Kurien et al. 2019. *Int. J. Vehicle Structures & Systems*, 11(1), 83-87
ISSN: 0975-3060 (Print), 0975-3540 (Online)
doi: 10.4273/ijvss.11.1.16

International Journal of
Vehicle Structures & Systems
Available online at www.maftree.org/eja

Geometric Design Validation of Oxidation Catalysis System in Composite Regeneration Emission Control System

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ABSTRACT:

Development of emission control systems for reducing the toxicity levels of exhaust emissions is one of the major challenges faced by automotive industry which rely on diesel engines owing to its thermal efficiency and service life. The major challenge faced for implementation of emission control system is the periodic regeneration of channels in diesel particulate filter to avoid clogging and backpressure rise inside the substrate. Commercial fuel based regeneration is leading to uncontrolled combustion inside the filter substrate affecting its service life. State of art of the emission control system has been detailed by conducting literature survey on the area and it has been found that these systems have a vital role in reducing emission levels to meet emission norms. Microwave based active regeneration has been proposed in this paper to improve the service life and effectiveness of diesel particulate filter. Three dimensional models of the axial flow, radial flow and cylindrical oxidation catalysis system are developed using Computer Aided Design software and flow analysis has been conducted using Computational Fluid Dynamics software (ANSYS FLUENT). Validation of the geometric design is done using simulation results and the pressure drop across the system is found to be in acceptable range.

KEYWORDS:

Computational fluid dynamics; Catalyst; Design; Emissions; Filtration; Particulate

CITATION:

C. Kurien, A.K. Srivastava and D. Kumar. 2019. Geometric Design Validation of Oxidation Catalysis System in Composite Regeneration Emission Control System, *Int. J. Vehicle Structures & Systems*, 11(1), 83-87. doi:10.4273/ijvss.11.1.16.

1. Introduction

Automotive vehicles are considered to be the major source contributing to the increasing levels of air pollution in major cities [1]. The carcinogenic nature of soot particles released by fossil fuel powered diesel engines has made it a serious threat to human life [2]. Development of emission control system has become a basic requirement for reducing the pollution levels and improving the sustainability of diesel engines [3]. Emission control systems are classified into pre-treatment and after treatments systems based on its application and working principle [4]. Pre-treatments systems include application of alternate fuels, engine modifications and optimization of various engine parameters. After-treatments systems have a higher impact on emission reduction and commonly applied emission control system consists of Oxidation Catalyst filter (DOC), Particulate Filter (DPF) and Nitrate trap [5]. Oxidation catalysis system consists of a substrate with honeycomb structure or square channels with a layer of alumina washout in which precious metal catalysts are impeded [6].

Precious metal catalysts like platinum, palladium and rhodium help in speeding up the oxidation of nitrates, hydrocarbons and organic fraction in the exhaust gas stream. Palladium is added to the catalyst layer along with platinum to avoid the coalescence of platinum by heating effect [7]. The heat rejected during the reactions can be utilized for continuous passive regeneration of accumulated soot particles in the channels of particulate filter [8]. Two stage catalysis setup developed in the early research works were found to be efficient where the reduction of nitrates over rhodium is the first stage and reduction of carbon monoxide and hydrocarbons over platinum and palladium is the final stage [9]. To reduce overall cost of the system, the precious metal catalyst is doped with non-noble metals [10]. The catalytic activity and sulphur resistance of platinum catalyst doped with vanadium in different ratios were tested in [11], where the highest performance was observed in the sample with vanadium loading of one weight percentage.

Supply of hydrogen in low concentration like 250ppm is found to have an influence on the catalytic activity by promoting the oxidation of nitrogen oxides [12]. The fouling of platinum catalyst by formation of platinum oxides can be reduced by introduction of carbon monoxide and propane to the exhaust flow [13]. A methodology for investigating the catalyst light off characteristics and carbon monoxide inhibition effect of the catalyst was developed by [6] in which the hysteresis of light off and light down was experimentally verified. The treated exhaust gases from the outlet side of the oxidation catalysis system are directed to the inlet of particulate filtration system where the soot particles get blocked in the channels of filter substrate [14]. Particulate filter works by depth filtration technique in which the soot particles are filtered by porous wall between adjacent filter channels as shown in Fig. 1.

