Computational Fluid Analysis on Catalytic Converter with More Surface Area Monolithic Structure

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ABSTRACT

Catalytic converters are used to convert toxic gases into less toxic residues. Monolithic honeycomb structure coated with Noble metals as catalysts are used for this purpose. Noble metals cause a redox reaction and put a check on the emission of toxic elements. Thus, increases in contact time with noble metals, lesser the emission. Hence the larger surface area is preferred in the monolithic structure of catalytic converter for coating Noble metals. This paper does a comparative study over a new monolithic structural design in place of the conventional honeycomb structure of the same dimensions with least weight and more contact area. Conventional used structure and proposed monolithic structure designs were simulated in ANSYS fluent software and the results are compared. The proposed design resulted in 9.23% increase of contact surface area and weight reduction of 64.18%. Exhaust flow analysis in terms of back pressure and exhaust temperature for the proposed structure are almost equivalent to the earlier design.

Keywords: CAD automation; catalytic converters; computational fluid dynamics; contact surface area; fractal curves; Hilbert curve; monolithic structure.

NOMENCLATURE

CAD	computer aided design
CFD	computational fluid dynamics
EGR	exhaust gas recirculation
SCR	selective catalytic reduction
E	turtle movement in east direction
F	forward
N	turtle movement in north direction
n	number of iteration.
S	turtle movement in south direction
W	turtle movement in west direction
3D	three dimensional

INTRODUCTION

At present, automobile industries are facing challenges and constrain in reducing exhaust gas emission. Industries are forced to adopt the new emission norms implemented by the pollution control policies. In comparison with exhaust gas recirculation (EGR), selective catalytic reduction (SCR) produces lesser NO_x emission compared to that of EGR. Here

EGR reduces NO_x by reducing the O_2 supply for combustion, which lead to a reduction in combustion efficiency [1], [2]. Chivate et al., [3] discussed the prospects and concluded that a separate catalytic converter is more efficient over EGR. Maheshappa et al. [4] and Bagus Irawan et al. [5] have discussed in their research, that catalytic converter's emissions are controlled by using a layer of small ceramic beads packed tight and held at the end of the converter with steel mesh. However, due to the gradual shifting of beads, they worn-out quickly. Currently, exhaust system uses a modern three-way catalytic converter which contains monolithic substrate, coated with rare earth metal as catalysts. The monolithic substrate is made up of either ceramic or with metals, where the latter exhibits better performance due to its good mechanical properties, long durability and high thermal stability during regeneration [6].

In Grigorios Koltsakis et al. [7] work, least light off temperature results in the emission of exhaust gas. Till light-off temperature is achieved, the catalyst will not start the redox reactions. To produce low light-off temperature, a separate unit is fixed which heat (electrically) the catalytic converter during cold start conditions. This lead to heating up of the catalytic converter, hence light-off temperature is achieved as early as possible and lead to an increase in the overall performance of the catalytic converter. Sua et al. [8], Subramanian et al. [9], Windmann et al. [10], Guojiang et al. [11] and Jeong et al. [12] have done research and concluded that light off temperature gets influenced by the flow of exhaust gas inside the catalytic converter. The light-off temperature depends upon various factors like the shape of the substrate and length of the substrate when more length substrate is used it increases the surface contact area that leads to earlier light-off temperature [13].

Chivate et al. [3] have briefly explained in his work about catalytic converters, variable design availability for the monolithic substrate is square, wire-mesh, corrugated, arrays of beads and honeycomb. Among all, honeycomb and square structures are commonly used due to its larger surface area within the same volume. The author has also concluded that the larger surface area of the substrate reduces the exhaust emission to a greater extent. Due to the maximum surface area, more quantity of catalyst is coated over the monolithic substrate to enhance redox reactions and reduce toxic emission. The same was explained by Mohan Laxmi et al. [6] where a larger surface area reduced pressure drop and fuel consumption with an increase in volumetric efficiency. Further pressure drop and uniform flow pattern increased the converter efficiency [14]. Benjamin et al., Kang et al., and Kim et al., reported that factors like high Reynolds number, pulsating flow, abrupt expansion and porous medium lead to non-uniform flow [14-16]. Catalytic converter must be designed in such a way that it should possess more uniformity. Subramanian et al., Ozhan et al., and Martin et al. have worked on a similar kind of problem and concluded that, to obtain a uniform flow pattern, the shape of the substrate, wash coat thickness, material, density, geometry and position of the converter should be optimised [9, 17, 18]. Furthermore, variation in substrate length ratio (front substrate and rear substrate) and the gap between them is also important which leads to needing for a longer substrate to maintain flow uniformity [8]. Computational fluid dynamics (CFD) is used as an optimised tool to solve the flow analysis in monolithic structure in terms of parameters such as pressure drop, uniform flow and velocity variation. Pandhare et al., Lai et al., and Hayes et al., have compared the various experimental values with CFD results and produced an optimum design for monolithic structure with help of CFD tool [19-22].

From this discussion, it is found that catalytic converter efficiency is depending on producing larger surface area, lesser specific volume. In this work, a new structure is

proposed for catalytic converter wash coat monolithic structure, which poses a greater surface area at the same volume and lesser specific volume. The CFD analysis was done on newly developed structure and its performance in terms of pressure drop and uniformity in flow is compared with conventional used honeycomb monolithic structure.

METHODOLOGY

This study is based on the idea that greater the surface area of a monolithic substrate, lesser the emission and a higher conversion efficiency obtained. For this objective, in this work, an attempt was made to investigate the use of advanced fractal curve based monolithic structure for the catalytic converter. Further, comparison was done between the conventional and proposed design using simulation software packages in terms of pressure drop, uniformity in flow.

