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Advancement in the Design of Automotive Catalytic Filter for Meeting Environmental Emission Norms

Caneon Kurien and Ajay Kumar Srivastava
Department of Mechanical Engineering, University of Petroleum & Energy Studies, Dehradun 248007, India

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ABSTRACT

Diesel engines used in automobiles and other industrial applications are found to be responsible for the emission of particulate matter and other toxic gases. The particulate matter is also carcinogenic in nature posing a serious threat to human life. Recent researches have shown that combined application of Diesel Oxidation Catalyst (DOC) filter, Diesel Particulate Filter (DPF) and Selective Catalytic Reduction (SCR) can reduce these emissions to a certain extent. In this paper, a detailed literature survey has been carried out in this area and it was found that the development of an effective regeneration procedure is one of the major challenges in the emission control using these devices. Composite regeneration technique using electromagnetic waves in the microwave region and fuel additives have been proposed in this paper. As an initial phase of the project, the analysis of the design aspects of the DOC filter has been carried out. Uniformity of catalyst coating in the monolith substrate is determined using metallurgical microscope. Models with different lofts have been designed in SOLIDWORK 2014 x 64 and its flow analysis is carried out in ANSYS FLUENT 16.2. The results of simulation showed that model with loft angle of 62 degree has the lowest pressure drop. Fabrication of system has been carried out based on simulation results.

INTRODUCTION

Diesel engines have become an integral part of the automotive industry as well as other industries because of their higher thermal efficiency and longer life compared to gasoline engines. But the exhaust emission from these engines is found to be toxic in nature, contributing a major part in environmental pollution. The exhaust emission from diesel engine includes carbon monoxide, nitrates, hydrocarbons and particulate matter. Particulate matter consists of soluble organic fraction and soot particles. Soot particles released from diesel engines are found to be carcinogenic in nature, creating a threat to human life. These emissions can be reduced by two techniques, namely pre-treatment and post-treatment. Engine modifications like exhaust gas recirculation, combustion cylinder alteration, fuel injection strategies and blending of fuels will come under pre-treatment techniques. Pre-treatment techniques are employed to reduce the generation of the toxic gases from the combustion inside engine. Post treatment techniques are used to treat the exhaust gases released from the engine by the use of systems for diesel oxidation catalysis, diesel particulate filtration and selective catalytic reduction. Tuler et al. (2016) is working currently with an objective to develop a simple emission control system which consists of a ceramic filter impregnated with combustion catalyst and a nitrogen oxide trap so that the reactions between nitrogen oxide and particles occurs, eliminating both the contaminants simultaneously. Combination of fuel injection strategies and DOC is found to remove the particulate matter emissions, both in nucleation mode and accumulation mode up to a certain extent with reference to the experiments performed by Guan et al. (2015). Diesel oxidation catalysis is done with the help of DOC filter, which has a monolith substrate with an alumina coating in which precious metal catalysts are impeded. Platinum, palladium and rhodium are mostly used as catalysts in these filters.

The expensive nature of these precious metals has made researchers to look for an effective replacement for these catalysts to meet the cost constraints. Wong et al. (2016) studied the effectiveness of a bimetallic catalyst which is a combination of platinum and palladium. Aging also has a significant effect on the performance of the catalyst since there will be loss of metal sites with aging. Platinum under oxidizing conditions will sinter to form large particles. The studies of Xiong et al. (2016) revealed that the sintering of platinum can be avoided by forming an alloy of platinum and palladium. The platinum species are allowed to diffuse on the surface of palladium oxide particles to form the required alloy of platinum and palladium. Vanadium has the ability to replace the platinum by an appropriate amount which will increase the catalytic activity and sulphur resistance of the catalysts. Huang et al. (2014) tested the catalytic performance of platinum vanadium / cerium zirconium oxide catalyst and the results showed that 1 weight percentage of the vanadium added to the platinum has the best catalytic performance and it also improved the dispersion of platinum. But excessive amount of vanadium will result in sulphur poisoning of platinum since it covers the active platinum sites. There are also chances for formation of platinum oxide in the DOC filter. Azis et al. (2015) proposed supplementation of hydrogen to reduce the formation of platinum oxide at low temperatures whereas in higher temperatures it was not applicable. Hydrogen supplementation also provided an increase in the yield of nitrogen dioxide. Arvajova et al. (2016) studied the impact of the carbon dioxide and propene pulses on the formation of platinum oxide and it was found that platinum oxide formation is reduced by introduction of these gases under lean conditions. The carbon monoxide and propene pulses were found to be most effective in the range of their light off temperature for oxidation. Herreros et al. (2013) found that introducing smaller concentrations of hydrogen to the exhaust gas prior to the DOC can improve the catalyst light off temperature as well as oxidation of nitrogen oxide.