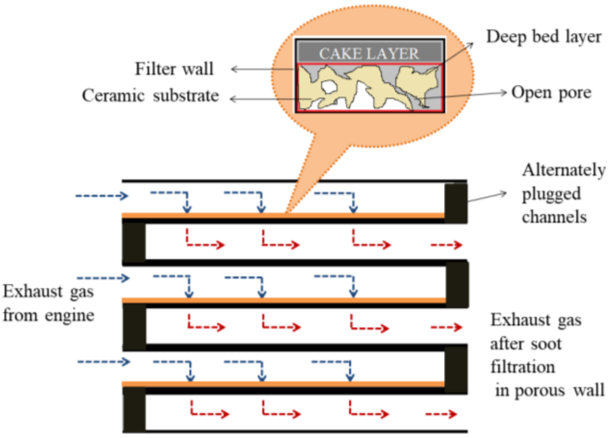

Fig. 1: Particulate filtration by depth filtration

As the thickness of soot particle layer in the filter channels starts increasing, the soot layer itself will act as a medium for filtering the soot particles leading to cake filtration which causes a rise in pressure drop across filter substrate resulting in backflow [15]. Hence periodic regeneration of the filter channels is a basic requisite for effective working of the emission control system. Commercially available method for regeneration involves injection of fuel which has self-ignition temperature in the same range as that of the exhaust gas. But it has been found that it is difficult to control the combustion of fuel during fuel based regeneration which will damage the filter substrate far before its service life period [16]. Regeneration of the clogged filter substrate without causing any damage to the filter is one of the major challenges faced by automotive industry. Results of previous studies on development of alternate regeneration technique using electric heaters, electrostatic precipitators, plasma discharge etc. showed that each technique is having an impact on the substrate material affecting its service life.

Electromagnetic radiations in microwave region is identified to be an effective alternate regeneration technique since it can penetrate through the filter substrate and burn the soot particles by selective burning of accumulated soot particles [17]. Passive regeneration of the particulate filter can be achieved by utilising the heat rejected during oxidation reactions taking place in the oxidation catalysis system. Passive regeneration can be enhanced by coating the filter channels with suitable catalysts like platinum and ceria in active phase [18]. Filter channels with 5% copper catalyst loaded with zinc oxide showed good catalytic performance due to the presence of copper ions in the surface even during cold start [19]. The nitrates present in the exhaust stream after treatment in the oxidation catalysis and particulate filtration system is removed by using reducing agent in the selective catalytic reduction system. Ammonia is mostly used as reducing agent which is generated by hydrolysis of urea [20].

Emission control system consisting of oxidation catalysis system, particulate filtration system and selective catalytic reduction system will be the best possible solution for meeting the stringent emission norms [21]. Regeneration of the accumulated soot in the filter channels has to be conducted by suitable alternate techniques other that commercial fuel based regeneration [22]. Electromagnetic waves in microwave region are considered to be an ideal alternate regeneration technique owing to the dielectric properties of ceramic substrate. Emission control system consisting of particulate filtration system with microwave assisted regeneration has been proposed in this paper. As an initial phase of the work, three dimensional models of the oxidation catalysis and particulate filtration substrate has been developed and geometrical validation of the same is conducted using computational fluid dynamics (CFD) software. CFD simulation is a proven tool for conducting the analysis of the designed models prior to the fabrication and also to reduce the number of experimental run [23].

Comparative analysis on the exhaust gas flow through axial and radial flow oxidation filtration system is conducted and results showed the presence of backflow near the sharp edges of the filter system. Based on the simulation results, cylindrical filter substrates are developed and flow analysis is conducted. The simulation results showed that cylindrical filter substrate has better flow properties compared to that of the axial and radial system with rectangular cross section. Models are developed using SOLIDWORKS 2010 software and the flow analysis is conducted using CFD software ANSYS FLUENT 16.2.

