CFD Letters

An Investigation of Three-Way Catalytic Converter for Various Inlet Cone Angles Using CFD

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ARTICLE INFO	ABSTRACT
	Three-way catalytic converters are utilized to minimize exhaust emissions. The efficient working of catalytic converter depends upon the flow field developed inside the converter. Due to the prevailing stringent norms, such as Bharat stage-VI, it is essential to create and design a high performing converter having uniform flow distribution within the converter to meet these norms. An easy way to gain an almost sufficiently homogeneous stream circulation is to compose the diffuser inclination minimally and correspondingly to manufacture the cone angle length long enough. The objective of the study is to examine an automobile catalytic convertor to present a detail and comprehensive report on the key parameters affecting the flow uniformity inside the converter and thus attempting to achieve minimum pressure drop across the converter to reduce the backpressure. They are modifying the existing geometry of the catalytic converter to have more uniform flow within the convertor. The analysis had been carried out with varying diffuser angles- 57.3, 52.3, and 45 degrees separately. Simulation program using computational fluid dynamics (CFD) software package STAR CCM + 11.02 was used. The monolith design with a 52.3º cone angle evaluated with computations provides an actual parabolic curve, which gives a laminar flow within the catalytic converter, which in turn will increase the conversion efficiency of the converter by 1.060 %. The pressure drop within the monolith is also reduced by 3.7 Pa. This accounts to be a reduction in backpressure up to 5%, thus reduces brake specific fuel consumption of automobiles. The results are validated with the literature. The result shows the overall pressure drop augments with velocity. The temperature effect on light-off performance also studied.

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1. Introduction

The catalytic converter aims to convert harmful gasses like nitrogen oxide, carbon monoxide, hydrocarbons into less harmful gasses like N_2, O_2, etc. Noble metals like platinum, rhodium, and palladium are the noble metals used for the catalytic reaction inside the steel tube. Rhodium is employed as a stimulant, whereas palladium assists as an oxidizing agent. Rhodium is used to reduce NOx into N_2. A cone angle of 6 to 10° has been established suitable. The mass flow rate (mean channel momentum) must be utilized while evaluating the evenness holdings H. Weltens *et al.,* [1]. Chakravarthy *et al.,* [2] employed an algebraic turbulence model for single convertor geometry in 2D and parameter such as temperature and reaction. The outcome was approved by applying experiments of Holmgren *et al.,* [3]. Benjamin *et al.,* [4] reported that accurate forecasting of maximum flow velocity is essential for the evaluation of catalyst deactivation and light-off time. The method is validated against the results of CFD. The results show flow profiles obtain by the CFD code and FRM technique to be a good agreement with experimental results. Subramanian *et al.,* [5] carried out a study applied on three guidelines viz. catalytic converter length, cell densities, and metal loading. Cell density was changed from 200 cells per inch (CPI) to 1200 CPI, and lengths from 70 to 180 mm commercially available CFD software was used S. Subramanian [5]. Augmenting the convertor length improves light-off and maximum conversion; with increasing cell densities, the conversion efficiency of species rises up to a certain level. Hayes *et al.,* [6] studied the effect of critical working parameters by changing the cell densities and wall thickness at constant wash coat loading.

Agrawal *et al.,* [7] presented a report on the synergy between movement, backlash, and thermal effects in a 2 Dimension axis-symmetric convertor. The parabolic velocity profile in the transverse direction is expected for laminar flow. The response did not have a significant impact on flow distribution. The literature review suggested that the most influencing key parameter is the inlet cone angle and inlet cone length, not much work had been reported in the literature so as to emphasize the effect of cone angle in the flow distribution within the converter. This paper aims to change the inlet cone angle of the diffuser and plotting the pressure and velocity fields and flow uniformity index fields and also evaluating pressure and velocity intensity at critical locations inside the converter to get the most uniform flow inside the converter.

2. Catalytic Converter Geometry

The monolith consists of a number of channels, inlet and outlet cones with a three-dimensional representation. Labeled geometry is represented in Figure 1 (a) and (b).

The monolith substrate used was 100 CPSI with standard wall thickness. The dimensions and physical properties of the substrate are given in Table 1.

Table 1
Monolith brick specification

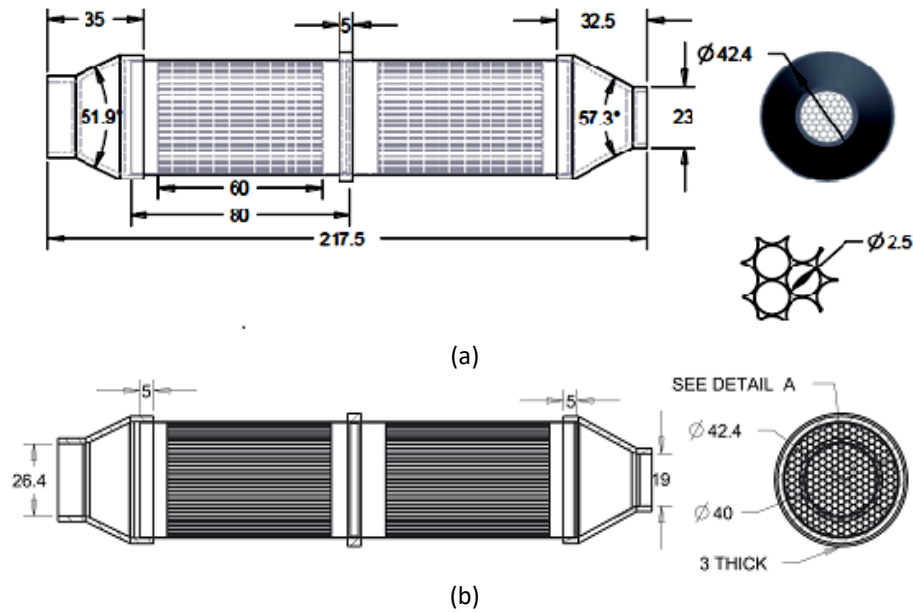| Properties	100CPSI
Wall thickness	0.10mm
Substrate Shape	Round
Open Frontal Area	0.72
Matrix Diameter	2.5 mm

