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Geometrical Modelling and Analysis of Automotive Oxidation Catalysis System for Compliance with Environmental Emission Norms

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ABSTRACT

Diesel engines find application in automotive and industrial areas owing to their higher thermal efficiency and longer life. The exhaust emissions from diesel engines pose a serious threat to environment and human health. Combined use of diesel oxidation catalyst filter (DOC), diesel particulate filter (DPF) and selective catalytic reduction (SCR) is found to reduce the exhaust emissions from the diesel engine. A detailed literature survey has been carried out in this paper to determine the current state of art. It was found that the regeneration of soot trapped in the filter is difficult and also it is reducing the life of the filter. Microwave technology has been proposed for conducting active regeneration of the filter without causing any damage to filter substrate. As an initial phase of the work, three dimensional model of DOC has been developed in SOLIDWORKS software. The flow analysis of the designed model is then carried out by importing the model to ANSYS FLUENT 16.2 as an IGS file. Geometric design of the model is validated by the results of simulation, and pressure drop is found to be in the acceptable range.

INTRODUCTION

Exhaust emissions from the diesel engine pose a serious threat to the environment and human health. The combined application of pre-treatment and post-treatment techniques is the only solution to reduce these emissions. Pre-treatment techniques include engine modifications like combustion cylinder alteration, injection timing retard, exhaust gas recirculation, fuel injection strategies and so on (Guan et al. 2016). Blending of diesel will also reduce the particulate matter emissions to a certain extent. Zhang et al. (2016) have conducted a study on the effects of blending of diesel with pentanol and butanol. Post treatment techniques involve the use of diesel oxidation catalysis, diesel particulate filtration and selective catalytic reduction. Diesel oxidation catalysis setup consists of a monolith substrate which has a wash coat impeded with a thin layer of catalyst and the whole setup is encased in a can (Hayes et al. 2012).

DOC is used for oxidation of hydrocarbons, nitrates and soluble organic fraction. It is suitably placed before diesel particulate filter since the oxidation of nitrates can be utilized for passive regeneration of the soot in the particulate filter. Precious metals like platinum, palladium and rhodium are used mostly as a catalyst. Taibani & Kalamkar (2012) performed catalysis in two stages, out of which initial stage involves reduction of nitrate emissions using a rhodium catalyst. The final stage is the reduction of carbon monoxide and unburnt hydrocarbons by oxidizing them over platinum and palladium catalyst. Expensive nature of precious metal catalysts has led to doping of non-noble metals into platinum based catalysts. An impregnation method for preparing a series of platinum-vanadium/cerium-zirconium oxide (Pt-V/Ce-Zr-O) diesel oxidation catalysts with different Pt/V ratios was developed by Huang et al. (2015), and the effect of vanadium on sulphur resistance and catalytic activity was investigated in detail. The results of the tests showed that Pt-V/Ce-Zr-O with only one weight percentage Pt catalyst showed the highest catalyst performance with vanadium loading of one weight percentage. Influence of hydrogen on the oxidation kinetics of exhaust gases was studied by Herreros et al. (2014) and the results showed that smaller concentrations of hydrogen is more effective in promoting NO oxidation as well as improving the catalyst light off temperature.

Oxidation of nitrates in DOC was enhanced by the addition of 250 ppm of hydrogen to the complete DOC feed mixture (Azis et al. 2015). Oxidation of nitrates in DOC is found to be hindered by formation of platinum oxides. Isothermal experiments were conducted by Arvajová et al. (2016) and the results showed that the introduction of carbon monoxide and propane pulses will reduce the formation of platinum oxide. The exhaust gases after oxidation in the DOC will be directed to DPF where the soot particles will get trapped in the porous walls of the filter. The soot particles get accumulated with time and will lead to clogging of the filter. Accumulated soot particles had to be regenerated by suitable methods to restore the flow of exhaust gases through the filter. Active regeneration is carried

Table 1: Specifications of axial and radial flow DOC.