2. Modelling and analysis of system

Oxidation catalysis system consisting of monolith substrate, inlet loft and outlet loft is modelled using SOLIDWORKSx64 software. The number of filter channels in the monolith substrate varies depending on the cell density of the substrate and application. Axial and radial flow oxidation catalysis system modelled in the present study has cell density of 240 cells per square inch. Designed models for axial and radial DOC with rectangular cross section are given in Fig. 1 and the model with cylindrical cross section after meshing is as shown in Fig. 2. Oxidation of exhaust gas takes place in the channels of filter substrate hence it must be made sure that the flow is uniform and the gases has considerable residence time in the system for the reactions to take place. Radial flow DOC would provide better uniformity in flow as compared to axial flow DOC. Cylindrical filter substrates would give better flow contour as compared to that of the rectangular substrate which has sharp edges.

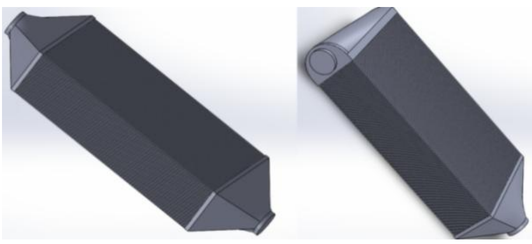

Fig. 2: Axial flow left and radial flow right oxidation catalysis system

CFD analysis has proven to be an effective tool in conducting analysis on performance of designed models in its application areas so that the prototype can be fabricated with optimized design parameters [24]. Simulations for flow of exhaust gas through the catalytic converter were conducted. The results showed that the performance of the system is affected by the presence of recirculation zone in the inlet loft [25]. Developed models are imported to the CFD software ANSYS and mesh is developed on the imported model for conducting iterative calculations on mathematical models [26]. The computational time for the simulation can be reduced by considering the cutting the models along its symmetrical axis as shown in Fig. 3. Mesh models of axial and radial flow filters after cutting along the symmetrical axis are shown in Fig. 4. Mesh is generated by considering coarse relevance centre and with a growth rate of 1.2. The number of nodes and elements in the three meshed models are given in Table 1.

The initial boundary conditions for radial and axial flow oxidation catalysis systems are detailed in Table 2. In the flow analysis for cylindrical oxidation catalysis system, the ceramic substrate is considered as porous zone by incorporating inertial resistance and viscous resistance in three directions as detailed in Table 3. Computations for the flow analysis of exhaust gas in the developed models are conducted by initializing the initial boundary conditions are detailed in Table 3.

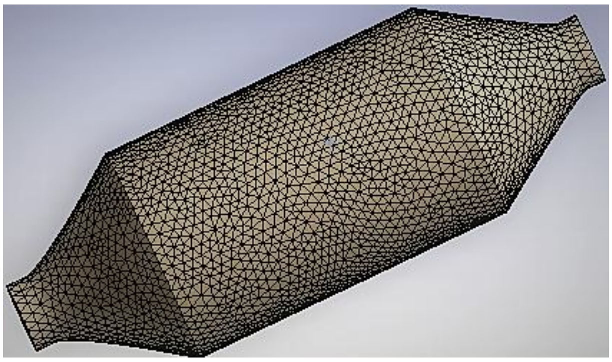

Fig. 3: Cylindrical filter substrate after meshing

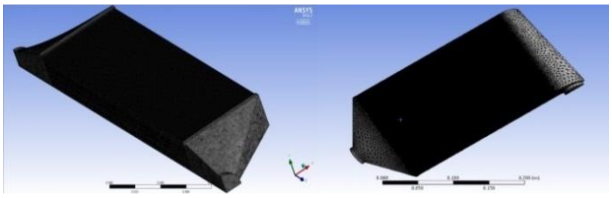

Fig. 4: Meshed models of axial and radial flow filters after cutting along the symmetrical axis

Table 1: Properties of mesh generated for simulation

Parameters	Axial DOC model	Radial DOC model	Cylindrical DOC model
Smoothing	High	Medium	High
Nodes	2087252	3486889	411195
Elements	4072844	5559220	391326

Table 2: Initial and boundary conditions of simulation for radial and axial flow oxidation catalysis systems

Parameters	Value
Type	Pressure based
Time	Steady
Turbulence model	K-omega
Fluid	Exhaust gas
Fluid density	0.5508 kg/m^3
Fluid viscosity	0.00003814 Pa
Fluid temperature	520 degree C
Inlet	Mass flow inlet
Mass flow rate at inlet	320 kg/hr
Pressure at inlet	220 milli bar
Outlet	Pressure outlet
Surface	Wall
Interior solid	Interior
Ratio of specific heats	1.4
Solution method scheme	Simple