(a)

(b)

Fig.1. Schematic view of catalytic converter assembly All dimensions are in mm

2.1 Inlet Velocity Calculation

The symbolic scope of momentum at the interior of block channels is 0 to 12 m/s. The mean velocity of 2 and 2.5 m/s into an individual monolith route is used for the geometries. As per geometry, 240 cells in 42.4mm diameter monolith are present. The Eqs. (1) to (7) are used to calculate inlet velocity.

$$V_{channel} = 2.5 m/s$$

$$Q_{channel} = \frac{\Pi d^2}{4} \times V_{Channel} \times density(\varsigma) \tag{1}$$

$$Q_{channel} = \frac{\Pi d^2}{4} \times V_{Channel} \times density(\varsigma) \tag{2}$$

$$Q_{channel} = \frac{3.14 \times (0.0025)^2}{4} \times 2.5 \times 1.136 = 0.00001394 kg/s \tag{3}$$

$$Q_{total} = 0.00001394 \times 240 = 0.003345 kg/s \tag{4}$$

$$Q_{inlet} = Q_{total} \tag{5}$$

$$0.003345 = 0.7854 \times 0.019^2 \times v \times 1.136 \tag{6}$$

$$V_{inlet} = 10.38 m/s \tag{7}$$

Similarly, for $V_{channel}$ = 2 m/s, the inlet velocity obtained is given by Eq. (8)

$$V_{inlet} = 8.31 m/s \tag{8}$$

Many authors [8-28] employed the Reynolds Averaged Navier-Stokes (RANS) mathematical statement having k-€ turbulence setup, where the k is the turbulent kinetic energy, and ω is the specific dissipation rate. In this present work, polyhedral mesh elements have been used to get accurate results and to reduce computation time. Meshed model is shown in Figure 2. The total mesh count was 7,537,067. The CFD package, STAR CCM + 11.02, is used for the analysis in present work.

Figure 3 shows three sections where pressure and velocity fields are evaluated. Three different geometry are analyzed: (a) base model geometry (cone angle 57.3°), (b) variant 01 geometry (cone angle 52.3°), and (c) variant 02 geometry (cone angle 45°). The central variation with the other efforts [2,6] is that they defined the block as a permeable element. Consequently, a multi-channel geometry was considered, as shown in Figure 1. Figure 3 shows three vertical lines (labeled v_1, v_2, and v_3) in a line is the cross-section area where the momentum study is interpreted comprehensively.
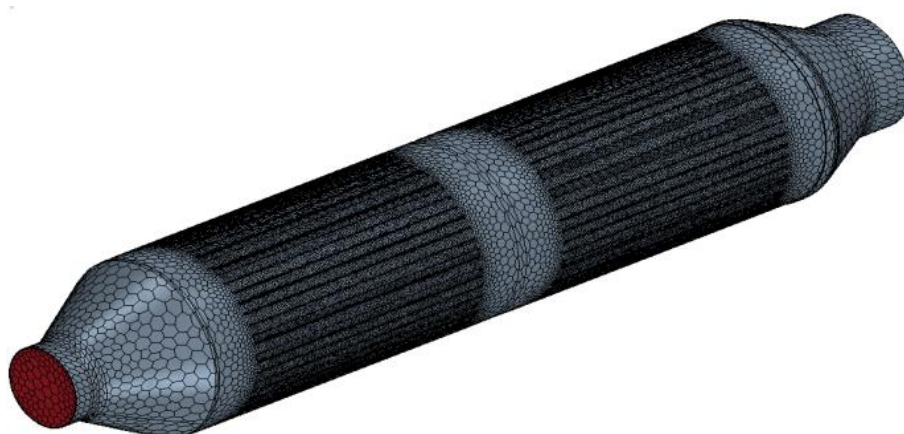

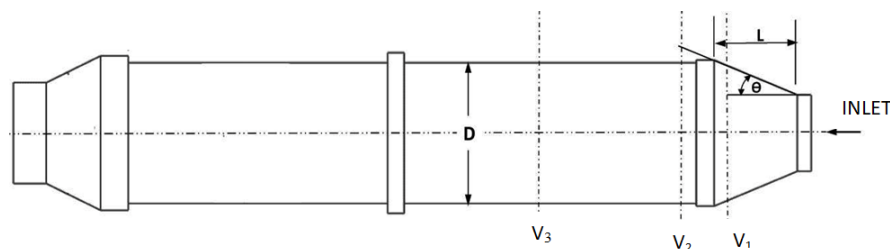**Fig.2.** The meshed fluid domain of catalytic converter

Fig. 3. Symbolic of even two-dimensional geometry of the catalytic converter

2.2 Inlet Boundary Requisite

At the inlet, to the catalytic converter, a velocity of 10.38 m/s and 8.31 m/s was considered. The inlet temperature is 27°C. For 10.38m/s situation, the Reynolds number (established upon hydraulic diameter) inside every brick carrier is $Re_{ch}=378$. The momentum at the interior of the brick carriers is laminar. The following parameters, like turbulence lens scale, solver setting, etc., chosen were default values as reported by H. Weltens *et al.,* [2]. The fluid is selected (nitrogen), and the properties and temperature are shown in Table 2.

