CFD Analysis of Catalytic Converter to Reduce Particulate Matter and Achieve Limited Back Pressure in Diesel Engine

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***Abstract*-The superior performance, higher output power and comparatively less-cost fuel make the diesel engines more popular in both heavy and light duty automobile applications. The main disadvantage in diesel engines is the emission of dangerous pollutants like oxides of nitrogen (NO_X) and particulate matter (PM) heavily, which affect seriously the environment and human health. 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 selected as filter materials. Models with filter materials of very fine grid size wire meshes packed inside the manifold develop more back pressure which causes more fuel consumption due to lower volumetric efficiency. Use of larger grid size wire meshes results in less back pressure, but the filtration efficiency is also reduced which may not be sufficient to meet the most stringent emission norms prescribed. Through CFD analysis, a compromise between these two parameters namely, more filtration efficiency with limited back pressure is aimed at. In CFD analysis, various models with different wire mesh grid size combinations were simulated using the appropriate boundary conditions and fluid properties specified to the system with suitable assumptions. The back pressure variations in various models are discussed in this paper.**

I. INTRODUCTION

With the introduction of the turbo charged high-speed diesel engines, the use of diesel engine vehicles in transport sector is increasing enormously. The main drawback in diesel engine is that it produces large amount of pollutants which include NO_X, CO, unburned HC, smoke etc. Apart from these unwanted gases, air borne Particulate Matter (PM) such as lead, soot, and other forms of black carbon are also produced in the diesel engine exhaust. All these pollutants are harmful to environment and human health. They are the main causes for greenhouse effect, acid rain, global warming etc. The simplest and the most effective way to reduce NO_X and PM, is to go for the after treatment of exhaust. The catalyst and filter materials placed inside the exhaust manifold increase back pressure This increase in back pressure causes more fuel consumption, and in most cases, engine stalling might happen. The filtration efficiency and back pressure are interrelated. If maximum filtration efficiency using very fine grid size wire meshes, is achieved, the back pressure will also be increased, which causes more fuel consumption. On the other hand, if larger grid size wire meshes are used, back pressure will be less, but the filtration efficiency will also be reduced, which does not help in meeting the present emission norms. With the help of CFD analysis, it is attempted to find out the optimum solution to get maximum filtration efficiency with limited back pressure developed inside the exhaust manifold.

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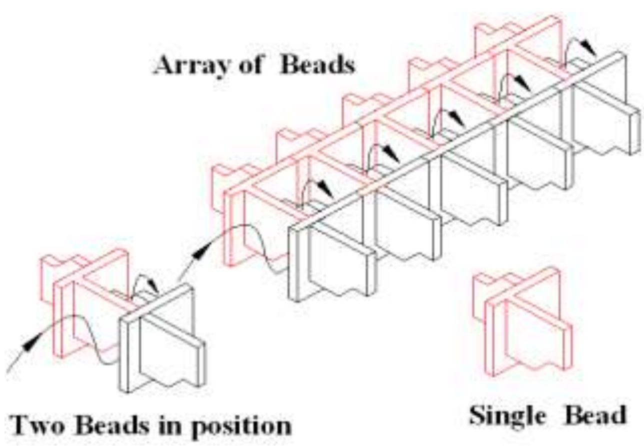
II. CATALYST

As this study deals only with the filtration efficiency of the trap system and the back pressure developed inside the exhaust manifold, the details pertaining to the type of catalyst, preparation of catalyst, reaction chemistry and NO_X conversion efficiency that can be achieved are not discussed in this paper. However, the shape of the catalyst bead which is relevant for the back pressure development inside the manifold is shown in Figure 1.



The flowing exhaust gas is free to move in all directions inside the manifold. As the movement of exhaust gas is not abruptly obstructed anywhere in its path, the back pressure is limited to minimum level. The porous nature of catalyst beads also help the gas to flow over the larger surface area of the catalyst enabling better reaction to take place for reducing NO_X as in the case of SCR system.