Modelling

Fractal curves

There are a variety of curves in nature which possess different kinds of geometry and features. A fractal is generally a rough or fragmented geometric shape that can be subdivided into parts, each of which is a reduced-size copy of the whole. This property is called self-similarity and are governed by various algorithms one among them is proposed by Family et al. [23]. Figure 1 depicts different forms of fractal curves. They possess various other properties like self-repeating space-filling, symmetry and maximum area occupancy in a given volume. Hilbert curve, which is a type of fractal curve, the area to the square made by it remains unchanged with an increase in the iteration values, thus when making a higher iteration curve then the effective length increases but the edge length remains the same. So the advantage is without increasing the size of the square it can incorporate an infinite length of the curve and as the length increases the effective current path also increases thus generating more area to collect power. Different methodologies are used to generate fractal curves. Some of the prominent methods are the L- system, space folding algorithm and the table-driven algorithm developed by Peitgen et al. and Griffiths et al. [24, 25]. Figure 2(a) and 2(b) depict the fractal curve for different iteration with algorithm axiom.

The algorithm used for generating Hilbert curve using the L-system. The creation of a Hilbert curve in L-system is explained as;

 i. Alphabets: A, B
 ii. Constants: F, +, -
 iii. Axiom: A

Production rules: A $\rightarrow$ -BF+AFA+FB- and B $\rightarrow$ +AF-BFB-FA+

The initial A and B in the L-system for a Hilbert curve of Order 0 are:

$n = 0$; A$\rightarrow$ -F+F+F-, B $\rightarrow$ +F-F-F+

Thus, the turtle movement is: -F+F+F-

The above-mentioned axiom was executed and output is shown in Figure 2(a). For a Hilbert curve of order 1, A and B are recursively produced as: $n =1$; A $\rightarrow$ - (+F-F-F+) F+(-F+F+F-) F(-F+F+F-) +F(+F-F-F+)- and B$\rightarrow$ +(-F+F+F-) F-(+F-F-F+) F(+F-F-F+)-F(-F+F+F-) +

And the turtle movement, which basically is the movement represented by A is: - (+F-F-F+) F+ (-F+F+F-) F (-F+F+F-) +F (+F-F-F+)-

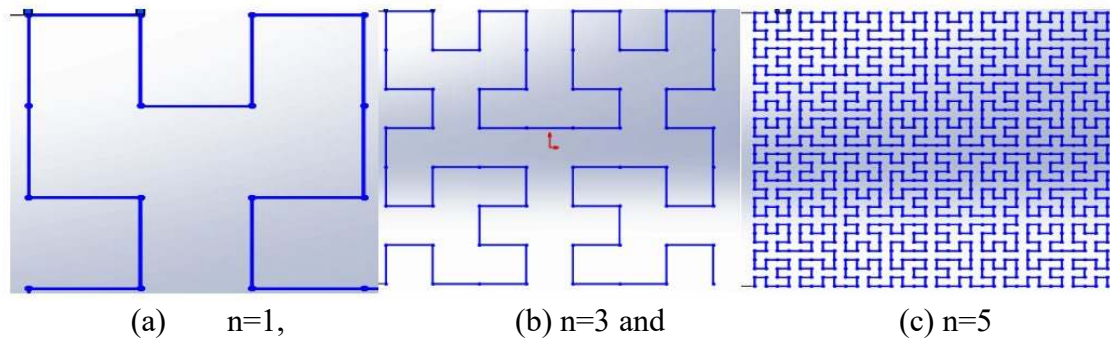(a)   n=1,   (b) n=3 and   (c) n=5

Figure 1. Different fractal curves for different iterations.

The above-mentioned axiom was executed and output is shown in Figure 2(b). Here n= number of iteration, '+'(plus) stands for 'turn right', '- (minus) stands for 'turn left', 'F' stands for 'move forward'. Applying the turtle movement for n=0, 1,4,5,7 and 9 the above axiom is executed, and the output are shown in the Figure 2 and Figure 3.

Currently, computer aided design (CAD) software does not have provision for the direct modelling of fractal curve model and manual sketching of fractal curve for higher iteration is tedious work. So for this work fractal curve sketch was drawn using VB script programming with algorithm discussed above and for the conventional model Honeycomb sketch was done using pattern options in CAD software as shown in Figure 4(a) and 4(c). From the sketch, a three-dimensional (3D) model as shown in Figure 4(b) and 4(d) was developed using extrude option in SOLIDWORKS 2015. The dimensions of 3D model are summarised below in Table 1.
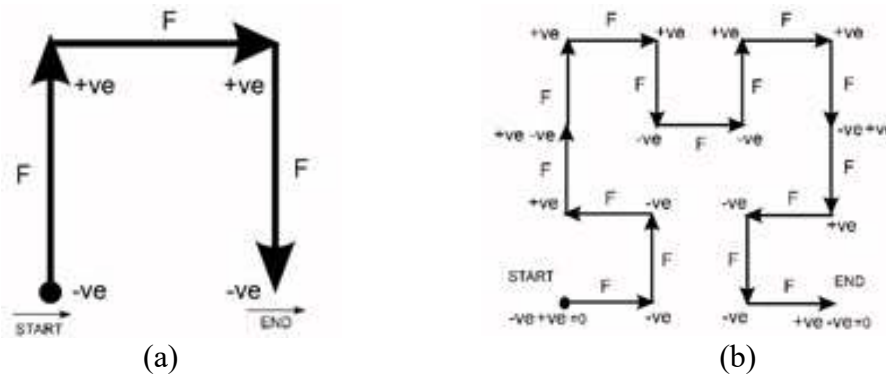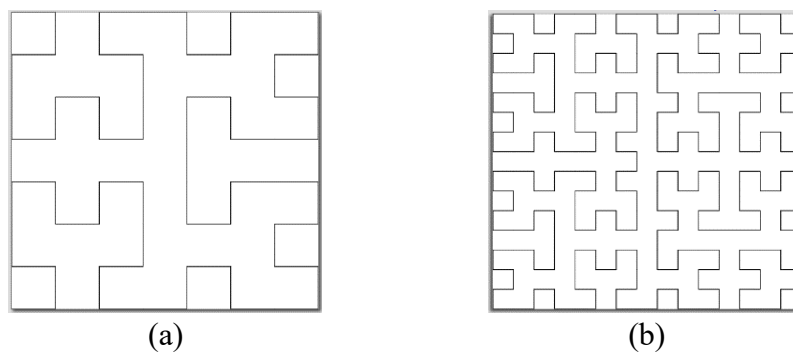