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Table 2
Functional conditions and variables for the catalytic convertor simulations

Brick carrier outline	
Brick dimension	60 mm
Carrier bore	2.5 mm
Wall thickness	0.10 mm
Average velocity	2.5 m/s
Channel Reynolds number	378
Inlet conditions	
Inlet velocity	V1=10.38m/s and V2=8.31m/s
Temperature	300 K
Pressure	1 atm
Density	1.136 Kg/m^3
Viscosity	1.6638*10-05 Kg/m-s

3. Results and Discussion

3.1 Validation

Before the parametric studies, the prediction of the base models was compared to some literature results. The result reported by Pushpavanam *et al.,* [7] have used 85 channels ceramic monolith with wall thickness 400 μm, the inlet diameter of 40 mm, the diffuser length was 53 mm, and the inlet flow velocity was 10.63 m/s.

It can be seen from Figures 4 and 5; the pattern of the literature result is similar to that of the simulated ones. The net deviation from the maximum centerline velocity is approximately 5%. This indicated that the established model is feasible and can be used to study the flow characteristics for the convertor with various configurations. There are many possible explanations for the errors between literature results and simulation results. They may be associated with turbulence model numerically inaccuracy or geometrical design.
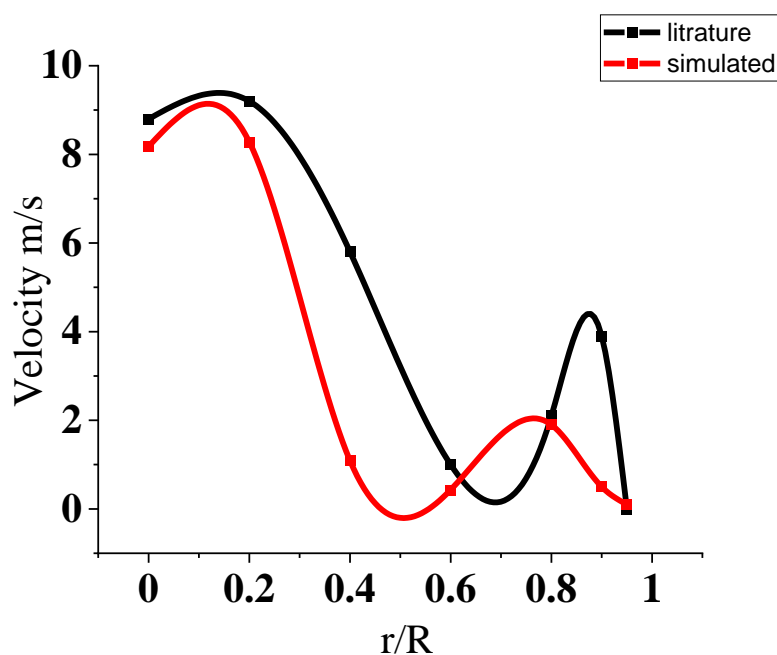

Fig. 4. Momentum intensity Vs. non-dimensional diagonal coordinate at location v_1
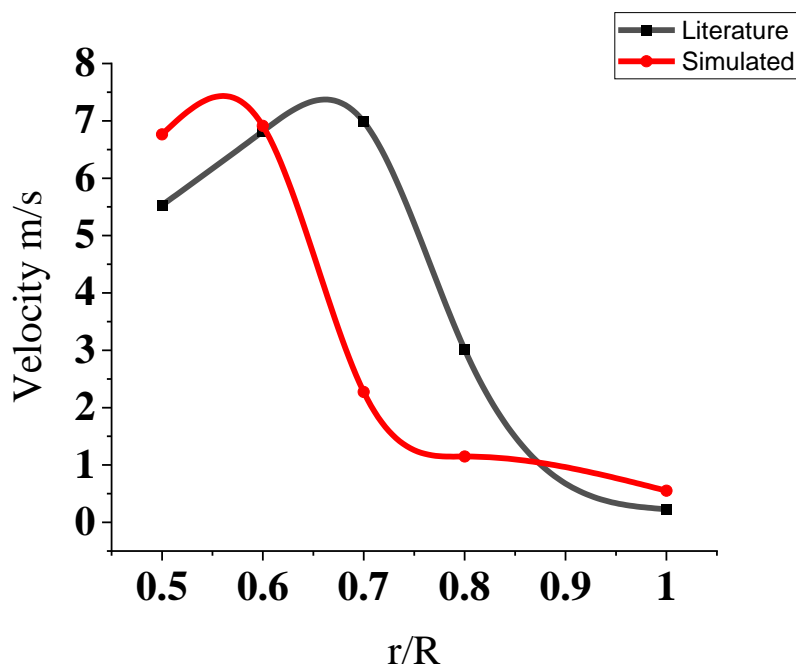
Fig. 5. Momentum intensity Vs. non-dimensional diagonal coordinate at location v_2

4. CFD Results

Three simulation run analysis results are presented for pressure drop characteristics and flow uniformity index, as shown in the Table 3.

Table 3
Geometry design for simulation confirmation

Cone angle (degrees)	brick dimension	brick bore	Inlet pipe diameter	Inlet pipe length
57.3	60	40	19	21.5
52.3	60	40	19	23.92
45	70	37.03	19	28.35

The grid independence test has been conducted for different mesh element sizes. Table 4 shows the results obtained by the CFD analysis at various mesh element sizes.