Parameters	Axial DOC	Radial DOC
Monolith material	Cordierite	Cordierite
Geometrical specification of monolith; l×b×h (mm)	250×160×60	250×160×60
Cell density (cpsi)	240	240
Wall thickness (mm)	0.04	0.04
Alumina washcoat (mm)	0.2	0.2
Inlet and outlet diameter (mm)	32	32
Inlet loft length (mm)	50	nil
Outlet left length (mm)	50	50
Radial flow inlet slope	nil	0.5
Initial pore size (mm)	0.8	0.8

out in traditional DPF by injecting the fuel to the filter and allowing it to burn the soot particles. Regeneration by injecting fuel will lead to uncontrolled combustion, reducing the efficiency and also causing damage to filter substrate (Jiaqiang et al. 2016). Alternate methods have to be adopted for regeneration of soot trapped in DPF. A feasibility study on application of microwave energy for regeneration purpose was conducted by Palma et al. (2015) and the results showed that application of microwave energy will reduce energy, time and temperature required for regeneration. Some passive regeneration methods are also adopted for continuous regeneration of DPF so that the time gap between active regenerations can be improved. Oxidation of nitrates in the DOC increases the temperature of exhaust gas and also nitrogen oxide is a good oxidizing agent for soot. Mathematical models are found to be very much effective for analysis purpose (Kurien & Srivastava 2017). Mathematical model for nitrogen oxide assisted regeneration was developed by Jiaqiang et al. (2016) and simulations were carried out which were verified by experiments. The results showed that the regeneration speed will be increased, since there will be an increase in temperature and concentration of nitrogen oxide and oxygen in the exhaust gas. The other method for passive regeneration is the catalytic combustion of soot by using suitable chemicals in the DPF. Pérez & Bueno-López (2015) investigated catalytic combustion of soot under realistic conditions with the help of an experimental setup in which the DPF loaded with platinum active phase and ceria active phase were compared. DPF with copper/zinc oxide catalyst was tested by Corro et al. (2015). Loading of copper was about 5% and there was high catalytic activity due to the presence of copper ions on the surface. Catalysed DPF is found to be very effective even at low temperatures during cold start. Exhaust gases leaving the outlet of DPF will be having a higher amount of nitrates in it. Selective catalytic reduction (SCR) method is used to reduce these nitrates by using ammonia as reducing agent. Ammonia for these reactions is generated by hydrolysis of urea (Qiu et al. 2014).

From the literature, it was evident that it is very much essential to develop a system for exhaust emission control which will meet the environmental standards. The main problems faced with the existing system include higher cost, efficiency reduction due to back pressure in DPF, packaging of system, urea slip in SCR and damage of DPF by uncontrolled combustion during regeneration. A system has been proposed with inference from the literature to develop a functional prototype of the exhaust emission control system which will be a combination of DOC, DPF and SCR. Alternate regeneration method using electromagnetic waves preferably microwaves have been suggested for improving the life of DPF filter and also to avoid clogging of filters leading to backflow. CFD analysis has been very much effective in optimizing the designed systems in a virtual environment so that manufacturing of the optimized design model can be done. As an initial phase of the research, designing and analysis of designed models have been carried out. The present work involves design and simulation of flow through the axial and radial flow DOC filter substrate. SOLIDWORKS 2010 software was used for designing of filters, and simulations for flow analysis were carried out in CFD software ANSYS FLUENT 16.2.

MATERIALS AND METHODS

Design of filters: Design of the DOC has been done in SOLIDWORKS x64 software. Diesel oxidation catalysis setup consists of an inlet loft, outlet loft and a monolith substrate with a thin layer of wash coat in which precious metals are impeded. Monolith substrate will be having a number of filter channels depending upon its cell density. Cell density of the model designed for the present study is 240 cpsi and length of monolith substrate is 250 mm (Lupše et al. 2016). Since DOC does oxidation of exhaust gases, it is essential that there must be a uniform flow of the mixture through all the filter channels and also enough residence time for the reactions to take place without hindering the flow.

Radial flow DOC would provide better uniformity in flow as compared to the axial flow DOC. Designed models for axial and radial DOC are provided in Figs. 1a & 1b. Designing has been done using parametric modelling methodology. The specifications of the designed models are given in Table 1.

CFD analysis: CFD analysis is an effective tool for determining the performance characteristics of designed models prior to the manufacture of a prototype. Three dimensional flow simulations of flow field in a catalytic converter were

Table 2: Properties of axial and radial generated mesh.