(a)   (b)

Figure 2. Hilbert curve for (a) n=0, turtle movement -F+F+F- and (b) n=1, turtle movement (- (+F-F-F+)F+(-F+F+F-) F (-F+F+F) +F(+F-F-F+)-.
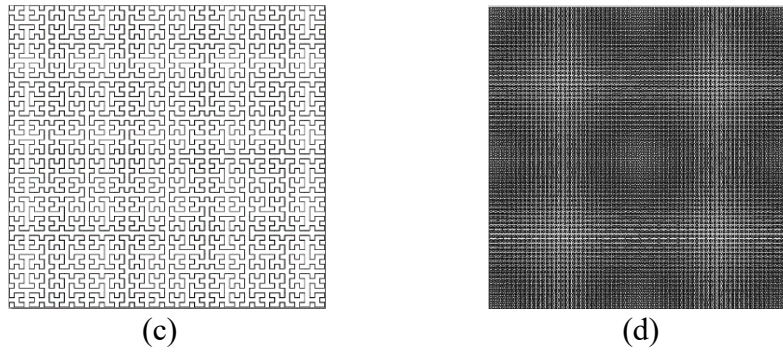

(a)   (b)

(c)   (d)

Figure 3. Hilbert curve for (a) n=4, (b) n=5, (c) n=7 and (d) n=9.
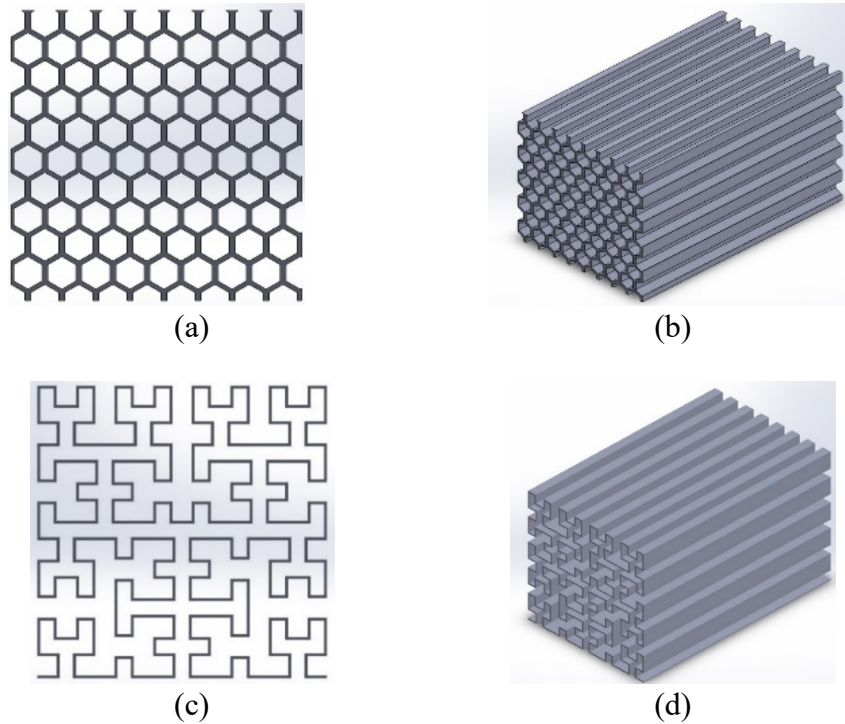

(a)   (b)

(c)   (d)

Figure 4. A 2-D and 3-D model of honeycomb (a), (b) and proposed structure (c), (d).

Table 1. Dimensions of monolith structures.

Parameter	Honey Comb Structure	Proposed Structure (Hilbert curve)
Length	100 mm	100 mm
Breadth	50 mm	50 mm
Height	50 mm	50 mm

Computational Fluid Dynamics

Meshing and Boundary conditions

Meshing was done in ANSYS Fluent with tetrahedron element. Table 2 summarises the meshing parameters of honeycomb model and proposed design. Model for the same is shown in Figures 5(a) and 5(b). The grid independent test was performed to finalize the

mesh size and the results were listed in Table 3 and Table 4 for the proposed model and honeycomb model respectively. The flow of gas was assumed as air with ideal gas properties. The ideal gas properties were imported from fluent data base. The boundary conditions used for analysis are listed in Table 5. The grid independent test was performed to finalize the mesh size to get the optimum results and they were shown in Figure 6. The Relevance option allows controlling the fineness of the mesh for the entire model. This number was to indicate a preference towards accuracy, the relevance value was varied from 0 to 100 and the analysis was performed, the pressure value was measured at a particular point at inlet and the result was shown in Figure 6. The finer the mesh, the more accurate the result. A coarse mesh provided less accurate results. From Figure 6 it was concluded that relevance value of 100 provides lesser deviation pressure in more accurate results and provides lesser error percentage hence, based on which meshing was finalised and analysis were performed further. Graphical result of honeycomb model's grid independent test was not mentioned since it also poses same kind of pattern.

Table 2. Meshing parameters for honeycomb and proposed model.