Table 3: Initial and boundary conditions of simulation for cylindrical oxidation catalysis system

Type	Pressure based
Time	Steady
Velocity formulation	Absolute
Model	K-epsilon
Fluid	Exhaust gas
Fluid density	0.5508 kg/m^3
Fluid viscosity	0.00003814 Pa S
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

3. Results and discussion

3.1. Axial flow oxidation catalysis system

Contours of pressure and velocity generated after completion of flow analysis in CFD software showed the presence of reversed flow by formation of eddies in the edges of the filter loft. There was continuous flow along the filter channels with considerable amount of pressure drop. Contour of total pressure for axial flow oxidation catalysis system is shown in Fig. 5. It can be seen that there is continuous flow along the filter channels in the center whereas there is a rise in pressure drop at the edges. Plot of axial velocity along the symmetrical quarter cross section of axial flow oxidation catalysis system is shown in Fig. 6.

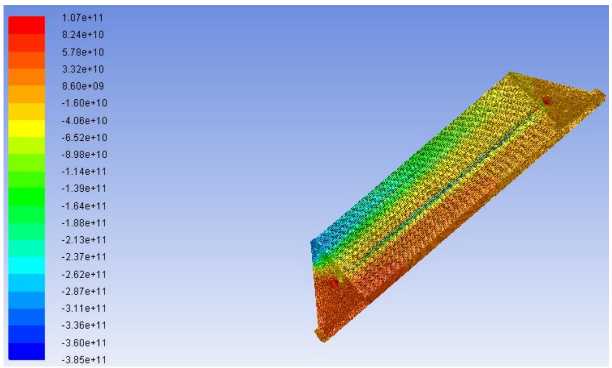

Fig. 5: Contour of total pressure across symmetrical quarter cross section of axial flow oxidation catalysis system

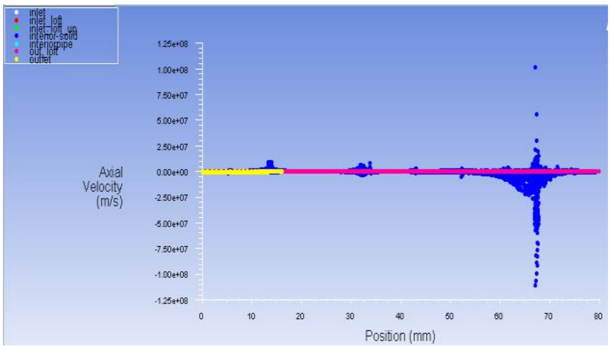

Fig. 6: Plot of axial velocity along the symmetrical quarter cross section of axial flow oxidation catalysis system

3.2. Radial flow oxidation catalysis system

The direction of exhaust gas flow changes its direction in radial flow oxidation catalysis system which enhances the residence time in the filter channels to escalate the catalyst reactions. The inlet to the system is in radial direction with the decreasing loft angle which will help to reduce the pressure drop. Contours of total pressure for symmetrical half cross section of radial flow oxidation catalysis system is shown in Fig. 7. It can be seen that it has more uniform and distributed flow characteristics as compared to axial flow oxidation catalysis system. The variation in the radial velocity along the x direction is as shown in Fig. 8.

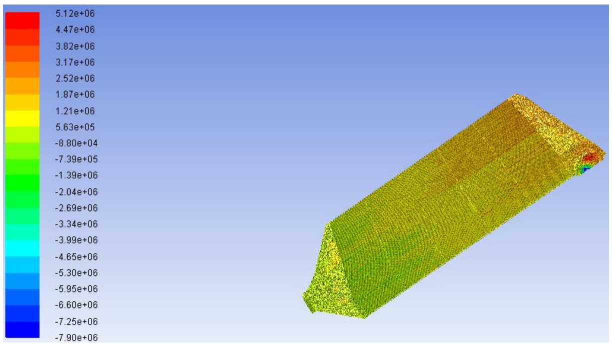

Fig. 7: Contour of total pressure for symmetrical half cross section radial flow oxidation catalysis system