1) SCR Catalyst System

Presently, ammonia derived from urea is used to reduce NO_X from diesel engines. This is achieved by allowing the ammonia plus exhaust gas to flow over the platinum coated ceramic substrates, and it has been proved as highly effective in reducing NO_X in heavy duty applications [2]. Ammonia is produced on-board by rapid hydrolysis of nonhazardous form of urea solution. The problem with this is, cost of on-board production of ammonia, cost of additional on-board air supply equipments, and high cost of rare metals like platinum etc. In this paper, rare earth metal catalyst is replaced by a specially prepared catalyst. This catalyst selectively reacts with NO and NO_2 species and effectively reduces them to form nitrogen and oxygen using SCR technology.

2) Diesel Oxidation Catalyst

DOC is made as a flow through device that consists of specially made catalytic beads and steel wire mesh material which are coated with metal catalyst. As the hot gases contact the catalyst and the coated wire mesh, most of the exhaust pollutants such as CO, gaseous hydrocarbons, unburnt fuel and lube oil, toxic aldehydes etc. are oxidized to CO_2 and water, thus reducing harmful emissions. DOC does not collect or burn the soot particles in diesel exhaust. But it is accomplished by oxidizing the soluble organic fraction of diesel PM.DOC can also produce sulphate particles by oxidizing the SO_2 present in the exhaust gas and thus increases the PM emission. This may not be a problem, if the fuel contains <50ppm of sulphur [3].

3) Volume Of Catalyst

The size of exhaust manifold is based on the engine exhaust flow rates. For maximizing catalyst applied surface area, the volume of catalyst must be 1.5 to 2 times the engine displacement [3]. The engine selected for this study is a four stroke twin cylinder (80mm bore and 110mm stroke length) water cooled diesel engine. The engine displacement is calculated as 603 cm^3/sec for the assumed velocity of 60 m/s. The total volume of catalyst used in the model is 1383 cm^3. The total trap material (catalytic beads plus coated wire meshes) kept inside the manifold occupies one third of its total volume. This means, the remaining volume is used for the exhaust gas to flow out freely. This helps for limiting the back pressure and ensuring effective DOC and SCR systems.

III. SELECTION OF FILTER MATERIAL

Ceramic monolith, ceramic foam, steel wire meshes, ceramic silicon fiber, porous ceramic honey comb are the few types of filter materials reported in the literature. Out of these filter materials, steel wire mesh is selected as trap material because knitted steel wire mesh material is ranked first [4] for its collection efficiency of PM. The other reasons for its selection are,

Thermal stability during regeneration.
Good mechanical properties.
Long durability.
Easy availability and less cost.

Wiremesh Specifications

In this analysis, the selected steel wire mesh grid sizes are 1.96, 1.61, 1.01 and 0.65mm. The specifications of these wire meshes are shown in Table 1. Three models are made, each using two different grid size wire meshes placed in two separate compartments. The details of wire mesh grid sizes used in different models are shown in Table 2.

Table 1: Wire Mesh Specifications

Wire Mesh size (gap) in mm	**Wire Dia (d) in mm**	**Open Area %**	**Wt in Kg/m²**	**Mesh per inch**	**CPSI**
1.96	0.58	59.3	1.71	10	100
1.61	0.51	57.7	1.56	12	144
1.01	0.41	50.8	1.51	18	324
0.65	0.25	51.8	0.92	28	576

Table 2: Models and Wire Mesh Grid Sizes

Model No.	**Wire Mesh Grid Size (in mm) in Compartment I**	**Wire Mesh Grid Size (in mm) in Compartment II**
Model 4	1.96	1.61
Model 5	1.61	1.01
Model 6	1.01	0.65

Since number of steel wire mesh pieces are stacked one over the other as a bunch, the gas flow cannot be straight, rather it is a zig-zag flow. This type of flow provides increased travel length and contact time so that more amount of DOC action can take place and hence more PM reduction is achievable.

IV. PHYSICAL MODEL

To meet the less ground clearance available in the present vehicles, the height of the manifold is restricted to 110 mm. The cross section is made as rectangular of size 176 x 110 mm. In CFD, the system consumes less memory space and less response time, if the rectangular cross section is assumed. However, in actual practice, the rectangular corners are suitably rounded off which ensures the smooth flow of exhaust gas with less turbulence near the wall sides.

a. Construction

The exhaust manifold designed for this study comprises two compartments. The first one is meant for filtration and DOC catalyst. The second compartment is meant for filtration and SCR system.