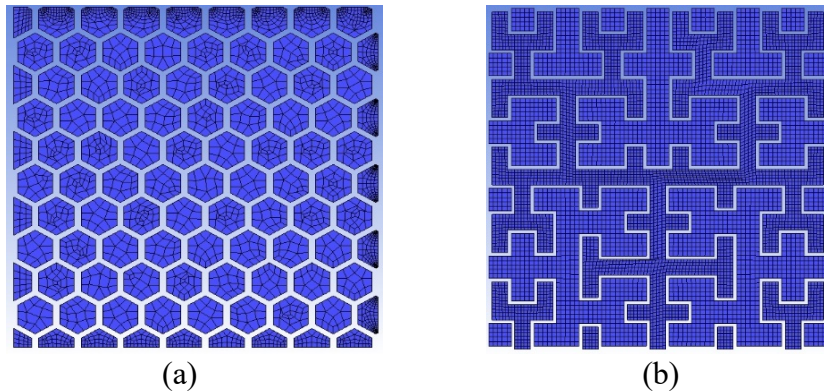| Type	Level	Number of elements	Nodes	Faces	Minimum volume range
Honeycomb	0	103200	176624	2061170	$1.9e^{-10}$
Proposed structure	0	122426	184426	3246589	$1.0e^{-09}$

(a)   (b)

Figure 5. Meshed (a) honeycomb model and (b) proposed fractal curve model.

Table 3. Grid independent test results for proposed model.

S.no	Relevance value	Number of elements	P_{max} (Pa)
1	0	38976	334.94
2	20	40260	334.64
3	40	67254	380.19
4	60	79272	378.56
5	80	110264	380.11
6	100	122426	381.38

Table 4. Grid independent test results for honeycomb model

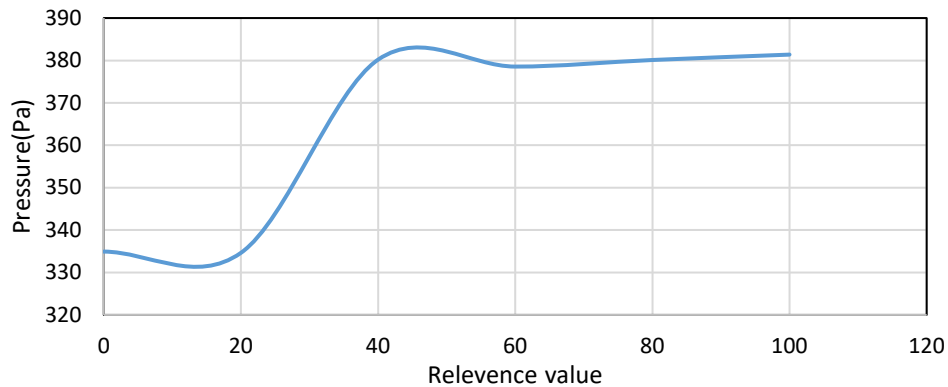| S.no	Relevance value	Number of elements	P_{max} (Pa)
1	0	35955	395.21
2	20	40600	395.48
3	40	43798	395.43
4	60	48180	395.38
5	80	949290	395.35
6	100	103200	395.32

Figure 6. Pressure Vs Relevance for proposed model

Table 5 Boundary conditions for analysis (Mohan Laxmi et al., [6])

Inlet boundary condition	
Type	Velocity inlet
Velocity	22.6 m/s
Outlet boundary condition	
Type	Pressure outlet
Pressure	101325 Pa
Target mass flow	0.0021732 kg/s

Governing Equation

The analysis was carried out based on the modified Navier stokes equation according to the application and the modification details are provided below. The general form of Naiver stokes equation is given in Eq. (1).

$$\rho\left[\left(\frac{\partial u}{\partial t}\right)+(u\,\nabla)u\right]-\mu\,\nabla^2+\,\nabla p=f \text{ on } \eth \, x(0,t) \tag{1}$$

Where, u is u(x,t) velocity vector, p is p(x,t) pressure field, ρ is constant density (incompressible flow), f is external body forces acting on the fluid and; μ is dynamic viscosity co-efficient. The flow was assumed as incompressible flow, steady state and 3-D flow. Hence the above Navier stokes equation can be modified based on assumptions:

$$\rho\left[\left(\frac{\partial u}{\partial t}\right)\right] - \mu \nabla^2 + \nabla p = f \ on \ \mho \ x(0,t) \tag{2}$$

The expanded form:

x momentum: $\rho\frac{\partial u}{\partial t} = \frac{\partial(\sigma_{xx})}{\partial x} + \frac{\partial(\tau_{xy})}{\partial y} + \frac{\partial(\tau_{xz})}{\partial z} + pf_x$ (3)

y momentum: $\rho\frac{\partial v}{\partial t} = \frac{\partial(\tau_{xy})}{\partial x} + \frac{\partial(\sigma_{xx})}{\partial y} + \frac{\partial(\tau_{xz})}{\partial z} + pf_y$ (4)

z momentum: $\rho\frac{\partial w}{\partial t} = \frac{\partial(\tau_{xz})}{\partial x} + \frac{\partial(\tau_{yz})}{\partial y} + \frac{\partial(\sigma_{zz})}{\partial z} + pf_z$ (5)

RESULTS AND DISCUSSION

After modelling, volume of honeycomb model and proposed fractal curve model was calculated using CAD software. Contact surface area of both the models and fluid domain area is summarised in Table 6. The proposed fractal curve model had higher surface area. Greater the surface area more quantity of catalyst could be coated to increases the redox reaction in catalytic converter. Proposed fractal curve model structure is having 9.2% of surface area more than honeycomb. New model occupies more area in given volume than honeycomb. Due to this greater surface area of the proposed fractal curve model, effects on pressure, velocity and flow distribution also varied. This was also explained by Chivate et al., Mohan Laxmi et al., and Om Griara Guhan et al., [3,6 & 26]. This will significantly reduce the weight of the catalytic converter also. Hence it possesses greater volumetric efficiency. The new model has lesser volume so weight of the component reduced and material cost also reduced.

