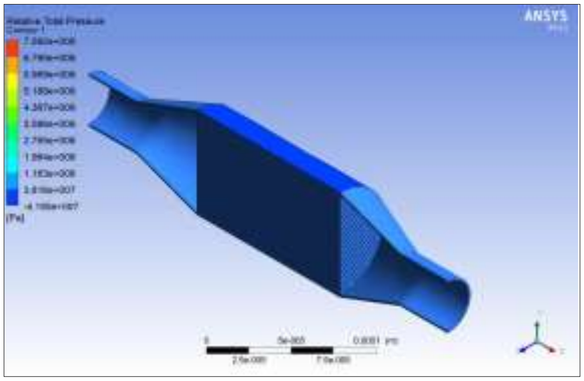


Figure 29 Dynamic pressure

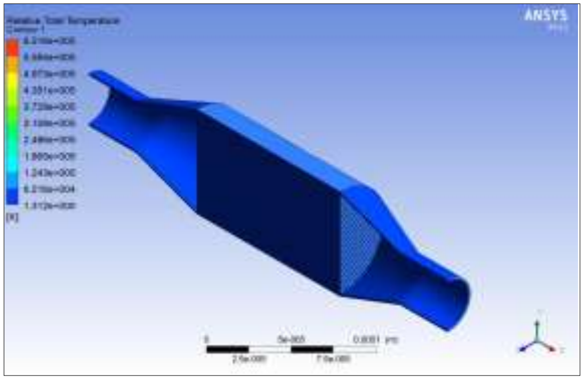


Figure 30 Wall temperature

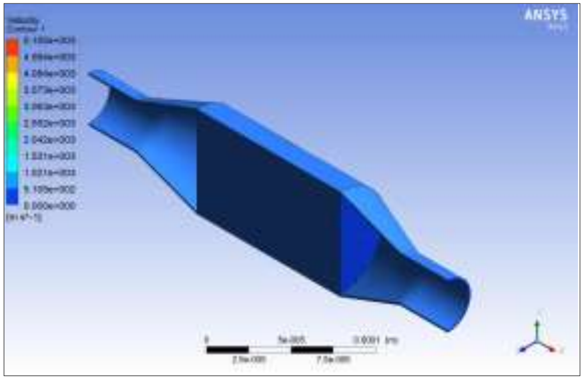


Figure 31 Velocity

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

Table 3 Numerical result comparison of square cross section

Sl.No.	Fluids	Dynamic pressure (P) in Pa (10^{11})	Wall temperature (T) in K (10^{8})	Velocity (V) in m/s (10^{4})
1	CO_2	1.203	7.525	8.870
2	CO	7.741	7.454	6.267
3	N_2	7.592	6.216	5.105

Numerical results of diamond cross section for H_2O

Fig.32 shows the dynamic pressure distribution inside the catalytic converter with Diamond (Honey comb) cross section for H_2O fluid flow. Maximum and minimum values of dynamic pressure distribution are -6.128×10^5 Pa and 2.239×10^7 Pa respectively.

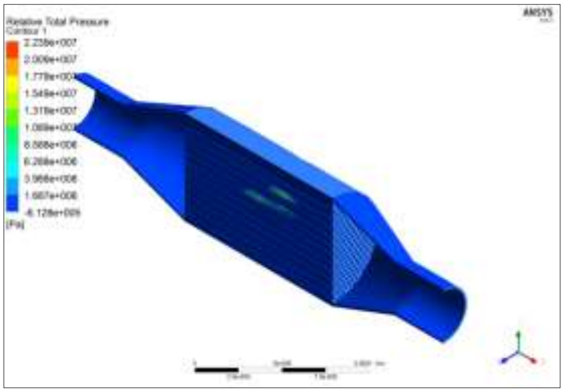


Figure 32 Dynamic pressure

Fig.33 shows the wall temperature distributions inside the catalytic converter with square cross section for H_2O fluid flow. Maximum and minimum values of wall temperature distributions are 1.398×10^1 K and 1.395×10^4 K respectively.