The nitrogen dioxide formed in the DOC increases the oxidation rate of the soot deposited in the particulate filter. This is the main advantage of placing the DOC before particulate filter so that the active regeneration of the accumulated soot will be done simultaneously. Jiaqiang et al. (2016a) developed a mathematical model for nitrogen dioxide assisted continuous active regeneration and verified it using simulations and experiments. The results showed that parameters like length of the filter, thickness and diameter of the channel wall has a tremendous effect on the nitrogen dioxide assisted continuous active regeneration. The results of the experiments conducted by Jiaqiang et al. (2016b) showed that the pressure drop in the diesel particulate filter during the continuous regeneration is dependent on various parameters like exhaust temperature, exhaust gas flow rate, oxygen concentration in the exhaust gas. In commercial diesel particulate filter, active regeneration of the accumulated soot particles is carried out by introducing fuel to the filter and then igniting it, which leads to uncontrolled combustion and also severe damage to the filters. Passive regeneration is required for complete regeneration of the accumulated soot particles since it is not achieved completely by active regeneration. Palma et al. (2015) studied the effectiveness of the regeneration by using microwave radiations. It was found to be effective and he suggested the combined use of catalyst and microwave regeneration system for improved performance of the system. Platinum can be used as a catalyst for improving the oxidation of accumulated soot, but still the expensive nature of platinum catalyst lead researchers to look for alternative catalysts to meet this application. Perez et al. (2015) developed an experimental setup to compare the performance of the diesel particulate filter (DPF) loaded with platinum active phase and ceria based active phase. Both the cases showed same performance until the level of soot loading was 0.6. The platinum phase exhibited better performance for higher soot loading composite materials, also find their application as a catalyst in the diesel particulate filter. Catalytic performance of hydrogen loaded zinc oxide was tested by Grisel Corro et al. (2014) and the results showed that the composite catalysts have the ability to oxidize the particulate matter at low temperatures.

The main objective of our work is to develop a functional prototype of intuitive emission control system, which is a combination of diesel oxidation catalyst filter, diesel particulate filter with composite regeneration and selective catalytic reduction. Composite regeneration of accumulated soot is proposed to be conducted with the help of electromagnetic waves in the microwave region and fuel additives to act as catalyst to improve oxidation of accumulated soot. CFD simulations have become more popular for analysis prior to the manufacturing of product, because it can save a lot of time and also the cost for developing the product will be reduced since the optimized model in the simulation will be only manufactured. Arthanareeswaren et al. (2015) conducted a CFD study to optimize the geometric design of the catalytic converter by modelling the substrate as a porous medium. Pressure drop and uniformity index of muffler, under body catalytic converter and close couple catalytic converter was calculated and required changes in the design were suggested after analysis. In the present work, detailed analysis of the ceramic monolith substrate for diesel oxidation catalysis is done to determine the uniformity of the catalyst coating on the substrate. Different models of the DOC filter have been designed in SOLIDWORKS and its flow analysis is carried out using CFD software ANSYS FLUENT.

MATERIALS AND METHODS

Analysis of monolith substrate: Simulation of rectangular shaped monolith substrate was carried out in our previous work where the conclusion was derived that the circular shaped substrates are more efficient on account of the reversed flow at the edges. The ceramic monolith substrate used in this work is shown in Fig. 1 and its details are provided in Table 1. Catalyst loading in the filter has to be checked for uniformity since it has an effect on the reactions taking place inside the substrate. Inverted metallurgical microscope has been used here for capturing the uniformity of the catalyst loading in the filter substrate. Random checking for the same was done and it has been found that variation in the uniformity of the catalyst layer is in the

Fig. 1: Monolith substrate placed in inverted metallurgical microscope.

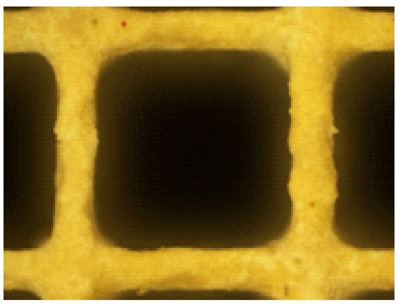

Fig. 2: Microscopic view of filter substrate (5x).

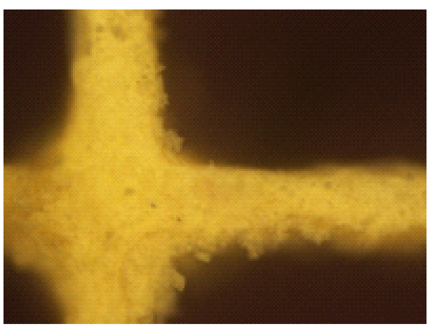

Fig.3: Microscopic view of filter substrate (10x).

acceptable range. The images captured by using the metallurgical microscope are shown in Figs. 2 and 3.