Table 4
The mesh dependency test for external flow

Mesh Max Size	Mesh Elements	Dimensionless Pressure
5	1351	0.997422734
4	1551	0.998361998
3	1970	0.998282478
2	12221	0.998697340
1	18795	0.999215397
0.5	134946	0.999209453
0.4	154641	0.999222551

4.1 Flow Distribution Inside the Converter
4.1.1 Flow velocity computations

Figure 6 shows that the base model transverse velocity profile is not following the parabolic curve. Near the circular boundary of the converter, there is higher resistance to flow offered, which introduces a considerable amount of non-uniformity within the converter and will result in lesser conversion efficiencies rates. The flow no more remains laminar near the boundary of the converter. Reducing the cone angle to 45° makes the transverse velocity profile more parabolic curve (expected for laminar flow).
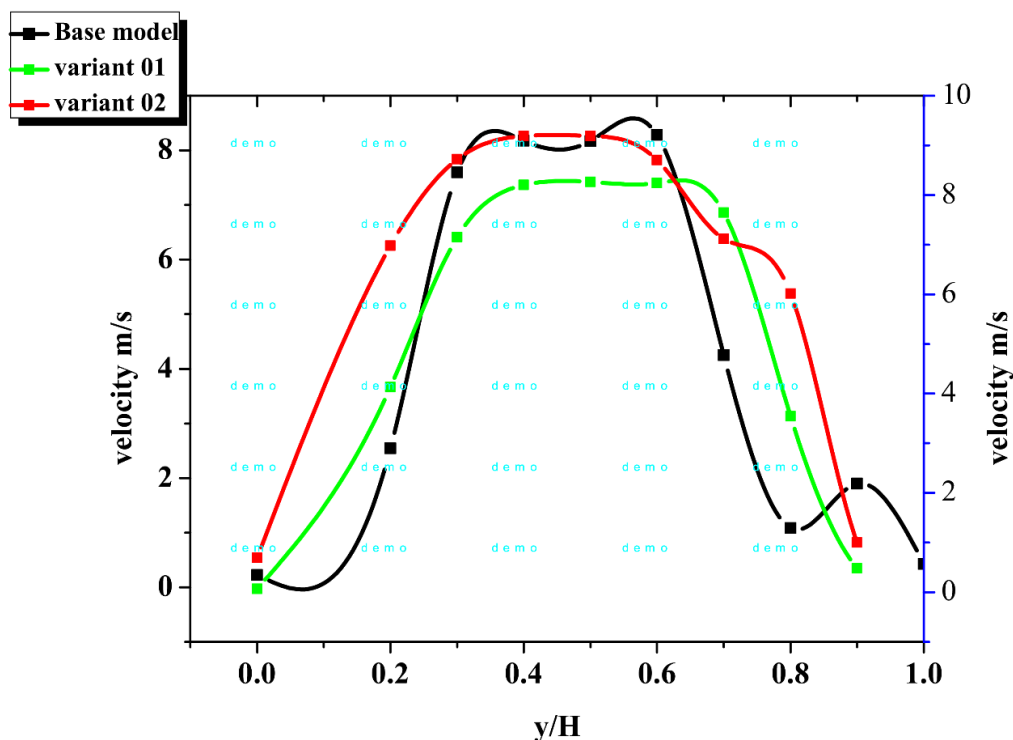

Fig. 6. The intensity of magnitude Vs the non-dimensional distance along with the diagonal path correlative to 10.38 m/s inlet velocity at v_1 location

This study aims to obtain a correct parabolic curve in nature so that the flow in the converter will be uniform flow, which will result in the highest conversion efficiency of harmful gasses into less harmful gasses, hence the more efficient design of converter is considered. Figure 7 shows the variant 02 model has a parabolic curve in nature, the maximum velocity at the center of the convertor 7 m/s.