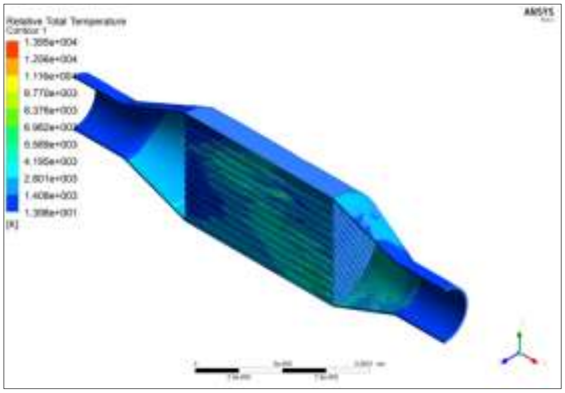


Figure 33 Wall temperature

Fig.34 shows the velocity distributions inside the catalytic converter with Diamond (Honey comb) cross section for H_2O fluid flow. A maximum and minimum value of velocity distributions is 0 m/s and 3.224×10^2 m/s respectively.

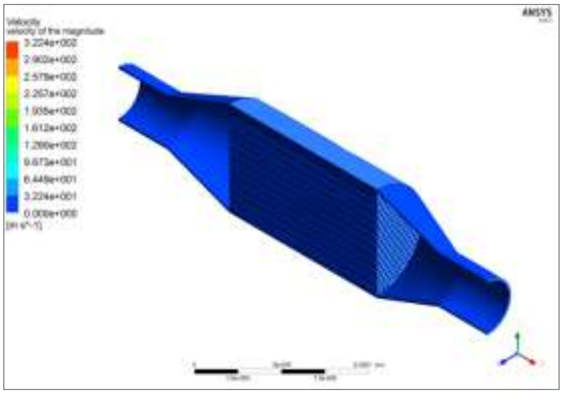


Figure 34 Velocity

Numerical results of diamond cross section for CO_2

Fig.35 shows the dynamic pressure distribution inside the catalytic converter with Diamond (Honey comb) cross section for CO_2 fluid flow. Maximum and minimum values of dynamic pressure distribution are -2.217×10^6 Pa and $2.243\times\times10^6$ Pa respectively.

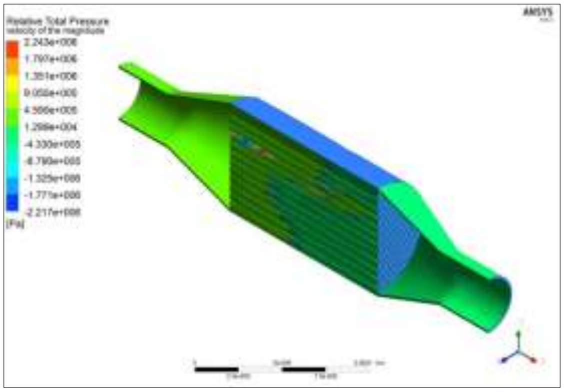


Figure 35 Dynamic pressure

Fig.36 shows the wall temperature distributions inside the catalytic converter with Diamond (Honey comb) cross section for CO_2 fluid flow. Maximum and minimum values of wall temperature distributions are 1.006 K and 5.775×10^3 K respectively.

Fig.37 shows the velocity distributions inside the catalytic converter with Diamond (Honey comb) cross section for CO_2 fluid flow. A maximum and minimum value of velocity distributions is 0 m/s and 3.224×10^2 m/s respectively.