Table 6. Comparison of area and volume properties for model and fluid domain
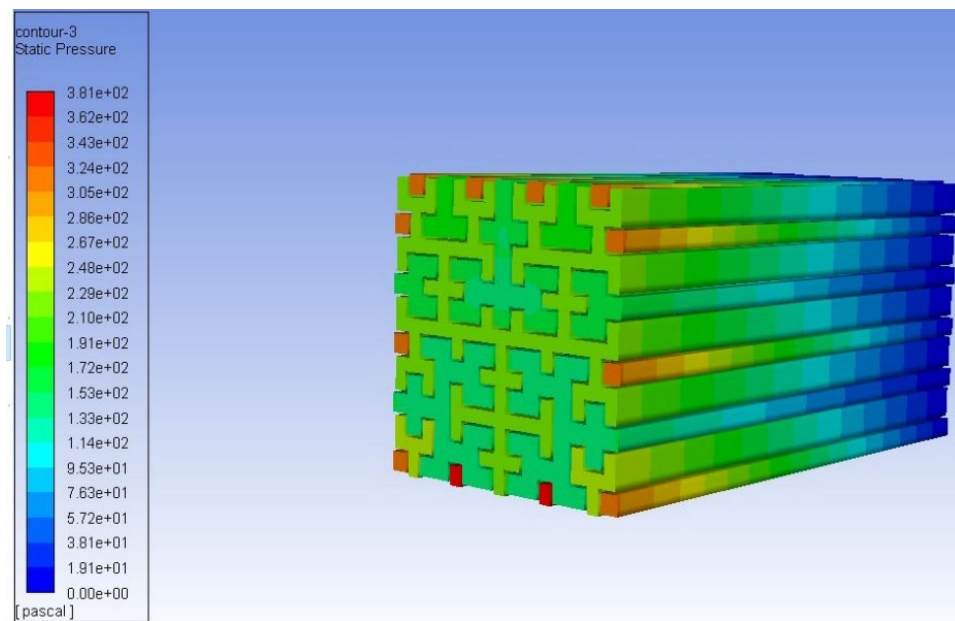
Properties	Honeycomb model	Proposed fractal curve model	Increment
Surface area for structure	123261.42 mm^2	134640 mm^2	9.23%
Area of fluid domain	0.61754612 m^2	0.95338597 m^2	54.38%
Volume of structure	55266 mm^3	33660 mm^3	- 64.18%
Volume of fluid domain	0.0001447339 m^3	0.00016434002 m^3	13.54%

The pressure contour of both conventional honeycomb and proposed fractal curve are shown in Figure 7(a) and 7(b). From the contours, it is observed that the proposed model possess higher pressure drop compared to honeycomb. Greater pressure drop than the conventional honey model, it could produce lesser noise and less damage to monolithic structure same was also experienced by Pandhare et al., Pandhare et al. [19,20]. The maximum, minimum and weighted average pressure of both models is summarised in Table 7. Pressure contour distribution for both models is almost same,

where the pressure gets increase from inlet to outlet. Though there is significance difference in static pressure, on average scale the pressure variation is not significance.
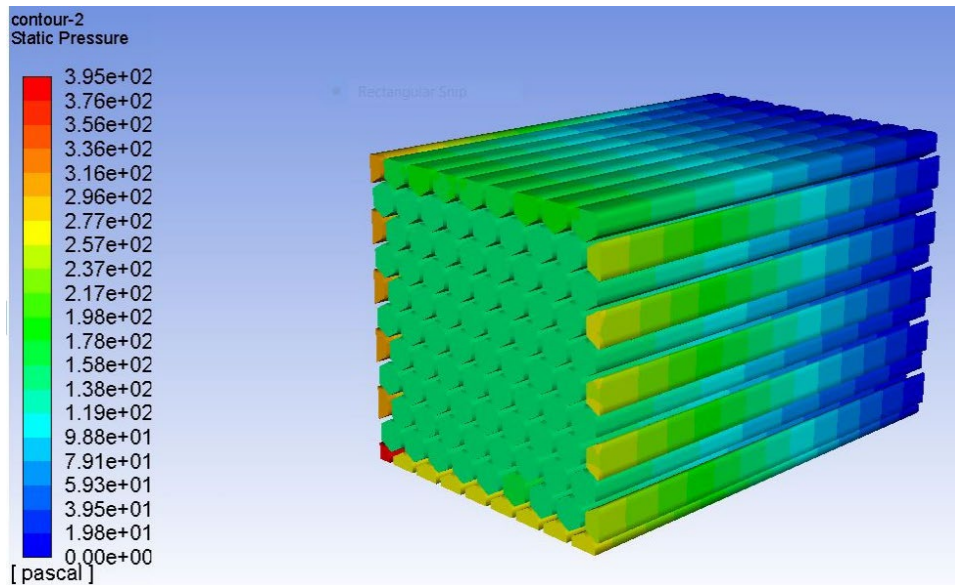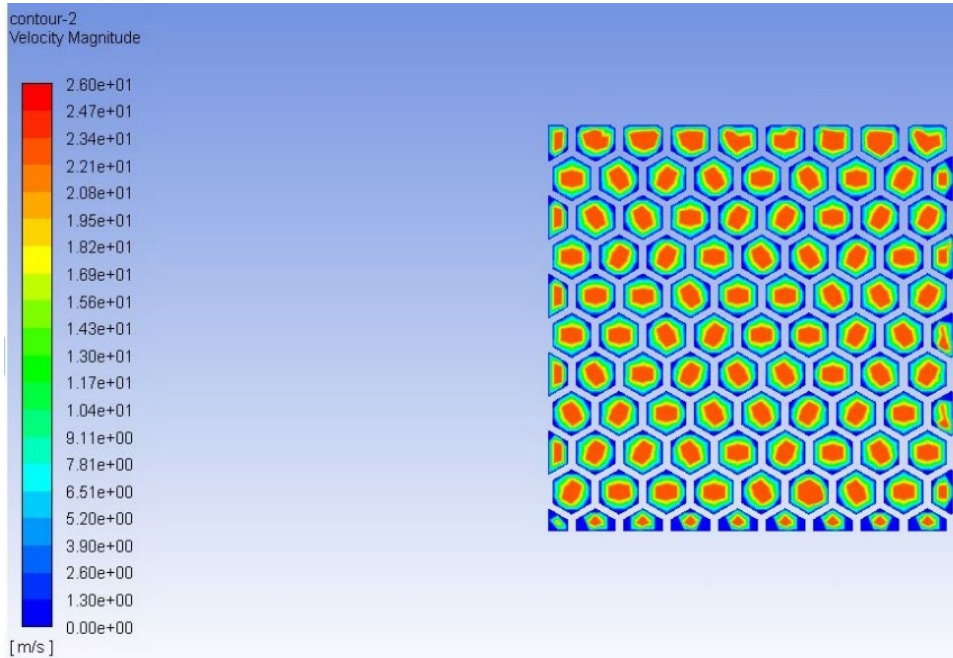

(a)

(b)

Figure 7. Pressure contour of (a) honeycomb and (b) the proposed fractal curve model.