Design of lofted inlet and outlet of DOC: Design of the lofted inlet and outlet for the monolith substrate has been done in SOLIDWORKS X64. The angle of loft is an important parameter deciding the pressure drop and also the flow uniformity of the gases into the cylinder. Nine models with different loft angles have been made using solid works. Details of these models are given in Table 2.

CFD analysis: Computational fluid dynamics analysis is carried out to determine the characteristics of a model in a virtual environment before manufacturing the prototype. The time consumed for experiments and also its developing

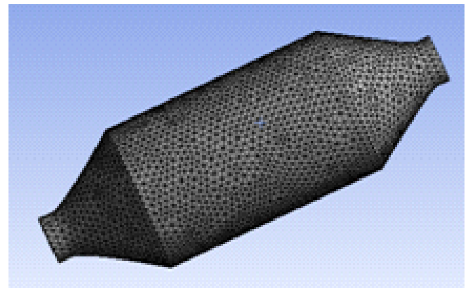

Fig. 4: Meshed model.

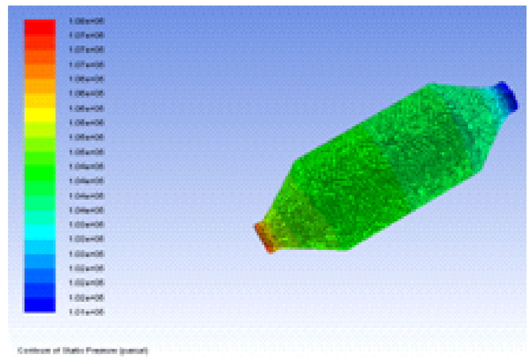

Fig. 5: Contour of static pressure.

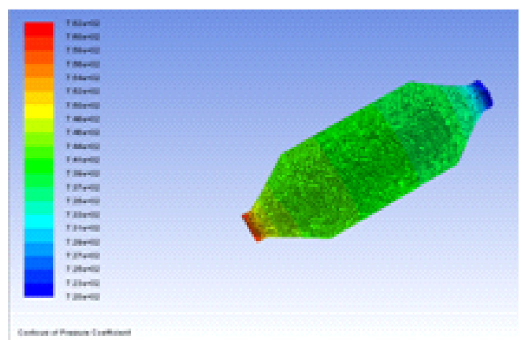

Fig. 6: Contour of pressure coefficient.

cost can be reduced by using CFD analysis. Taibani et al. (2012) conducted CFD simulations to analyse the performance of catalytic converter, where the species concentrations before and after the catalytic converter were measured. The results of the simulation showed that radial flow catalytic converter has better performance as compared to axial flow catalytic converter owing to higher residence time. Here, we have used CFD analysis to determine the pressure drop and flow uniformity of the exhaust gases through the filter for different loft angles. Models designed in SOLIDWORKS are imported to ANSYS workbench as an IGES file. Monolith substrate is considered as a porous medium and it is also considered to be impermeable in other directions. Inlet and outlet sections of the model will have turbulent flow while the substrate will be having laminar flow. Structured mesh is generated in the model with fine relevanceas shown in Fig. 4. Meshed model is then imported to ANSYS FLUENT for carrying out simulation. The model is scaled in millimetre and the quality of the mesh is also checked. Minimum orthogonal quality and maximum ortho skew of the mesh in all models were found to be in acceptable region. Pressure based type solver with absolute velocity formulation was used for analysis and time is considered as steady. K-epsilon turbulence model is used where the first variable is the turbulent kinetic energy and the second variable is the dissipation rate of kinetic energy. This model is commonly used for flows with small pressure gradients and also in cases where Reynold stresses are important. Fluid flowing through the filter is assumed to be exhaust gas by providing its density and viscosity. The ceramic substrate is considered as the porous zone with laminar flow by providing the viscous resistance and inertial resistance in three directions. The inlet is assumed as velocity inlet and outlet as pressure outlet. The details of the initial and boundary conditions are given in Table 3.

Table 1: Specifications of monolith substrate.

Material	Ceramic
Cell density	300 cpsi
Catalyst	Pt:Pd (1:1)
Catalyst Loading	20 g/cubic cm
Size	100 mm diameter*152.40 mm

Table 2: Specifications of designed models.