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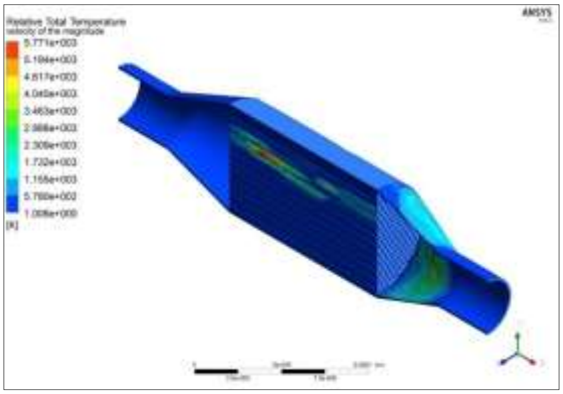

Figure 36 Wall temperature

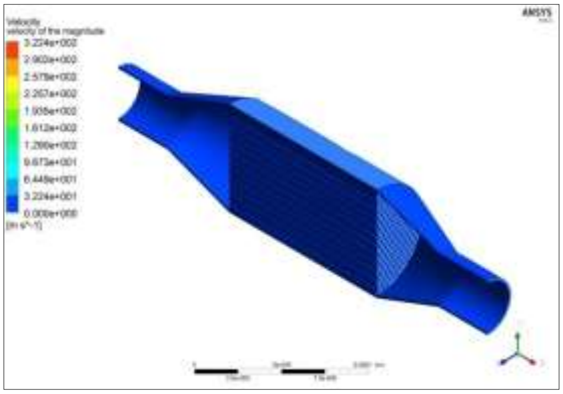

Figure 37 Velocity

Numerical results of diamond cross section for N_2

Fig.38 shows the dynamic pressure distribution inside the catalytic converter with Diamond (Honey comb) cross section for N_2 fluid flow. Maximum and minimum values of dynamic pressure distribution are -3.029×10^{9} Pa and 2.052×10^{10} Pa respectively.

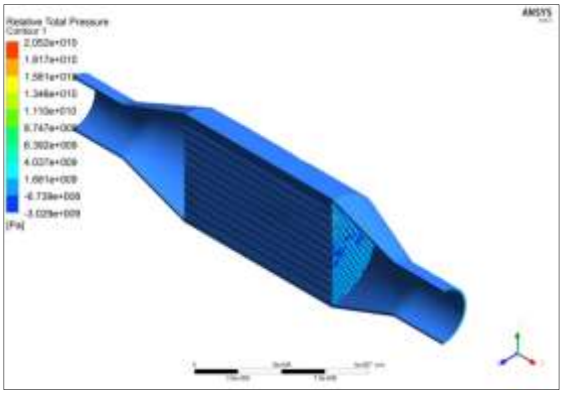

Figure 38 Dynamic pressure

Fig.39 shows the wall temperature distributions inside the catalytic converter with Diamond (Honey comb) cross section for N_2 fluid flow. Maximum and minimum values of wall temperature distributions are 6.897×10^{2} K and 1.352×10^{7} K respectively.

Fig.40 shows the velocity distributions inside the catalytic converter with Diamond (Honey comb) cross section for N_2 fluid flow. A maximum and minimum value of velocity distributions is 0 m/s and 6.292×10^{5} m/s respectively.