Table 7. Range of pressure contour between both structures

Honeycomb		New model	
Minimum	Maximum	Minimum	Maximum
0 Pa	101720.3 Pa	0 Pa	101706.38 Pa

Velocity plots were analysed and compared between both models. The velocity contour plots for both models are shown in Figures 8 and 9. The rise in velocity was

recorded in both the monolithic structures. The minimum velocity rise was recorded in newly developed structure when compared with result of conventional honeycomb structure. From the velocity plot of simulation, it can be concluded that newly developed model possess does not have significant change in velocity of flow. Maximum, minimum and weighted average velocity is summarised in Table 8.
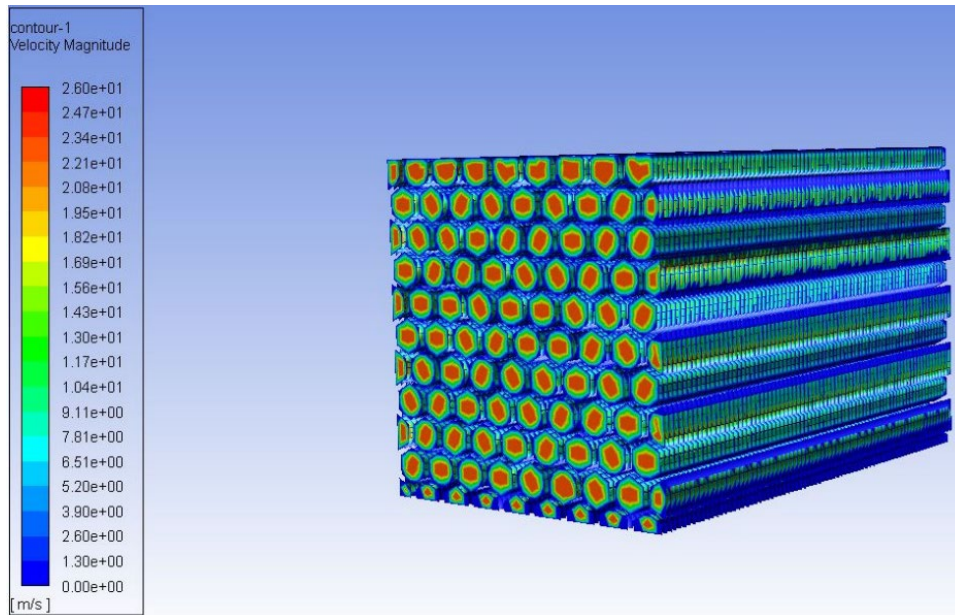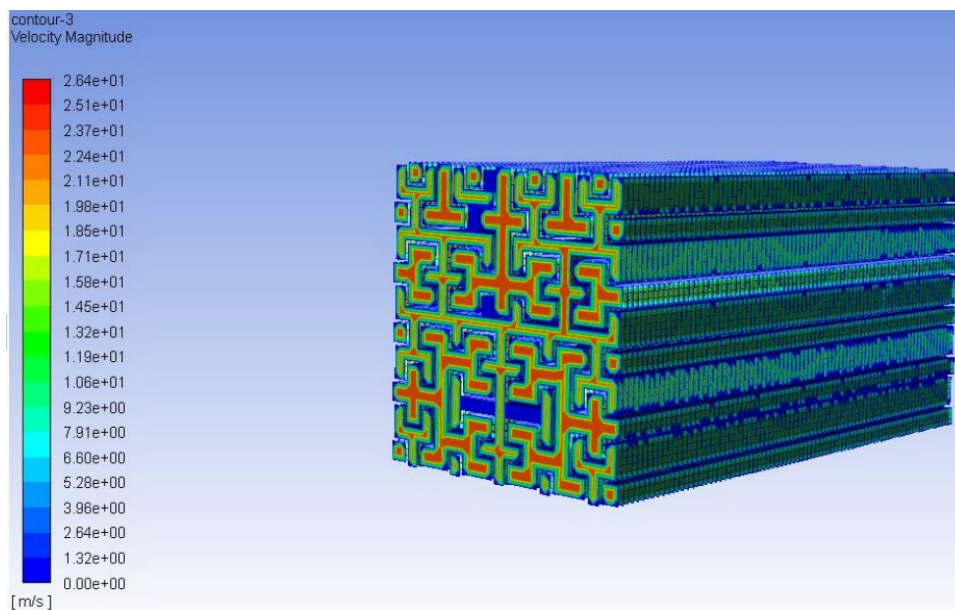