Model No	Length (mm)	Loft angle (degree)	Taper Length (mm)
1	45	66	110
2	50	63	112
3	55	61	114
4	60	59	117
5	65	57	119
6	70	55	122
7	75	53	125
8	80	51	128
9	85	49	131

Table 3: Initial and boundary conditions.

Type	Pressure based
Time	Steady
Velocity formulation	Absolute
Model	K-epsilon
Fluid	Exhaust gas
Fluid density	0.5508 kg/cubic meter
Fluid viscosity	0.00003814 Pascal second
Substrate	Porous zone
Viscous resistance	Direction 1: 3.846e+07 (m^{-2})
	Direction 2: 3.846e+10 (m^{-2})
	Direction 3: 3.846e+10 (m^{-2})
Inlet	Velocity inlet
Inlet velocity	22.6 m/s
Outlet	Pressure outlet
Outlet pressure	101325 pa
Surface	wall

RESULTS AND DISCUSSION

Calculations were carried out for different models of the diesel oxidation catalyst filter and the simulation started from the inlet of the DOC which provided initial and boundary conditions.

Pressure drop across DOC: The exhaust gases from the engine are directed to the inlet of the DOC filter and there will be a drop in its pressure due to lofted inlet and also due to the flow through the monolith porous substrate. The filter with lowest pressure drop is considered to be most suitable for this application since these gases will be directed for further treatment to diesel particulate filter (DPF). The calculations were carried out for each model with different lofts until the results are converged. Contours of the pressure coefficients and static pressure have been generated using the results obtained from ANSYS FLUENT as shown in Figs. 5 and 6. From the contours, it can be seen that there is a substantial fall in the pressure as the gas flows from inlet to outlet. The pressure in the inlet side is at higher end as indicated by red colour and at the outlet side is at lower end as indicated by blue colour. The values of the pressure at the inlet, interior solid and the outlet are derived from the report generated after the simulation. A graph is plotted to determine the variation in the static pressure and pressure coefficient with different models as shown in Figs. 7 and 8. The pressure drop in each case is then calculated using the obtained results and a graph has been plotted between the length of loft and difference in pressure at the inlet and outlet of the DOC as shown in Fig. 9.

From Fig. 9, it can be seen that the pressure drop increases from 5400 pascal to 6000 pascal when the loft length increases from 45 mm to 50 mm. Then there is a sudden reduction in pressure drop when the loft length is about 55 mm. From this point the pressure drop is found to increase as the loft length increases up to 75 mm and then there is a sudden drop and rise when the loft length is increased to 80 mm and 85 mm. From the results, it can be seen that the loft length of 55 mm with a loft angle of 61 degree is found to be more suitable for the fabrication of the DOC since it has the lowest pressure drop and also due to its stability in the manufacturing point of view. Even though the model with loft

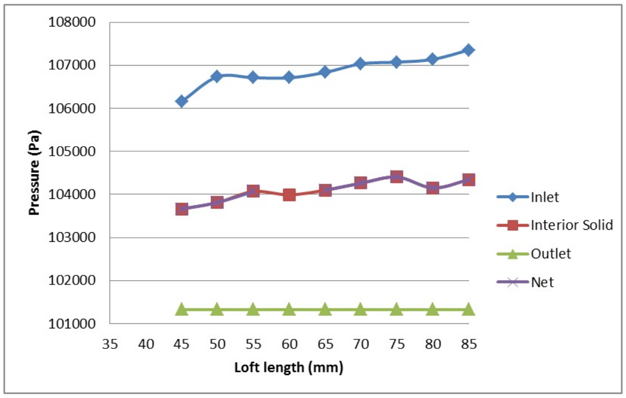

Fig. 7. Effect of the loft length on the static pressure.

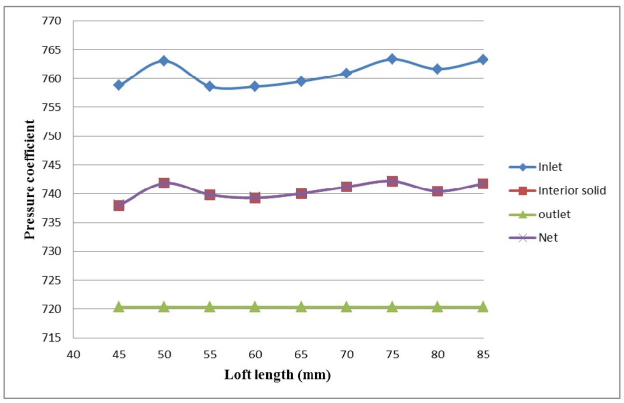

Fig. 8: Effect of loft length on pressure coefficient.