Parameters	Axial DOC model	Radial DOC model
Relevance center	Coarse	Coarse
Initial size seed	Active assembly	Active assembly
Smoothing	High	Medium
Transition	Slow	Slow
Span angle center	Fine	fine
Curvature	-	Default (18.0)
Element size	0.001	-
Min size	-	0.0001m
Max face size	-	0.019345m
Max size	-	0.038689m
Growth rate	1.2	1.20
Min edge length	0.00020	0.00020
Inflation	Smooth transition	Smooth transition
Transition ratio	0.272	0.272
Pinch tolerance	Default	0.0009
Defeaturing tolerance	Default	0.0005
Nodes	2087252	3486889
Elements	4072844	5559220

Table 3: Initial and boundary conditions.

Parameters	Value
Type	Pressure based
Time	Steady
Turbulence model	K-omega
Fluid	Exhaust gas
Fluid density	0.5508 kg/cubic meter
Fluid viscosity	0.00003814 Pascal. second
Fluid temperature	520 degree C
Inlet	Mass flow inlet
Mass flow rate at inlet	320 kg/hour
Pressure at inlet	220 milli bar
Outlet	Pressure outlet
Surface	Wall
Interior solid	Interior
Ratio of specific heats	1.4
Solution method scheme	Simple
Under Relaxation Factor (pressure)	0.3
URF Turbulent viscosity	0.7
URF Turbulent kinetic energy	0.8
Absolute criteria	0.001

performed by Fornarelli et al. (2015), where the results showed that there is non-uniform flow in the monolith inlet due to sudden expansion creating an annual recirculation zone which would lead to performance downgrade of the converter. Simulations in this work were carried out in ANSYS creating a virtual environment of real application by providing mathematical equations with boundary conditions. Models designed in SOLIDWORKS were imported to ANSYS workbench as an IGS file for analysis purpose.

Geometries are cut in their symmetrical axis for reducing computation time. Axial flow model is symmetrical in both x and z plane. So a quarter of the model was generated by using the symmetry tool. Mesh is generated in the model for analysis. The details of the mesh in axial model are given in Table 2 and meshed model is shown in Fig. 2. Radial flow model is symmetrical in x plane alone since it has radial inlet and axial outlet. Half section of the geometry is generated by symmetry tool and unstructured mesh is generated as shown in Figs. 2a & 2b.

RESULTS AND DISCUSSION

Calculations were carried out for both axial and radial flow DOC filters after initializing all the initial and boundary conditions. Computations were started from inlet of the DOC.

Axial flow DOC filter: Pressure contours and velocity contours were generated after the completion of the simulation calculation in the software. Contours of pressure coefficient, total pressure and axial velocity are shown in Figs. 3-5. Contours showed that there is continuous flow of the fluid through the filter even though there is some pressure loss leading to reversed flow in some faces at the edges due to formation of eddies. Plots of axial velocity and pressure coefficient in x direction are shown in Figs. 6 and 7.

Radial flow DOC filter: Contours of pressure and velocity generated after the completion of simulation calculation are shown in Figs. 8-10. Similar to the case of axial flow DOC there was reverse flow in the edges owing to the formation of eddies. Radial flow DOC has an inlet loft of decreasing area which will increase the flow velocity and reduce chances of pressure drop which would lead to reverse flow. Reverse flow in radial flow DOC is less as compared to axial flow DOC and also the flow is more uniform and distributed. Plots of radial velocity and pressure coefficients in x direction are shown in Figs. 11 and 12. In radial flow DOC filters, the direction of the flow changes inside the DOC from axial to radial increasing the conversion efficiency of the filter.

Analysis of contours: The comparison of contours generated from simulation of axial and radial flow DOC indicates that the flow is more uniform in the case of radial flow DOC as compared to axial flow DOC. Radial flow filter has inlet in radial direction with decreasing area of 0.5 slopes, which reduces the chances of pressure drop and also the chances for reversed flow will be reduced. While in axial flow DOC, there is a sudden enlargement in the area which leads to pressure drop and reduction in velocity. Reversed flow in the edges can be eliminated by changing the shape of the filter from rectangular to cylindrical.