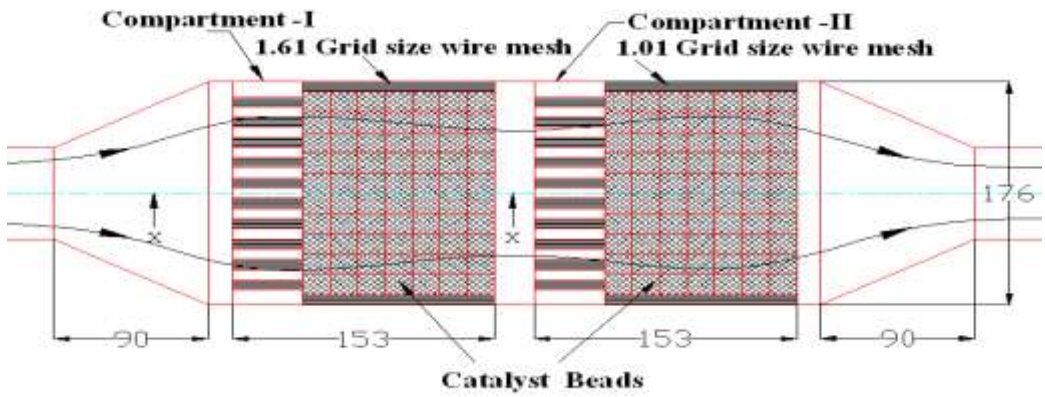


Figure 2: Sectional Plan Showing Two Compartments

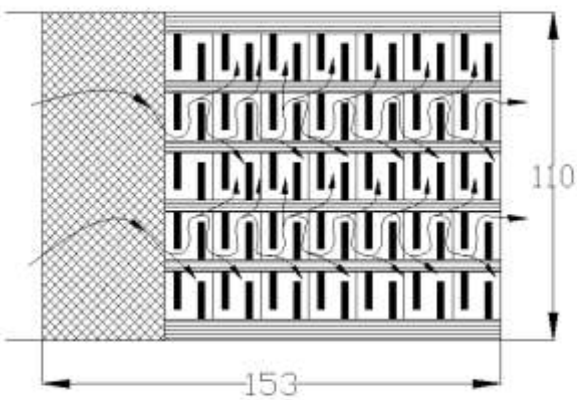


Figure 3: Sectional Elevation at x-x

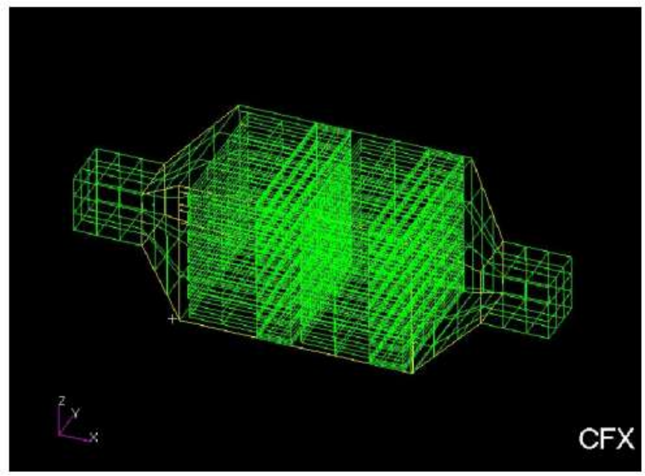


Figure 4: Meshing of Elements

The upstream of the first compartment is filled with steel wire meshes for about one-fourth of its length. These wire meshes are placed vertically with their surface being parallel to the flow of gas. Sufficient gaps are provided amongst the bunch of wire meshes which make the gas to flow crosswise also for better filtration and reduce back pressure as shown in Figure 2. The enlarged view showing the flow directions of exhaust gas is shown as sectional elevation in Figure 3.The downstream of first compartment is filled with catalyst beads and steel wire meshes arranged in alternate layers. The beads are arranged horizontally in a single layer so that the gas can enter at one end of the bead and come out in the opposite end. During its travel, the gas follows the up and down movement and meets the entire inner surface area of the catalyst as shown in Figure 3. There are 322 catalytic beads of size 16x16x16 mm placed in each compartment. More contact surface area of the catalytic beads enables the better catalytic reaction to take place between the catalyst and the flowing exhaust gas. The beads are designed so that the top and bottom portions are open and the gas can go up and down to the next layer of beads through the steel wire mesh layers which are also horizontally placed as shown in Figure 3.