(a)
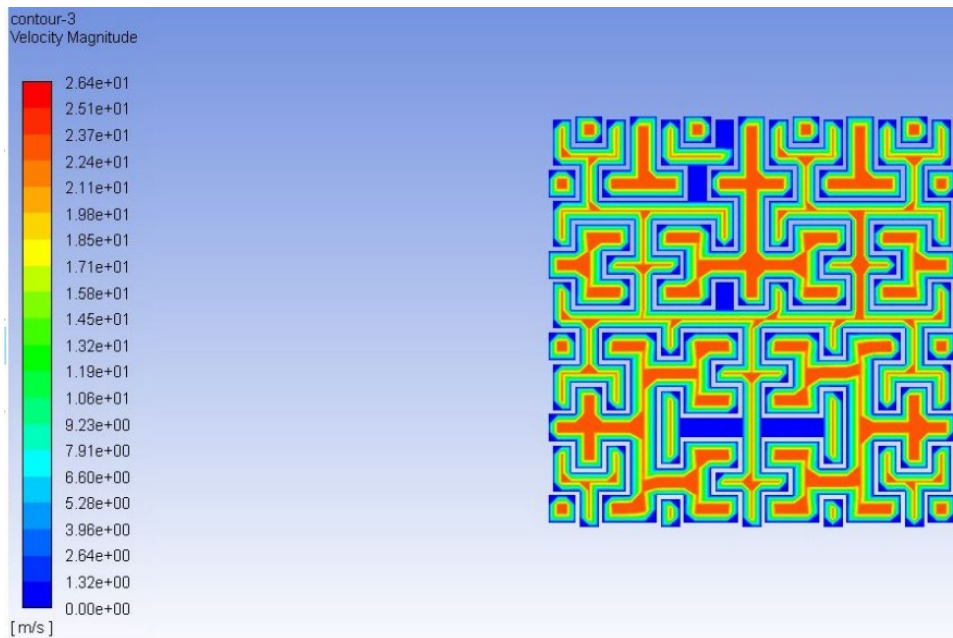
(b)

Figure 8. Velocity contour of (a) honeycomb and (b) proposed fractal curve model at inlet.

(a)

(b)

Figure 9. Velocity contour of (a) honeycomb and(b) proposed fractal curve model.

Table 8. Comparison of velocity contour between both structures

Honeycomb		Newly developed model	
Minimum	Maximum	Minimum	Maximum
0 m/s	26.02 m/s	0 m/s	26.39 m/s

Flow distribution over both the monolithic substrate was analysed with help of stream line plots. Through which we could find out which monolithic substrate possess less disturbance in flow. This parameter will influence the light off temperature of the catalyst. Greater the uniform flow quickly can achieve the light off temperature. The flow

distribution results of both honeycomb and proposed fractal curve model is shown in Figures 10(a) and 10(b).
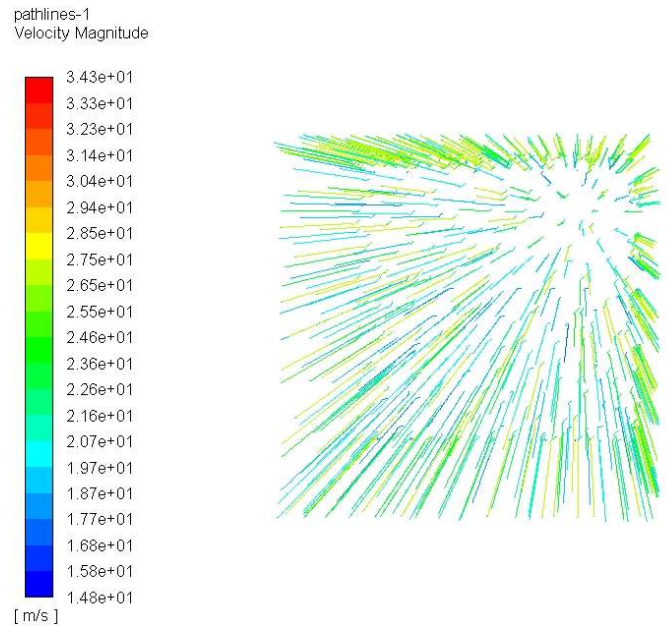
(a)
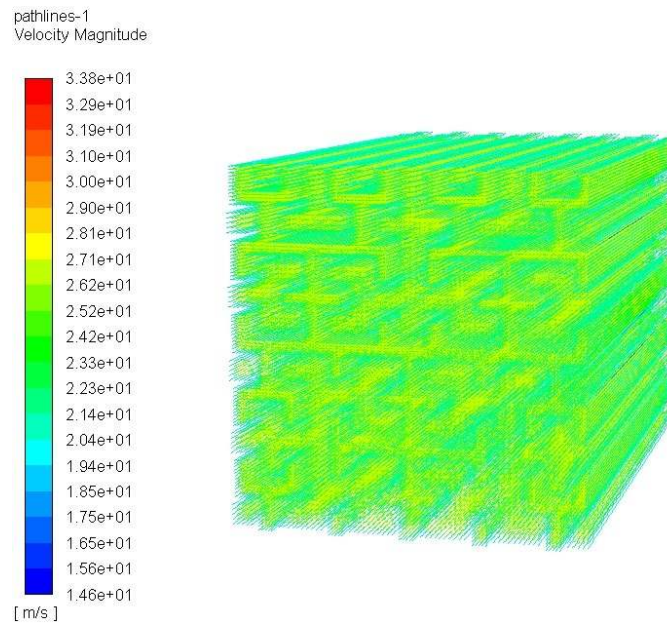
(b)

Figure 10. Flow distribution of (a) honeycomb and (b) proposed fractal curve model.

       More disturbances are observed in conventional honeycomb structure while comparing with the newly developed structure. This result shows that newly developed structure will have fewer disturbances due to which it can have higher conversion efficiency than conventional honeycomb Sua et al., Ozhan et al. and Martin et al., [8,17,18]. The above results imply that the newly developed model has higher uniform flow when it is compared with conventional honeycomb. From which it can be concluded that the proposed fractal curve structure will achieve quicker light off temperature for the

catalyst Gasser et al., [13]. Quickly achieved light off temperature of catalyst lead to a quicker response of catalyst with exhaust gas so we could have a lesser emission while comparing with conventional honeycomb structured monolithic Grigorios Koltsakis et al., Windmann et al., Guojiang et al. and Jeong et al. [7, 10 -12]

CONCLUSION

In this work an attempt to understand the effect of the fractal curve based monolithic structure for monolithic wash coat in catalytic convertor. From the detailed study of surface area, volumetric efficiency velocity distribution, pressure contour, flow distribution and pressure drop on both conventional honeycomb structure and proposed model the following conclusions are obtained.

   i.   Newly developed model has 9.2% greater surface area than honeycomb structure so it could be coated with more quantity of catalyst.

   ii.   The volume of the proposed model is 64.2% lesser volume when compared with honeycomb structure. This will result in high performance to weight ratio in the catalytic converter.

   iii.   Performance of Fractal curve model in terms of pressure drop and velocity of flow is almost the same for both fractal and honeycomb model.

   iv.   Flow distribution results suggest that lesser disturbance of flow occur in the newly developed model so it will have greater conversion efficiency and have more uniform flow and less light off temperature while comparing with honeycomb

In future, this proposed fractal curve manufacturing feasibilies and its performance in the experimental setup can be studied.