CONCLUSION

CFD analysis of the designed models was carried out and the results were analysed. The contours of flow in the mod-

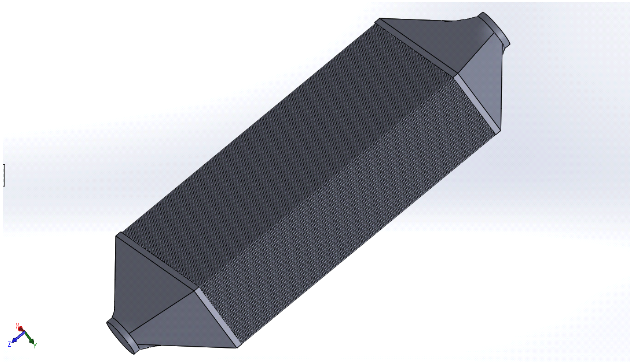

Fig. 1a: Axial flow DOC model.

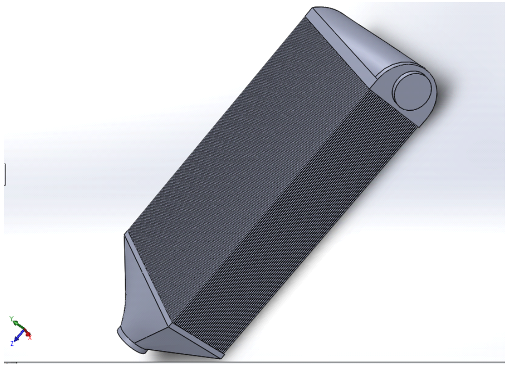

Fig. 1b: Radial flow DOC model.

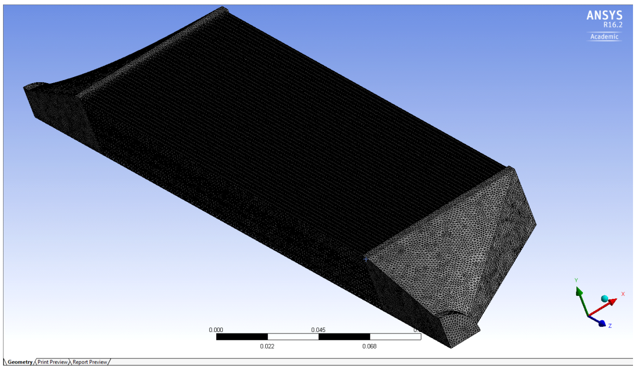

Fig. 2a: Meshed axial flow DOC model.

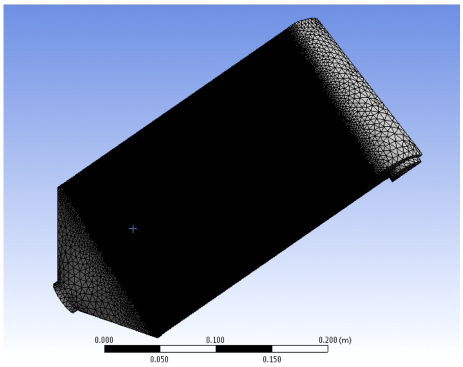

Fig. 2b: Meshed axial flow DOC model.

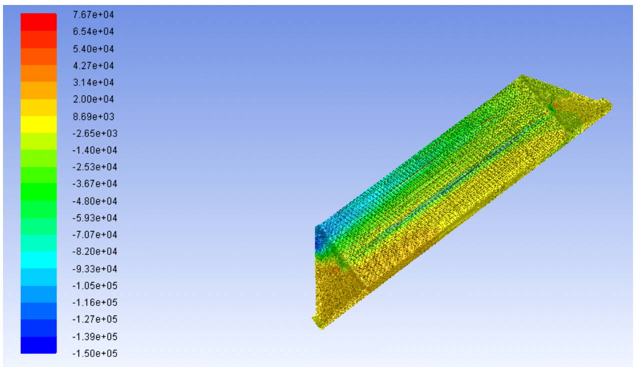

Fig. 3: Contour of pressure coefficient for axial flow DO.