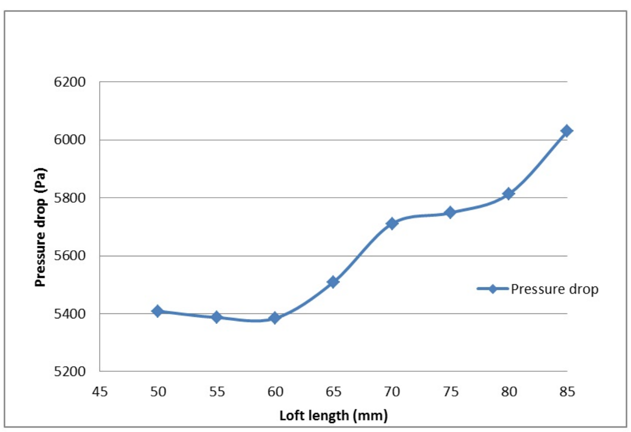

Fig. 9: Variation in pressure drop with loft length.

length of 45 mm has lowest pressure drop, the structural stability of the model is very low.

Flow uniformity index: Level of uniformity or how uniform is the flow through the model is determined by the uniformity index. Model with more uniform flow is consid-

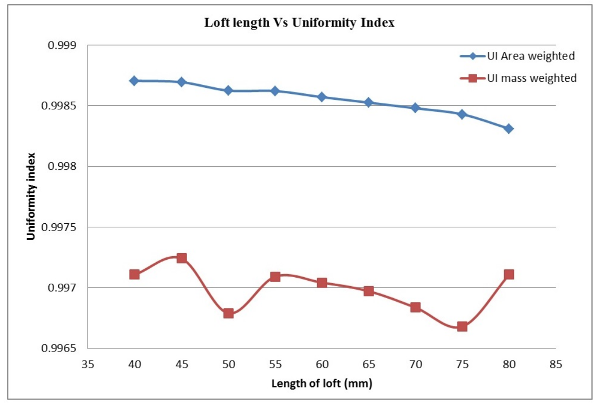

Fig. 10: Variation in uniformity index with loft length.

Fig. 11: Fabricated DOC with inlet and outlet lofts.

ered to be more suitable for this application. The uniformity index for all the models is derived after simulation and a graph is drawn as shown in Fig. 10 to study the variation in the uniformity index as the loft length of the model increases. From the plots, it can be seen that the area weighted uniformity index decreases as the loft length increases and the mass weighted uniformity index also shows a similar pattern as an average. The changes in the uniformity index are very low and it can be neglected.

Analysis of the simulation results: The results of the simulation are plotted and from the Fig. 9, it is evident that the lowest pressure drop is achieved in the third case where the loft length is 55 mm. Therefore it can be suggested to fabricate the DOC filter with a loft length of 55 mm for flow with low pressure drop. The uniformity index of the model with the loft length of 55 mm is also in the acceptable range from Fig. 10 and the lofts have been fabricated with observed results as shown in Fig. 11.

CONCLUSION

The monolith substrate for the fabrication of DOC filter has been studied using a metallurgical microscope. The uniformity of the catalyst coating in the filter substrate is observed under the microscope and it was found that the coating is uniform with small amount of variations which can be neglected. The inlet and outlet loft has to be designed for the monolith substrate. The length of the loft and the loft angle is an important parameter which decides the flow through the substrate. Inlet loft has to be designed in such a way that the pressure drop occurring in the flow due to its effect must be as low as possible. For determining the loft length with lowest pressure drop, CFD simulations have been carried out for different models of the diesel oxidation catalyst filter designed in SOLIDWORKS. Calculations were carried out in ANSYS FLUENT by importing the model as an IGES file. The exhaust gas is considered as the fluid flowing through the filter and the turbulence model as k-epsilon. The results of simulation showed that the pressure drop is lowest in the case of the model with a loft length of 55 mm and loft angle of 61 degree. Fabrication of the emission control system has been initiated and the results of the simulation are considered for the fabrication of the diesel oxidation catalyst filter. The use of the diesel engines for automotive and other industry applications has increased tremendously in the past decades. The increasing rate of automobiles has also increased the emission of toxic gases which in turn has a negative impact on environment. Researches are going on in most of the developing countries for implementing EURO VI emission norms. The oil companies and automobile companies are facing the challenge to develop a system which is economically feasible to meet this challenge of environmental pollution. DPF system has been used in European countries to meet these norms, but the main problem faced is the failure to regenerate the accumulated soot particles leading to clogging of filter which reduces the efficiency of engine. The main aim of our research work is to develop a functional prototype of an emission control system which uses electromagnetic waves and fuel additives for the composite regeneration of the accumulated soot particles.

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