The flow is also near to laminar flow for the variant 01 models shown by the parabolic curve in the above Figure 8. From Figures 6, 7, and 8, the most promising model is variant 01, which is showing nearly a parabolic curve at all three locations Viz: v_1, v_2, v_3. The flow behavior at these three locations is qualitatively similar to that obtained for the inlet velocity corresponding to 8.31 m/s.
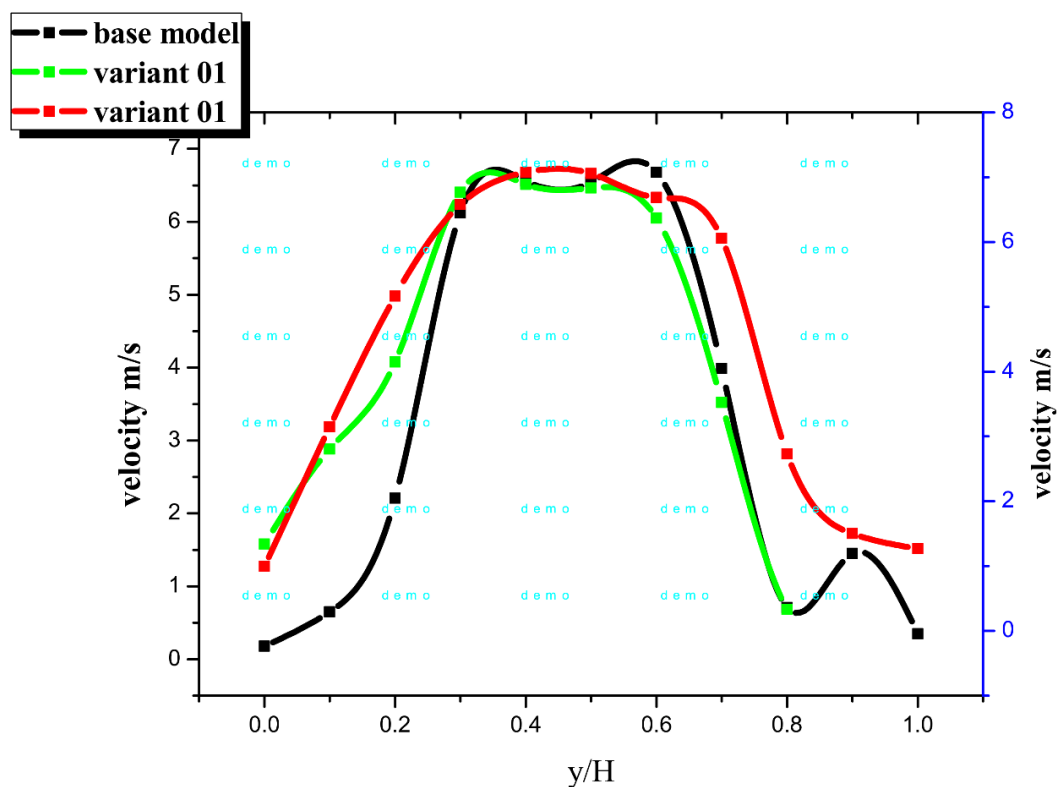
Fig. 7. The intensity of magnitude Vs. the Non-dimensional distance along with the diagonal path correlative to 10.38 m/s inlet velocity at v_2 location
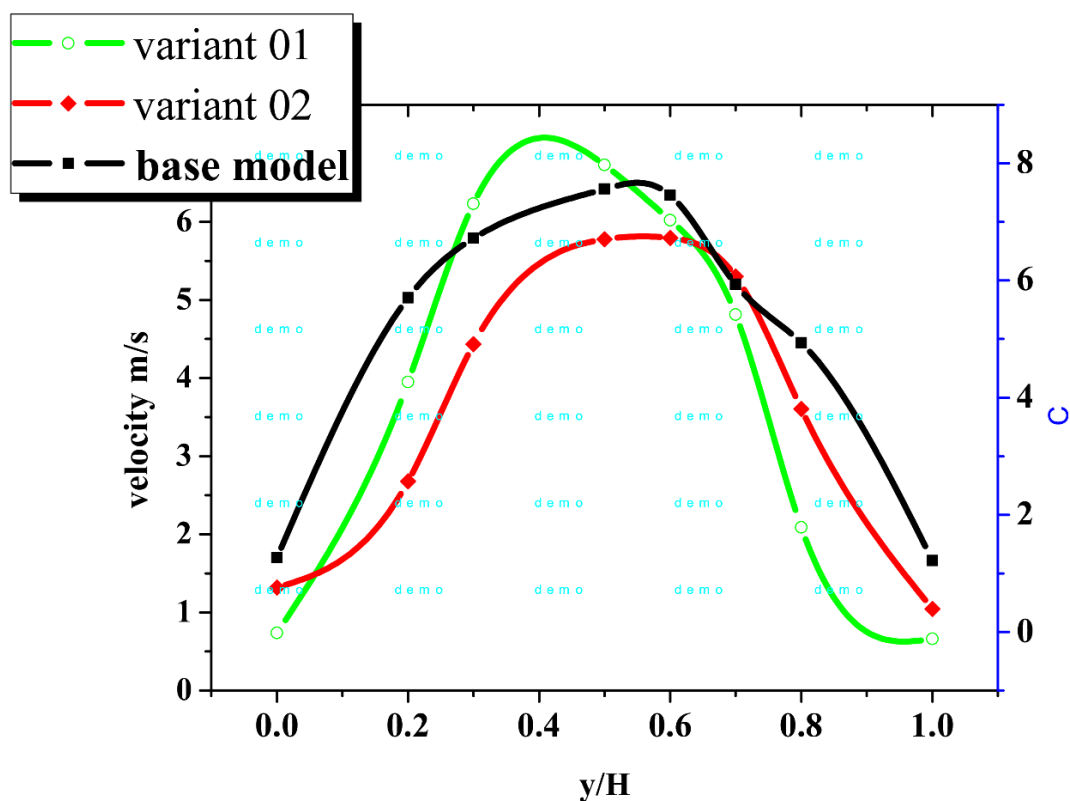

Fig. 8. The intensity of magnitude Vs. the non-dimensional distance along with the diagonal path correlative to 10.38 m/s inlet velocity at v_3 location

4.1.2 Pressure computations

The Pressure analysis is also evaluated at these three locations, and the graph is plotted for calculated inlet velocities. The pressure graph from Figure 9 indicates a rise in pressure in the transverse direction in variant 02 is high as compare to option 01 and the base model. The pressure here is 62 Pa for variant 02, a value higher than 17 Pa as compare to other designs. Also, the peak pressure rise is lower in the variant 01 models as compared to the base model. Small growth in pressure will not introduce vorticity within the flow, and flow will remain uniform within the converter.
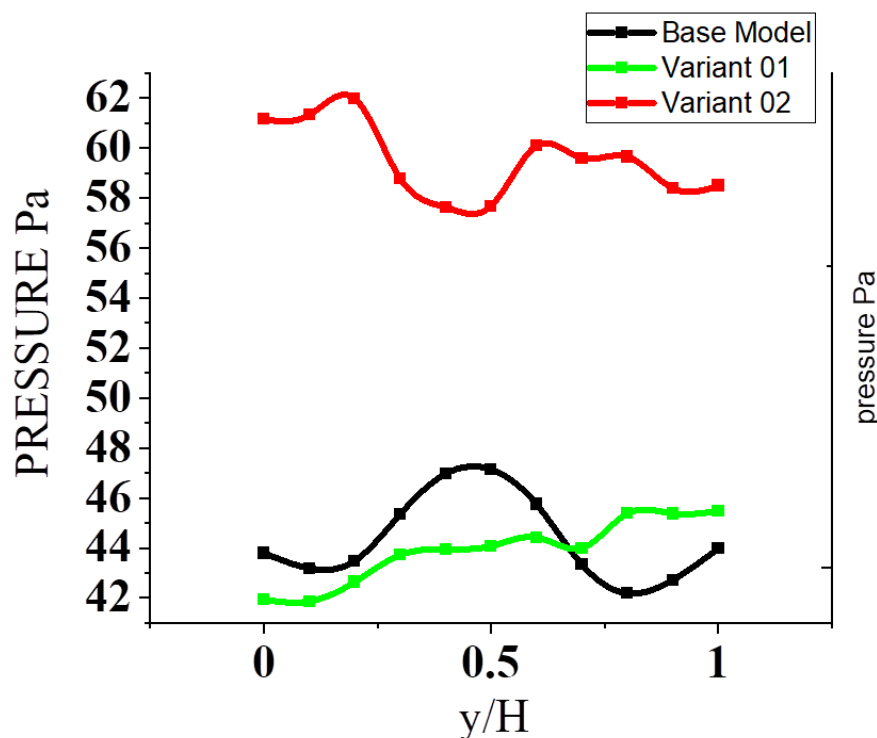