b. Operating Principle

A part of the exhaust gas passes through the wire mesh layers which trap a portion of the soot. The remaining exhaust gas flows out to the neighboring bead placed in the same line – similar to a flow-through substrate. The soot trapped in the wire mesh material is combusted by the NO_2 that is generated by the upstream catalyst and thus the filter is regenerated continuously. If a situation occurs where filter regeneration is stopped and a saturation point occurred with the collected soot, the wire meshes placed over the catalytic beads will not plug as happened in wall flow filter. In this condition, the exhaust gas can flow out through the catalytic beads which are similar to a flow-through substrate. However, much larger part of exhaust gas flows through the catalytic beads in the direction as shown in Figure 3.As the path of the gas is not totally blocked, the back pressure developed inside the exhaust manifold is very much limited and no further increase in back pressure can happen beyond certain limit, irrespective of the soot loading over a period of time.A compressed air cleaning process is suggested to clean the PM deposition on steel wire meshes and catalytic beads. In this process, two numbers of compressed air inlet points are placed in between two compartments at diametrically in opposite position. By using compressed air available air at the fuel filling stations, the cleaning operation can be carried out. A hinged door of very thin size provided at the inlet end of the exhaust manifold will act as a non-return valve. This will prevent the cleaned PM dust going back into the engine while cleaning.It can be estimated and proved that, with the existing volume of catalyst and steel wire meshes, the cleaning may be required for every 10,000 Kilometers of engine run, for efficient fuel consumption.

V. Mathematical Modelling

Air is used as fluid media, which is assumed to be steady and compressible. High Reynolds number k-ε turbulence model is used in the CFD model. This turbulence model is widely used in industrial applications. The equations of mass and momentum are solved using SIMPLE algorithm to get velocity and pressure in the fluid domain. The assumption of an isotropic turbulence field used in this turbulence model is valid for the current application. The near-wall cell thickness is calculated to satisfy the logarithmic law of the wall boundary. Other fluid properties are taken as constants. Filter media of catalytic converter is modelled as porous media using coefficients. For porous media, it is assumed that, within the volume containing the distributed resistance there exists a local balance everywhere between pressure and resistance forces such that

$$-K_i u_i = \frac{\partial p}{\partial \xi_i}$$

Where ξ_I (i = 1, 2, 3) represents the (mutually orthogonal) orthotropic directions.

K_i is the permeability

u_i is the superficial velocity in direction ξ_iThe permeability K_i is assumed to be a quasi linear function of the superficial velocity. Superficial velocity at any cross section through the porous medium is defined as the volume flow rate divided by the total cross sectional area (i.e. area occupied by both fluid and solid).

VI. Three Dimensional CFD Study

A three-dimensional model of a catalytic converter is generated in CFD tool CFX for the analysis.

1) *Modeling And Meshing*

The geometry of the element is made as tetrahedral mesh, with a refined mesh near the wall. The RNG K-E turbulence model is used, with standard wall functions for near-wall treatment. The model has approximately 0.8 million tetrahedron fluid elements, and the same is shown in Figure 4.

2) *Governing Equations*

Commercial CFD solver CFX is used for this study. It is a finite volume approach based solver which is widely used in the industries. Governing equations solved by the software for this study in tensor Cartesian form are

Continuity:

$$\rho\left(\frac{\partial u_j}{\partial x_j}\right) = 0$$

Momentum:

$$\rho\frac{\partial}{\partial x_j}\left(u_j u_i\right) = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} + S_{cor} + S_{cfg}$$

Where ρ is density, u_i and u_j Cartesian velocity, p is static pressure, τ is viscous stress tensor.

3) *Boundary Conditions And Solver Modeling*

The inlet boundary condition is defined with the static pressure and temperature, and the outlet boundary condition is defined with the outlet static pressure. Exhaust gas is used as working fluid with initial pressure of 1.35 bar and 350^o C.Isothermal heat transfer model is for the entire domain. For outlet, the static pressure is specified as 1.15 bar. No slip boundary condition is applied on all wall surfaces. The discretisation scheme used is second order in space. The convergence criterion is set to a maximum residual equal to $1x10^{-4}$ for all the equations.