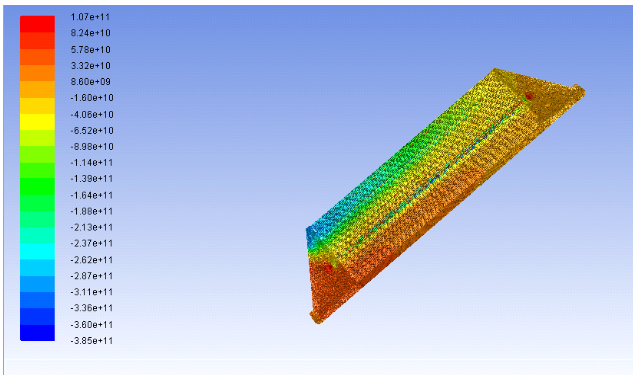

Fig. 4: Contour of total pressure for axial flow DOC.

els showed that there is continuous flow inside the filter. Pressure drop in both the cases was well within limits. In axial flow DOC, there was reversed flow in the edges due to sudden expansion of loft leading to pressure drop. Radial flow DOC had a uniform flow contour compared to axial flow DOC. It will also provide much better residence time for the reactions to take place. Rectangular filters were designed for better packaging of the components in exhaust systems since it is also an issue in the case of light commercial vehicles. These developed models can be simulated for chemical analysis and heat treatment for much better results. Future scope of this work includes chemical analysis of the designed models and design and simulation of DPF by taking outlet conditions of DOC as its inlet conditions. Also, since reversed flow was observed in this analysis, cylindrical shaped DOC filters are suggested in place of rectangular filters. Manufacturing and fabrication of the proposed system is initialized with reference to the results ob-

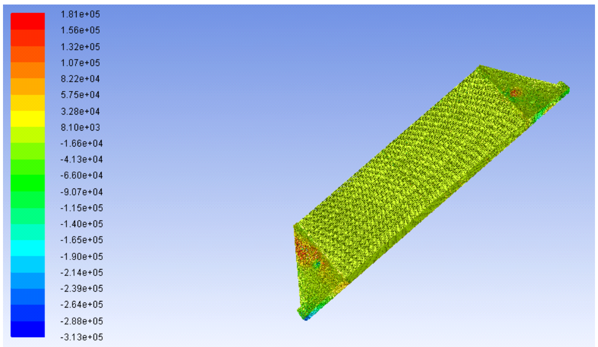

Fig. 5: Contour of axial velocity for axial flow DOC.

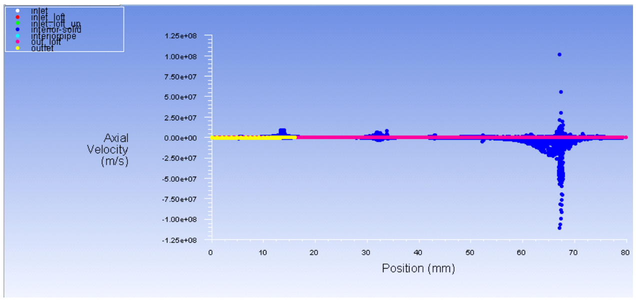

Fig. 6: Plot of axial velocity for axial flow DOC.

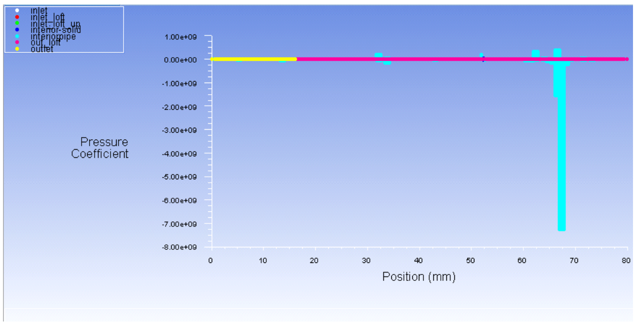

Fig. 7: Plot of pressure coefficient for axial flow DOC.