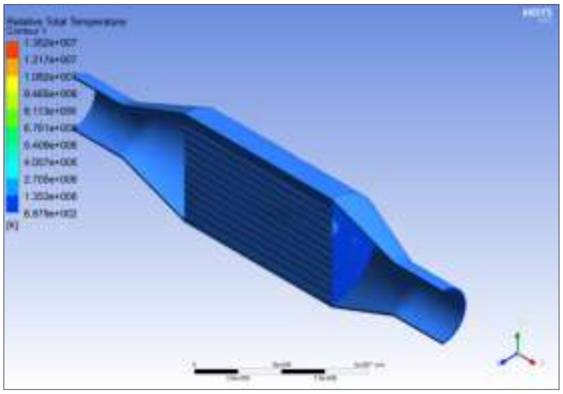

Figure 39 Wall temperature

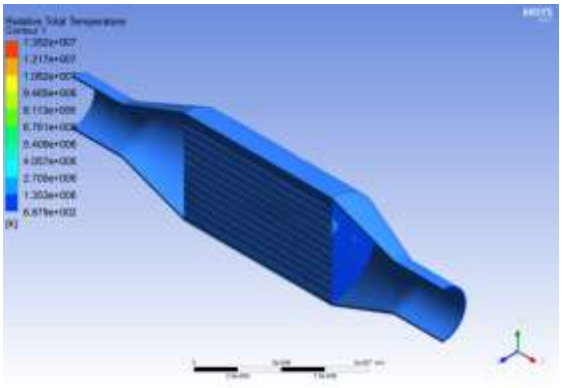

Figure 40 Velocity

Table.4 shows the Numerical result comparison of diamond cross section with different fluid flow conditions.

Table 4 Numerical result comparison of diamond cross section

Sl.No.	Fluids	Dynamic pressure (P) in Pa (10^8)	Wall temperature (T) in K (10^5)	Velocity (V) in m/s (10^3)
1	CO_2	2.243	5.775	3.224
2	H_2O	2.239	1.395	3.224
3	N_2	2.052	1.352	6.292

Effects of dynamic pressure

Fig.41 to 43 shows the effect of dynamic pressure in different cross section profile of the catalytic converter under the H_2O , CO_2 and N_2 fluid flow conditions.

Effects of wall temperature

Fig.44 to 46 shows the effect of wall temperature in different cross section profile of the catalytic converter under the H_2O , CO_2 and N_2 fluid flow conditions.

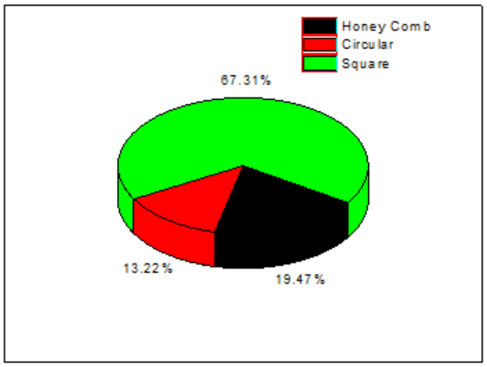

Figure 41 Effects of dynamic pressure in H_2O fluid flow for different cross section

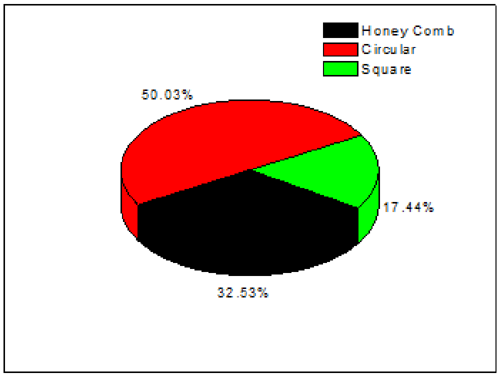

Figure 42 Effects of dynamic pressure in CO_2 fluid flow for different cross section

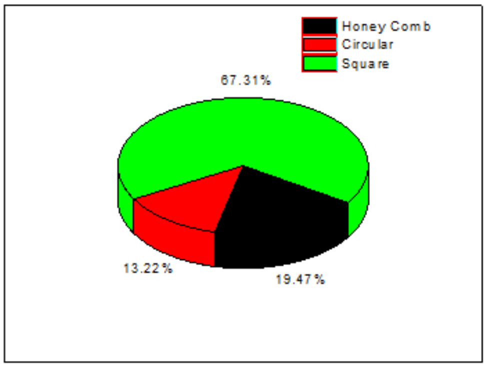

Figure 43 Effects of dynamic pressure in N_2 fluid flow for different cross section

Effects of velocity

Fig.47 to 49 shows the effect of velocity in different cross section profile of the catalytic converter under the H_2O , CO_2 and N_2 fluid flow conditions.