VII. Methodology

In the present study, the CFD analysis is carried out in two different stages as Stage I and II.

STAGE I

In Stage I, the length of conical portions of inlet and outlet of the exhaust manifold is varied as 70, 80, and 90 mm and are named as model 1, 2, and 3 respectively and the flow pattern is studied in CFD. The model which offers less back pressure is selected for further analysis.

STAGE II

In Stage II, 1.96 and 1.01 mm grid size wire meshes are filled in first and second compartments respectively. This particular combination is named as model 4. Similarly, the model with 1.61 and 1.01 mm grid size wire mesh is named as model 5. The model 6 contains 1.01 and 0.65 mm grids size wire meshes. After the CFD analysis, the best one from these three models is selected for further analysis.

VIII. Results And Discussions

The primary aim of this CFD analysis is to find out the right grid size of the filter material for the exhaust manifold which can offer minimum back pressure with maximum filtration efficiency of PM, using new catalyst for NO_X reduction. At present, the wall flow ceramic substrate are used as filters which are costly and also offer more back pressure resulting more fuel consumption. In the present study, steel wire meshes with coarse, fine and very fine grid sizes are used as filter materials.

a) *Back Pressures In Models 1, 2 & 3*

It is observed that the back pressure in model 1, 2 and 3 are found to be 0.907, 0.812 and 0.784 bar respectively as shown in Figure 5. The back pressure is found to be reduced with the increase in length of taper for the same inlet and outlet bound conditions. The back pressure variations are shown in graphical form in Figure 6.