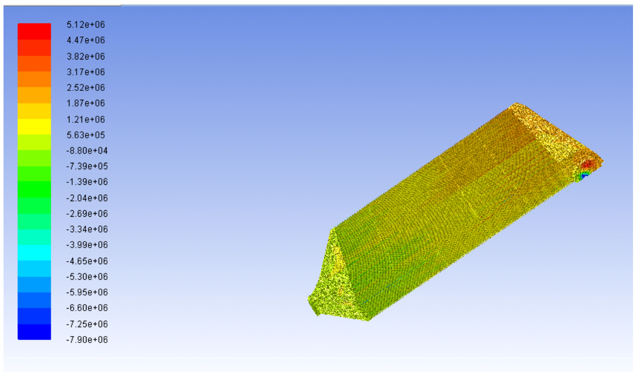

Fig. 8: Contour of total pressure for radial flow DOC.

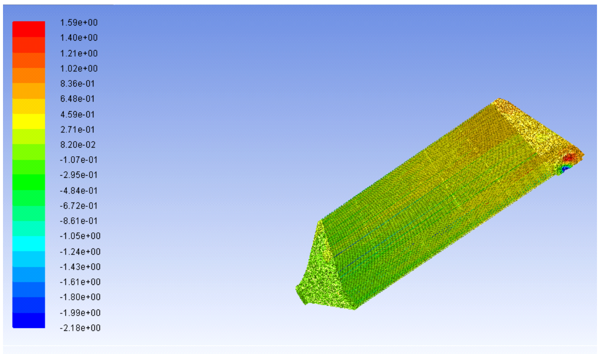

Fig. 9: Contour of pressure coefficient for radial flow DOC.

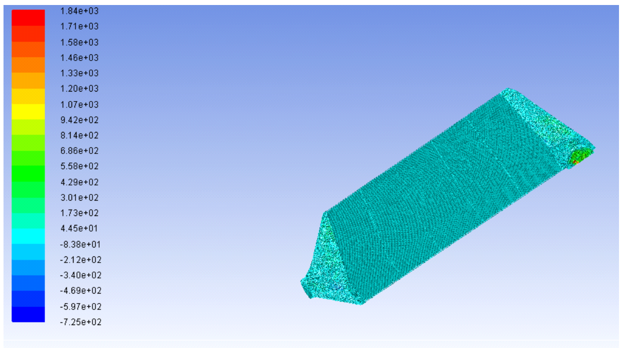

Fig. 10: Contour of radial velocity for radial flow DOC.

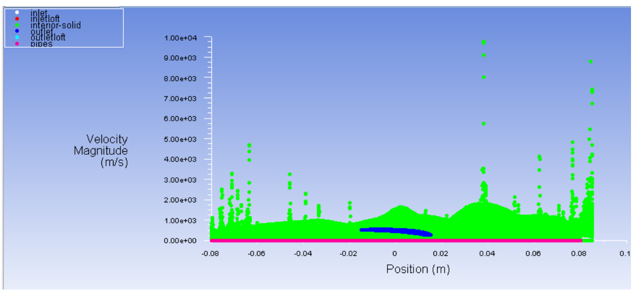

Fig. 11: Plot of radial velocity for radial flow DOC.

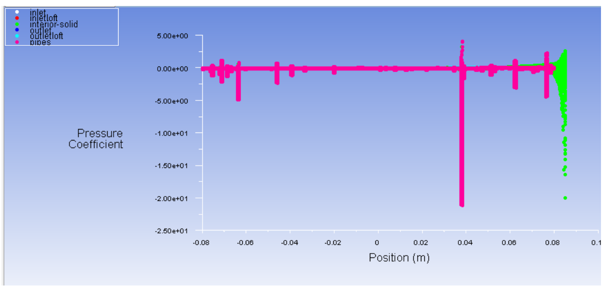

Fig. 12: Plot of pressure coefficent for radial flow DOC.

tained from this work. Electromagnetic waves (preferably microwaves) have been proposed to be used for regeneration of soot particles in the DPF to avoid damage to the filter due to uncontrolled combustion of injected fuel and also to improve efficiency.

The main challenges for implementing emission norms are faced by the automobile companies and the oil marketing companies. Automobile companies have to design changes in vehicles and oil marketing companies have to upgrade the fuel quality. Vehicles have to be fitted with exhaust control devices (DOC, DPF and SCR) and also the new designs must cope up with the Indian driving roads and ambient conditions. This research aims to develop a functional prototype which can be fitted to automobiles so that their emission can be controlled to meet EURO VI emission norms.

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