ACKNOWLEDGEMENT

REFERENCES

[1]   Jiang L, Wanga LW, Wang RZ, Roskilly AP. Performance analysis on a novel self-adaptive sorption system to reduce nitrogen oxides emission of diesel engine: Applied Thermal Engineering; 2017; 127:1077–1085.

[2]   Sagar D, Chaitanya SV. Comparision between EGR & SCR technologies. In: International Conference on Ideas, Impact and Innovation in Mechanical Engineering, pp. 856-861; 2017.

[3]   Chivate A, Dengale P. Design, analysis & testing of catalytic converter for emission reduction & backpressure optimisation. In: IRF International Conference, pp. 28-32; 2017.

[4]   Maheshappa H, Pravin VK, Umesh KS, Veena PH. Design analysis of catalytic converter to reduce particulate matter and achieve limited back pressure in diesel engine by CFD. International Journal of Engineering Research and Applications; 2013; 3(1): 998-1004.

[5]   Bagus Irawan RM, Purwanto P, Hadianto H. Optimum design of manganese-coated copper catalytic converter to reduce carbon monoxdie emissions on gasoline motor. Procedia Environmental Sciences;2015; 23: 86-92.

[6]   Laxmi MK, Kumar VR, Rao YVH. Modeling and simulation of different gas flows velocity and pressure in catalytic converter with porous. International Journal of Computational Engineering Reasearch; 2013; 3(4): 28-41.

[7]   Grigorios Koltsakis C, Dimitrios Tsinoglou N. Thermal response of close-coupled catalysts during light-off. SAE Technical Paper: 01: 1876; 2003.

[8]   Sua Q, Xiea L, Shuaib S, Wangb J, Songc J, Li Z. Optimisation of automotive catalytic converter by numerical modeling and simulation with detailed mechanism. Catalysis Today; 2013; 216: 292– 298.

[9]   Subramanian M, Gajendra Babu MK, Subrahmanyam JP. Optimisation of catalytic converter for cost and effective conversion for spark ignition engine. SAE Technical Paper: 28: 0008; 2004.

[10]   Windmann J, Braun J, Zacke P, Tischer S, Deutschmann O, Warnatz J. Impact on the inlet flow distribution on the light-off behavior of a 3-way catalytic converter. SAE Technical Paper: 01: 0937; 2003.

[11]   Guojiang W, Song T. CFD simulation of the effect of upstream flow distribution on the light-off performance of a catalytic converter. Energy Conversion and Management; 2005; 46: 2010-2031.

[12]   Jeong SJ, Kim WS. Three-dimensional numerical study on the use of warm-up catalyst to improve light-off performance. SAE Technical Paper: 01: 0207; 2000.

[13]   Gasser I, Rybicki M, Wollner W. Optimal control of the temperature in a catalytic converter. Computers and Mathematics with Applications; 2014; 67: 1521–1544.

[14]   Benjamin SF, Roberts CA, Wollin J. A Study of the effect of flow pulsations on the flow distribution within ceramic contoured catalyst substrates. SAE Technical Paper: 01: 1996; 2001.

[15]   Kang KN, Jung MS, Kim CM, Lee JK, Kim MY. Numerical study on the mixing flow characteristics with a vane-type static mixer in a diesel exhaust system for urea scr application. Proceedings of the KSAE Spring Conference, pp. 532-538; 2012.

[16]   Kim YD, Jeong SJ, Kim WS. A numerical study on the flow uniformity and pressure drop in dual monolith catalytic converter during the rapid acceleration/deceleration driving. Transactions of the KSAE; 2007; 15: 63-71.

[17]   Ozhan C, Fuster D, Costa PD. Multi-scale flow simulation of automotive catalytic converters. Chemical Engineering Science; 2016; 116: 161–171.

[18]   Martin AP, Will NS, Bordet A, Cornet P. Effect of flow distribution on emissions performance of catalytic converters. SAE Technical Paper: 980936; 1998.

[19]   Pandhare A, Atul Padalkar S. Experimental and simulation study of design engine for lower exhaust emissions. SAE Technical Paper: 26-0136; 2013.

[20]   Pandhare A, Lal A, Vanarse P, Jadhav N, Yemul K. CFD analysis of flow through muffler to select optimum muffler model for CI engine. International Journal of Latest Trends in Engineering and Technology; 2014; 4(1): 12-19.

[21]   Lai MC, Lee T, Kim JY, Cheng CY, Li P, Chui G. Numerical and experimental characterizations of automotive catalytic converter internal flows. Journal of Fluids and Structures; 1992; 6(4): 451-470.

[22]   Hayes RE, Fadic A, Mmbaga J, Najafi A. CFD modelling of the automotive catalytic converter. Catalysis Today; 2012; 188: 94-105.

[23]   Family F, Vicsek T. Dynamics of fractal surfaces. 1st ed. Singapore: World Scientific Publishing Co Pte Ltd; 1991.

[24]   Peitgen HO, Jürgens H, Saupe D. Chaos and fractals. 2nd ed. New York: New Frontiers of Science, Springer; 2004.

[25]   Griffiths JG. Table-driven algorithms for generating space-filling curves. Computer-Aided Design; 1995; 17(1): 37-41.

[26]   Om Griara Guhan CP, Arthanareeswaren G, Varadarajan KN. CFD study on pressure drop and uniformity index of three cylinder lcv exhaust system. Procedia Engineering; 2015; 127: 1211-1218.