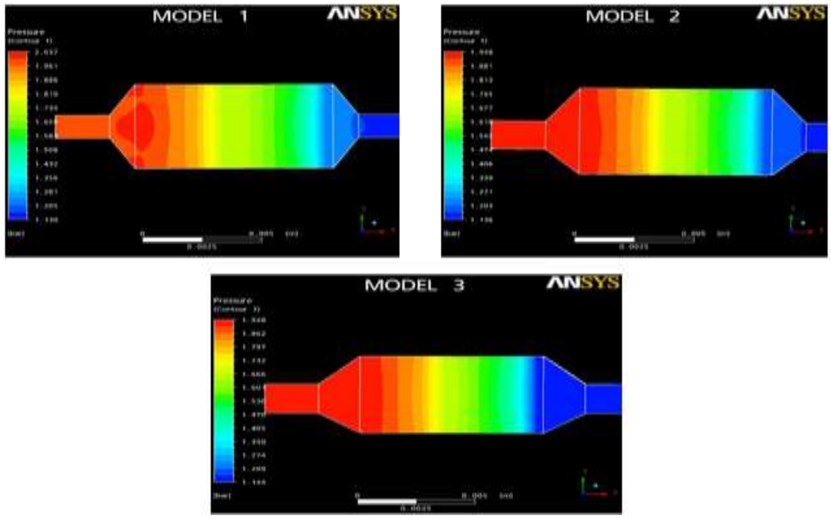


Figure 5 – Pressure Variations

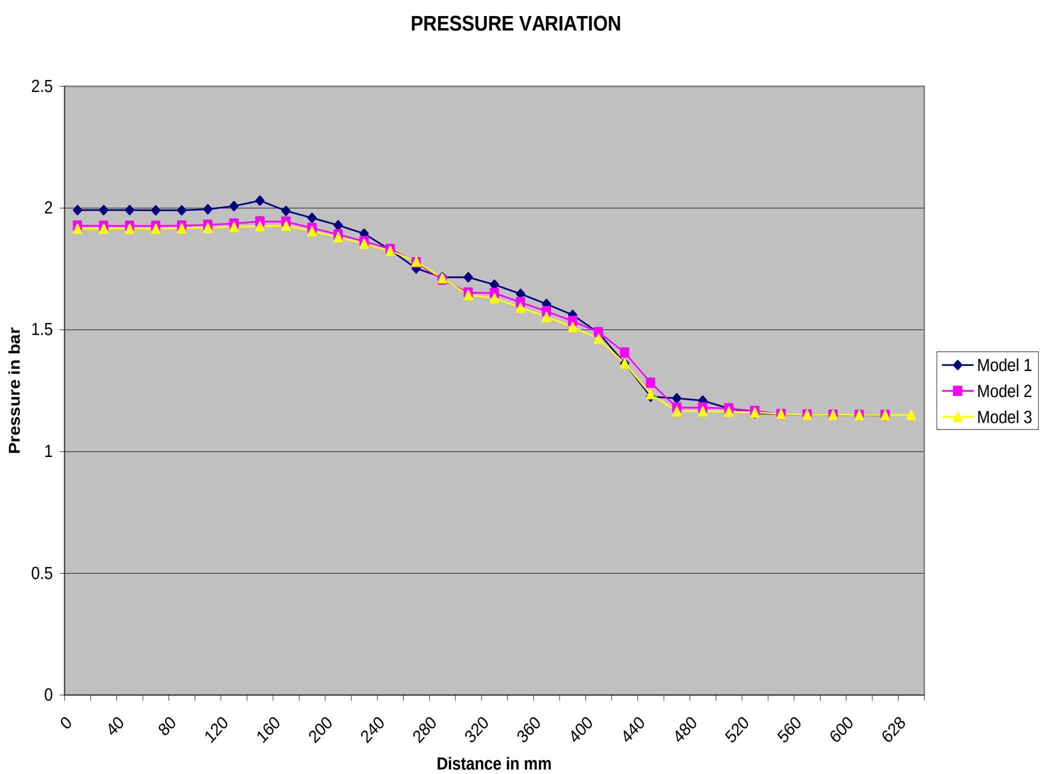


Figure 6 – Pressure Variations (Graphical)

b) Back Pressures In Models 4, 5 & 6

For the same input pressure of 1.142 bar, the outlet pressure is found to be varied as 2.399, 1.975, and 2.148 bars in model 4, 5, and 6 respectively as shown in Figure 7. The model 5 with medium grid size of 1.61 and 1.01 mm combinations offer minimum pressure drop of 0.833 bar.

The Figure 8 clearly indicates that in Model 4 the back pressure is very high in first compartment, and it is low in second compartment, whereas, in Model 6, it is reversed. But in Model 5, the back pressure is found to be less in first compartment. In second compartment, the back pressure is slightly higher but less than that of Model 6, which is due to the wire mesh grid size of 144 cpsi placed in the first and 324 cpsi placed in second compartment. Figure 8