Fig. 9. Pressure Vs. the non-dimensional distance along with the diagonal path correlative to 10.38 m/s inlet velocity at v_1 location

There is a rise in pressure for variant 02 in a transverse direction, indicating a value of 80 Pa in Figure 10 as it was 62 Pa at v_1 location for the same geometry. There is also a rise in pressure values for other designs as compared to pressure values at the same places.

Based on the obtained results from Figures 9 and 10, it is concluded that decreasing the diffuser angle gives rise to pressure in a transverse direction. It is observed from Figure 11 that just at the upstream location of the diffuser, the flow is highly non-uniform because at such a high-pressure rise introduces turbulence in the flow of gas. It is a highly undesirable flow and must be avoided by changing specific design parameters.
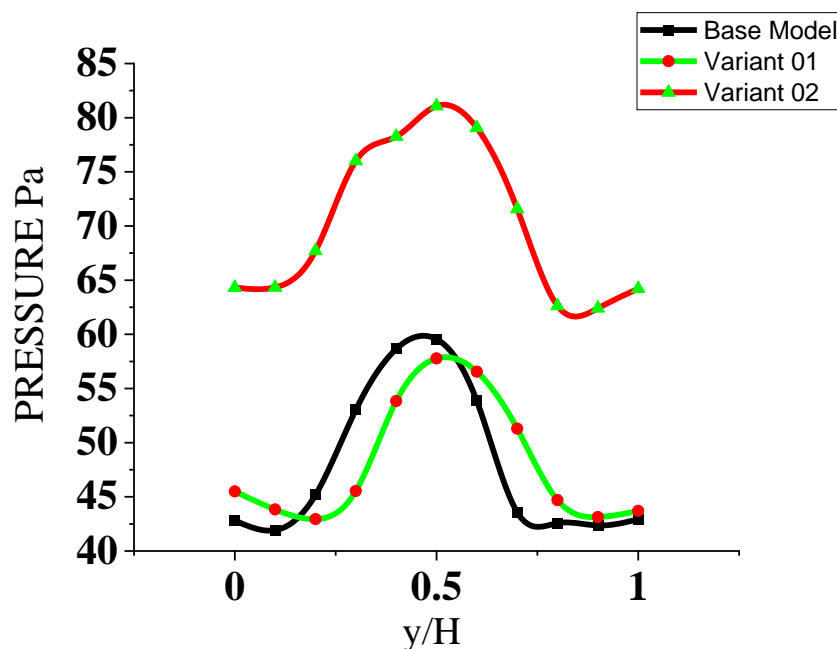
Fig. 10. Pressure Vs. the non-dimensional distance along with the diagonal path correlative to 10.38 m/s inlet velocity at v_2 location
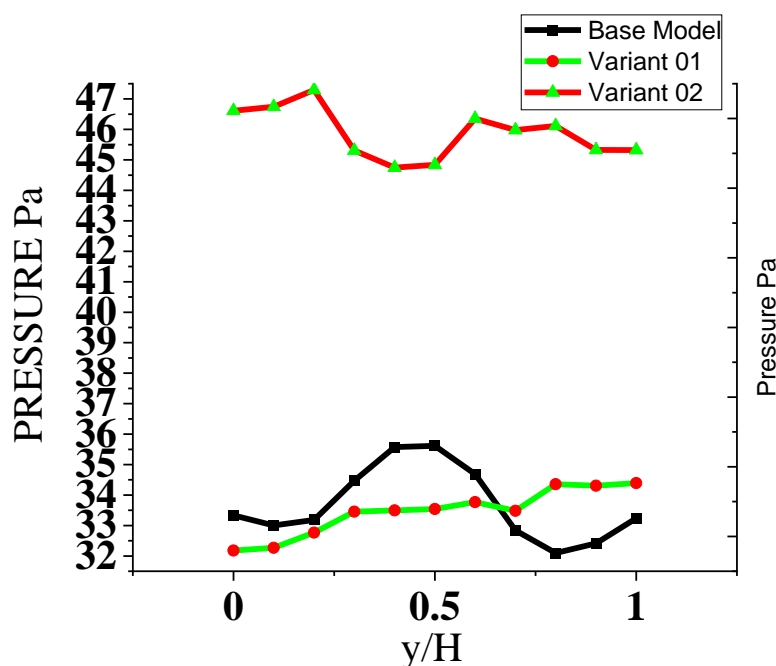

Fig. 11. pressure Vs. the non-dimensional distance along with the diagonal path correlative to 8.31 m/s inlet velocity at v_1 location

From Figure 12, it can be conferred that the value of maximum velocities for all three variants is less concerning to corresponding values of velocities at 10.38 m/s inlet.