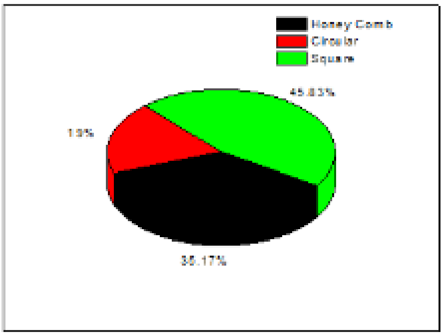

Figure 44 Effects of wall temperature in H_2O fluid flow for different cross section

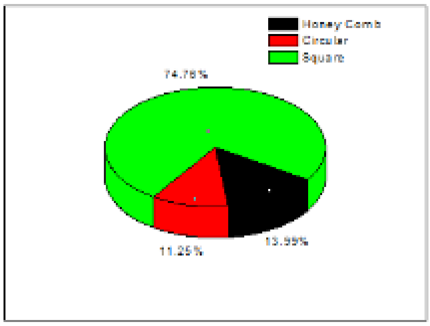

Figure 45 Effects of wall temperature in CO_2 fluid flow for different cross section

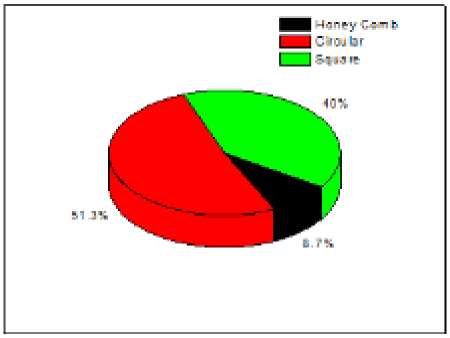

Figure 46 Effects of wall temperature in N_2 fluid flow for different cross section

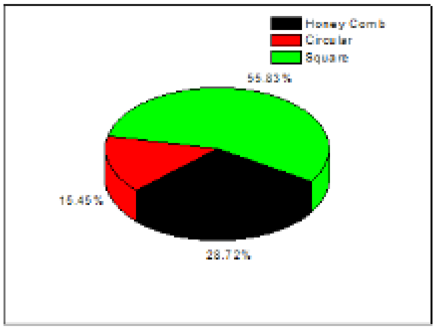

Figure 47 Effects of velocity in H_2O fluid flow for different cross section

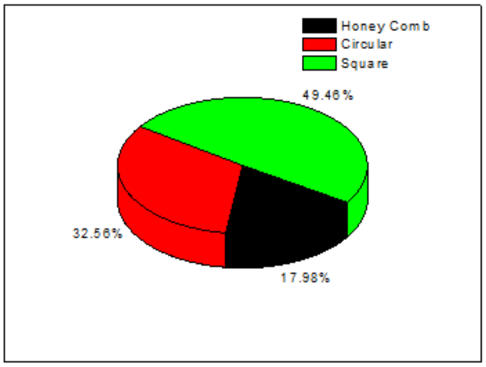

Figure 48 Effects of velocity in CO_2 fluid flow for different cross section

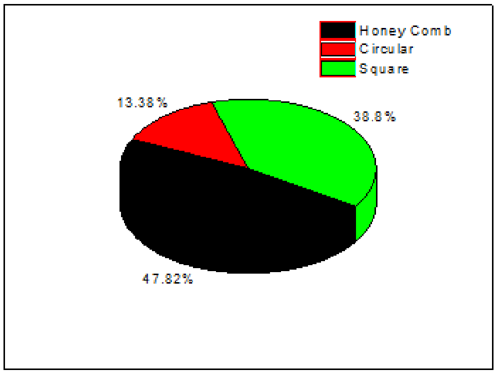

Figure 49 Effects of velocity in N_2 fluid flow for different cross section

Conclusions

Dynamic pressure

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

Relative outer surface temperature

From the above numerical analysis results and graphs we have concluded that the catalytic converters with diamond cross section posses the minimum temperature distribution towards the outside.

Velocity magnitude

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

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