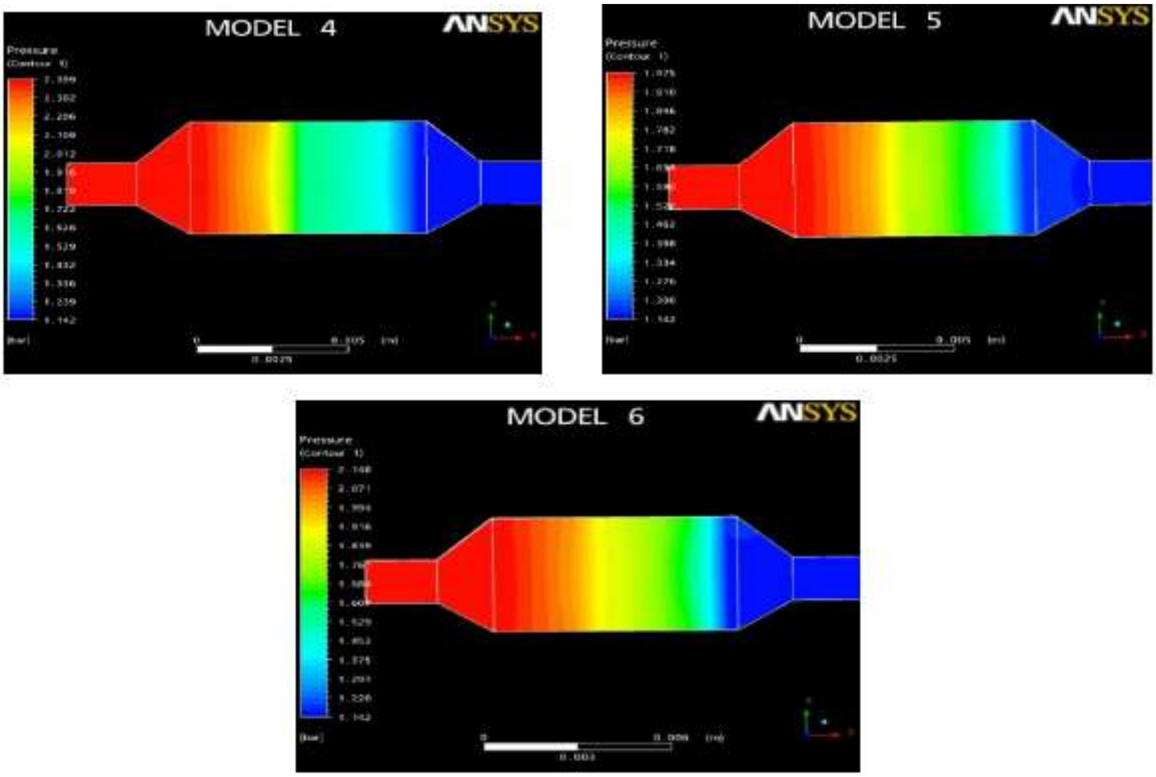


Figure 7 – Pressure Variations

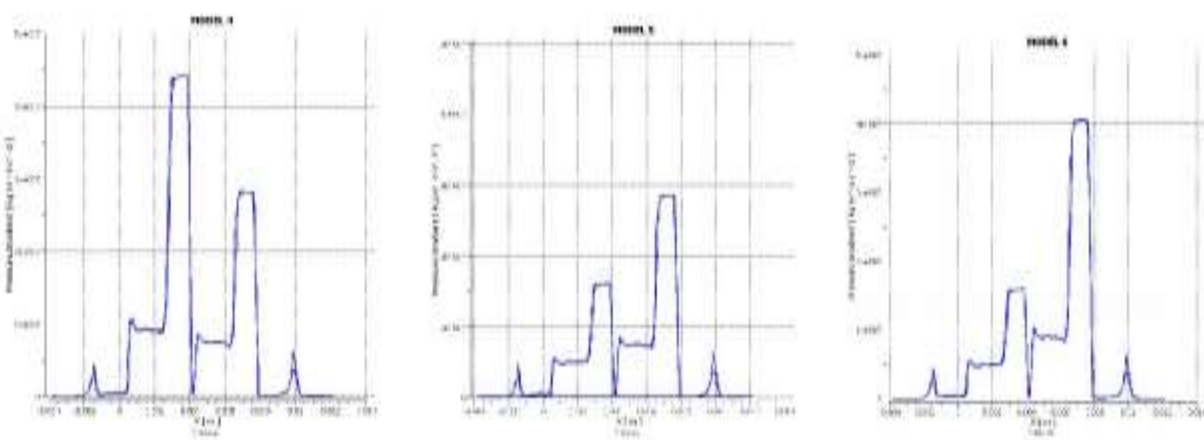


Figure 8 – Pressure Variations (Graphical)

IX. Conclusion

Based upon the work presented in the paper, the following conclusions can be drawn. The special shaped catalytic beads allow the exhaust gas to flow freely without making any obstruction or blocking. Since the partial flow technology is used, it helps to limit the back pressure to the minimum level resulting in better engine performance and fuel saving. The process of regeneration of PM through DOC is continuous. Even if the automatic regeneration is saturated with the collected soot over a period of time, the system will not fail as it happens in wall flow filter, rather all the exhaust gases can flow straight to the other end of the neighboring catalytic bead, similar to flow through substrate. It is estimated that, with the existing volume of catalyst and steel wire meshes, the cleaning may be required for every 10,000 Kilometers of engine run, for efficient fuel consumption. As the catalytic beads are very hard, no wear and tear of catalyst can take place, and hence long life of catalyst is assured. This also ensures no chance of washout catalytic materials coming out along with the exhaust gas adding further pollution to the environment. This after treatment technology for PM reduction is cost effective and robust which needs no interaction with the engine management system and is totally independent.

Abbreviations

CFD – Computerized Fluid Dynamics
NO_X – Oxides of Nitrogen
PM – Particulate Matter
DOC – Diesel Oxidation Catalyst
SCR – Selective Catalytic Reduction
CPSI – Cells Per Square Inch

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