From Figure 12, it can be seen that the velocity profile for variant 01 is parabolic in nature, which is termed as the maximum centerline velocity for the variant 01 model is 6m/s. The trend for the velocity profile is exact as compared to the inlet velocity of 10.38m/s at location v_1. The maximum pressure rise in the transverse direction is 33 Pa for variant 01 model, which is the comparatively lesser value at the same location corresponding to inlet velocity 10.38 m/s. This indicates at higher velocities and flows, mal-distribution will be higher.
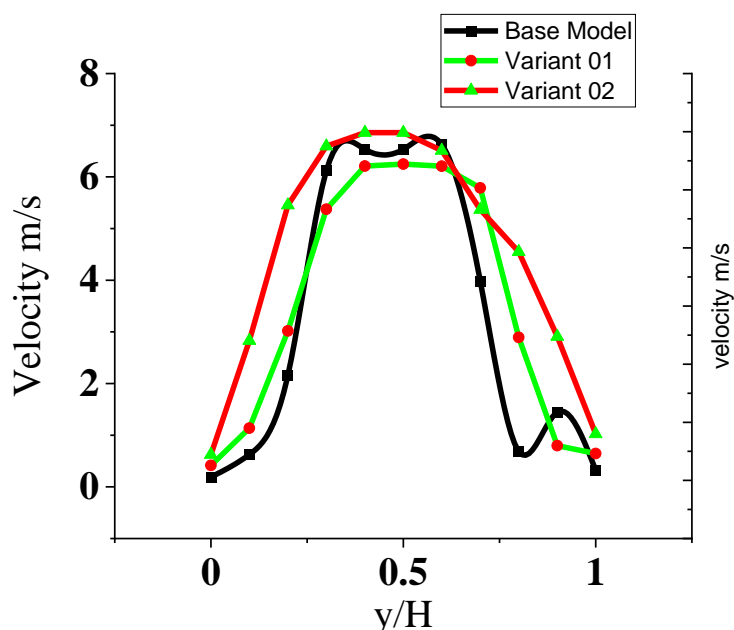
Fig. 12. Velocity Vs. the non-dimensional distance along with the diagonal path correlative to 8.31 m/s inlet velocity at v_1 location

4.1.3 Pressure drop characteristics

The pressure drop characteristics, i.e., pressure difference at inlet and outlet of the converter, are also studied by estimating the numerical values of pressure across the catalytic converter. The Figure 13 indicated the minimum value of pressure drop is for variant 02 is 62.7 Pa, corresponding to 52.3° cone angle for inlet velocity 10.38 m/s, decreasing the additional amount of diffuser angle increases the pressure drop. Similarly, for 8.31m/s, the value of pressure drop is less as compared to inlet velocity 10.38 m/s, for cone angle 52.3° is 45.4 Pa.
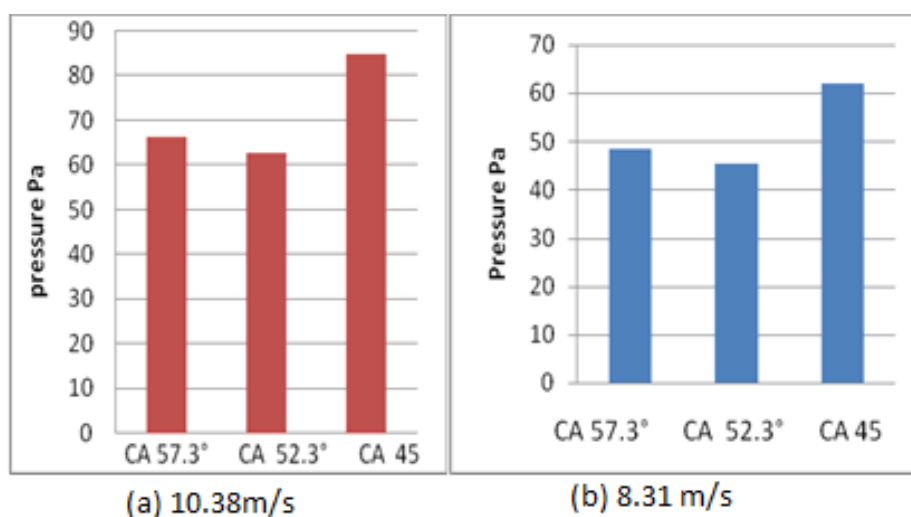

Fig. 13. Influence of cone angle (CA) on pressure drop corresponding to inlet velocity 10.38m/s and 8.31 m/s

5. Flow Uniformity Index

A dimensionless parameter-flow uniformity index (γ) indicates the range of flow mal-distribution inside the monolith channels. Ideally, γ should be one for normal- distribution inside the monolith. The flow index value is 1.9 at the center of the channels. Figure 14 shows a uniform flow inside the catalytic convertor for variant 02 model, followed by the variant 01 models as compared to base geometry design.

The flow index for the variant 02 models is 1.62, which is a lower value as compared to the inlet velocity of 10.38 m/s at the same location. This shows that flow mal-distribution is higher at higher velocities. In summary

i. The variant 01 model offers a lower pressure drop value as compared to other geometrical designs and also has uniform flow as compared to the base model design.
ii. A decrease in the cone angle makes the flow inside the convertor a uniform flow but increases the pressure drop characteristics across the convertor.