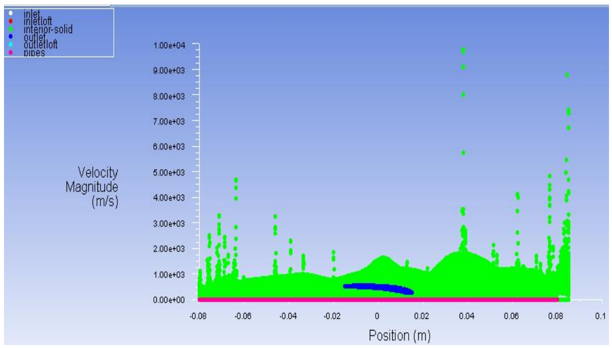

Fig. 8: Plot of radial velocity for symmetrical half cross sectional radial flow oxidation catalysis system

3.3. Cylindrical oxidation catalysis system

Cylindrical oxidation catalysis system has better flow characteristics since the chances of reverse flow is reduced by the elimination of sharp edges as compared to that of system with rectangular cross section. The major factor considering the pressure drop in the case of cylindrical oxidation catalysis system will be the loft angle at inlet and outlet side. The contour of pressure co-efficient at different sections of the system is shown in Fig. 9. It can be seen that there is continuous flow through the system. Velocity distribution at the inlet of the system is shown in Fig. 10. Area weighted uniformity index of the flow through the system is found to be 0.998572 and mass weighted uniformity index of flow through the system is found to be 0.997042. The pressure drop across the system is found to be 5384 Pa.

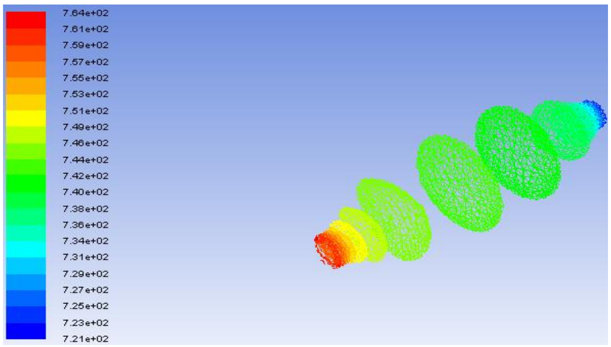

Fig. 9: Plot of pressure co-efficient at different sections of the cylindrical oxidation catalysis system

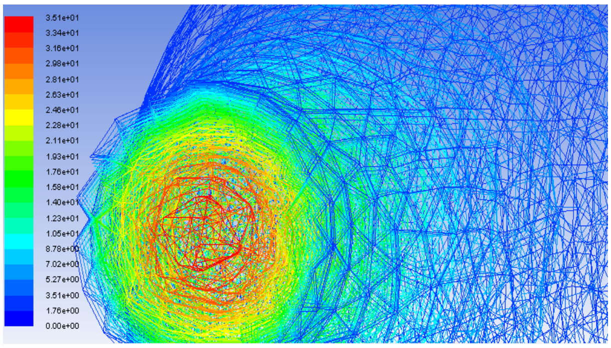

Fig. 10: Contour of velocity magnitude at the inlet section of cylindrical oxidation catalysis system

4. Conclusion

Geometric design of the three dimensional models of the oxidation catalysis system has been validated by conducting CFD simulations. Continuous flow without any backpressure has been observed with minimal pressure drop in the case of three models considered for the study. In axial flow DOC, there was reversed flow in the edges due to sudden expansion of loft leading to pressure drop. Exhaust gas flow is found to be more uniform in the case of radial flow and cylindrical oxidation catalysis system. Radial flow system provides better residence time for the catalytic reactions to take place inside the filter channels but the sharp edges of the rectangular cross section will lead to formation of eddies. System with rectangular cross section was considered for study to facilitate the packing of system in the engine exhaust. But the reversed flow at the edges has proved that the system with cylindrical cross section has better flow properties as compared to that with rectangular cross section. The flow simulations for the second stage of the post treatment emission control system can be conducted by considering the outlet conditions of the simulation results in the present study as inlet conditions of the particulate filtration system.

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