From Figures 14 and 15, the flow is more uniform at the center of the monolith as compared to near the inner walls of the catalytic converter. It may be as there are vortices created in the flow near the walls due to this, there is flow mal-distribution near the circumference of the catcon, and at the center, and there is the greater amount of mass flow rates.
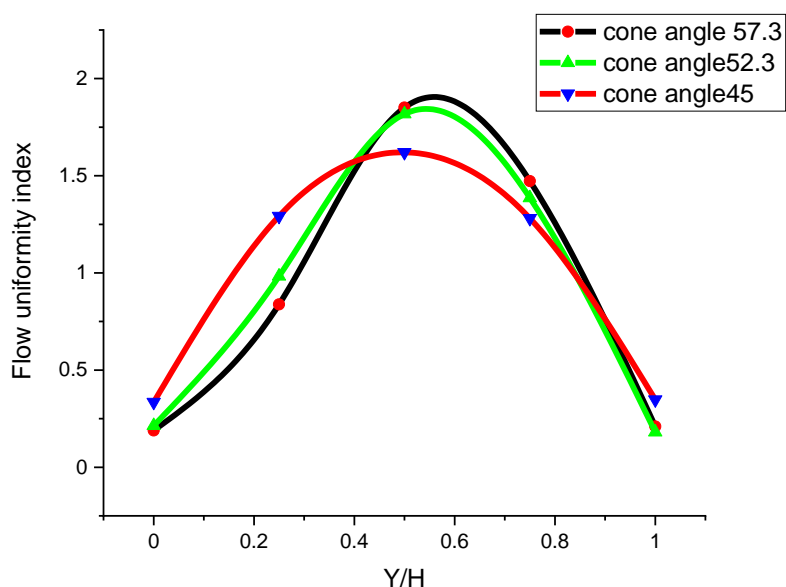

Fig. 14. Flow index Vs. the non-dimensional distance along with the diagonal path correlative to 10.38 m/s inlet velocity at v_3 location
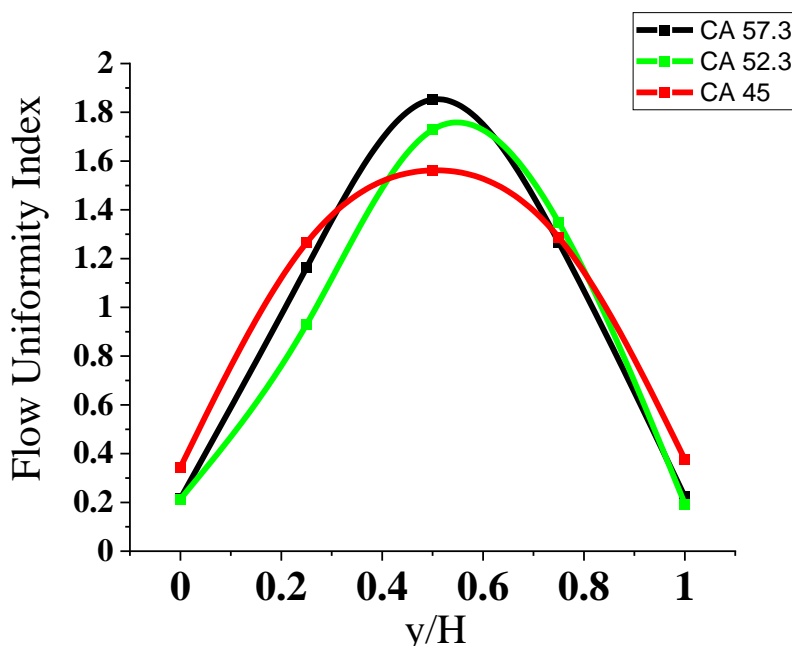
Fig. 15. Flow index Vs. Non-dimensional distance in the transverse direction corresponding to 8.31 m/s inlet velocity at v_3 location

6. Conclusions

The stream circulation in a base design brick is uneven because of the geometry of the estuary features and catalytic monolith. Due to the presence of powerful recirculation zones, the flow is termed as non-uniform. The velocity profile curves for inlet velocity 10.38 m/s for base design geometry at the different transverse location was compared with the existing literature results. The trend depicted was similar in both cases. The deviation from maximum velocity is within an acceptable range of 3%. This shows that the model is established and can be modified to obtain different analysis results.

As seen from the results, to minimize the flow mal-distribution within the convertor, the critical parameter is optimizing diffuser geometry. Flow separation occurs within the distribution leading to a non-uniform flow. There is an increase in pressure filed values in the transverse direction at v_2 location; this is because the diffuser increases the pressure of the fluid at the expense of its kinetic energy.

The overall pressure drop increases with an increase in inlet velocities. For 10.38m/s, the total pressure drop is 84.9 pa, corresponding to the 45° cone angle. There is a reduction in flow separation as the cone angle reduces to 45°, minimizing the flow maldistribution within the converter. One of the reasons for the increase in overall pressure drop at reduced diffuser angle is, the flow area of the diffuser will become smaller and smaller as the inclined angle reduces, thus decreasing the flow uniformity index and increasing the pressure loss.

The variant 01 models with diffuser angle 52.3° shows favorable conditions with a limited overall pressure drop value of 62.7 pa as compared to the base design value of 66.4pa corresponding to inlet velocity 10.38 m/s, the design can achieve an improvement in pressure drop value of 3.7 pa. The result is similar for inlet velocity 8.31 m/s, here a pressure drop improvement value is 2.7 pa. The engine exhaust backpressure is directly proportional to the pressure drop across the converter. The minimum amount of the pressure drop will exert lower back pressure on the engine. Reduction in backpressure will lead to reduced specific fuel consumption. The flow uniformity index value is enhanced as compared to the base design, indicating a more uniform flow than its original geometry.

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