Design Optimization of Automotive Emission System using Computational Fluid Dynamics

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***Abstract*- The increasing demand on the automotive industry to reduce emissions from diesel engines entails more knowledge about modelling of exhaust gas after treatment systems. One of the major pollutants in diesel exhaust is nitric oxide (NO_x) which has adverse effect on both human health and the environment. The exhaust gas mainly contains the pollutants like soot, CO, nitric oxides. In order to control the soot, diesel particulate filter (DPF) is used which removes particulate matter from diesel exhaust by physical filtration, for the control of CO the diesel oxidization catalyst (DOC) is used. In DOC the oxidation process takes place which convert CO to harmless gas. To reduce the NO_x the Ad blue (32.5 wt% of urea in water) solution is sprayed in to the exhaust gas and it evaporates into water and urea. The urea further thermally decomposes into NH_3 and isocyanic acid. The isocyanic acid further undergoes hydrolysis in presence of catalyst. The NH_3 produced during thermolysis and hydrolysis is used as reducing agent to convert NO_x to N_2 and O_2. In order to enhance the mixing and evaporation of UWS (urea water solution) droplets a mixer element is used in SCR systems. In this study two types of mixing elements are designed and analysed using CFD. Three cases were considered, base case without mixer element, case 2 with mixer-1 and case 3 with mixer-2. Mixer-1 has two baffle plates each consists of 8 blades arranged circumferentially. The blades are titled to 45 deg. to change the direction of the fluid. In mixer -2 a hole is made in the baffle plate to reduce the pressure loss.**

Keywords*- *Automobile Emission, Ad-Blue, Back Pressure, Diesel Particulate Filter, Diesel Oxidation Catalyst, Nitrogen Dioxides, Hydrocarbon, Carbon Monoxide, Urea.

1. INTRODUCTION

The requirement for cleaner air continues to demand improvements in exhaust after treatment devices and components (e.g. three-way catalysts, diesel oxidation catalysts, lean nitrogen oxide traps or selective catalytic reducers) and also the engine as well as controls and sensors. Until recently, much of the design and engineering process to optimize various components of the engine and emission systems has relied heavily on the use of experiments and prototype testing. Meeting stricter emission regulations by improvement in the engine and emission systems would require comprehensive and quantitative understanding of the various complexes, transient and coupled physical and chemical processes that occur in these systems. Because of the overall complexity and increased costs associated with these factors, mathematical (i.e. computer-based) modelling continues to be pursued as a method of obtaining valuable information supporting the design and development process associated with exhaust emission system optimization.

Optimization of the urea dosing system to maximize de-NO_x performance and to minimize NH_3 slip during load changes is one of the main challenges for the mobile application of the urea-SCR (selective catalytic reduction) system. A mobile SCR system is restricted to a short distance between the engine exhaust and the catalyst entrance. Therefore, it is likely that urea residence time may not be adequate for complete thermolysis at the catalyst entrance. The key factors affecting the automobile application of SCR technology are the rapid thermolysis, good mixing of ammonia and gas, and reduction of ammonia slip.

Computer-based models can provide a very good understanding of the qualitative behaviour of a system. However, to obtain a quantitatively accurate result, these models need to be calibrated and later validated with experimental data. These models are only as good as the experimental data and they cannot be expected to out-perform the quality of the experimental data. Hence, to arrive at a model that can make quantitatively accurate predictions, good-quality experimental data are needed.

2. EXPERIMENTAL SETUP

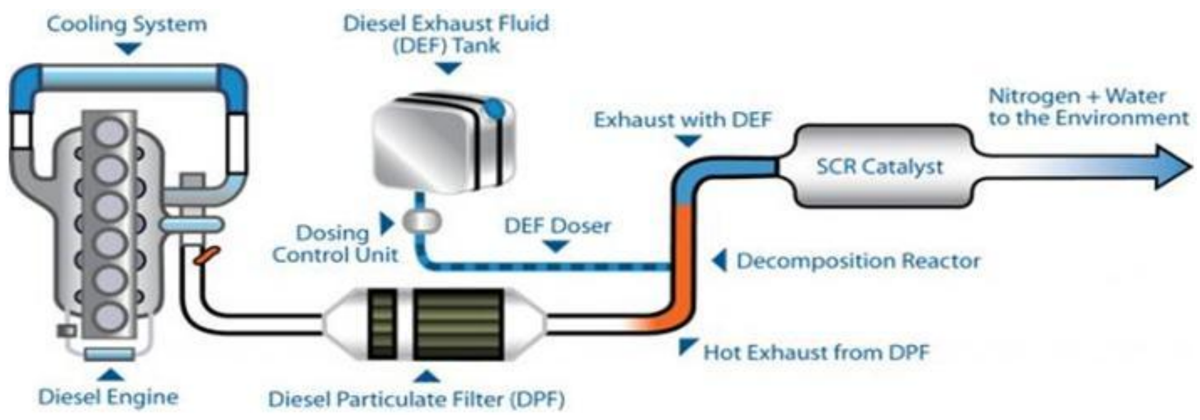

Fig 2.1 Line diagram of experimental setup

A 4 cylinder, 1986cc, diesel Volkswagen Passat engine is used for conducting the experiment. For analyzing the exhaust gas for the engine, Crypton 295 Gas Analyzer is used. Thermocouple and pressure probes are used at suitable places for measuring the temperature and pressure respectively. All the controls and readings are controlled and recorded through an instrumentation system connected to a computerized central control system.

Exhaust gas system consist of the fallowing process

I. **DPF** (Diesel Particulate Filter)
II. **DEF** (Diesel Exhaust Fluid)
III. **SCR** (Selective Catalytic Reduction)

3. EXPERIMENTATION AND RESULTS

Experimental Input Parameters

At the Inlet

Mass flow rate	2128 kg/hr
Inlet velocity	128.4 m/s
Inlet temperature	700 k
Density	0.5658 Kg / m3

Table: 3.1 Input Parameters

Material Properties

Fluid	Air
Molecular Viscosity	3.225e-05 kg/ms
Molecular Weight	28.97
Conductivity	0.02847 W/ m K
C_p	1003 J/ Kg K

Table: 3.2 Material Proprieties

Note: With or Without Mixer or Baffle plates there would be no changes in the inlet parameters.

Experimental Procedure

This experiment setup consist of the ad-blue which is been sprayed with the standard nozzle diameter for dispersing the nozzle used for the DEF is 19mm and the diameter of the diesel nozzle is 22mm. The consumption of DEF is 2% of diesel fuel consumed which is the ratio of 50 to 1 ratio of diesel. The DEF which is called as the Ad Blue is sprayed after the DPF (Diesel Particulate Filter) using the nozzle which is similar to the diesel nozzle which is sprayed and mixed with the exhaust gas.

The ammonia is mixed with the exhaust gas in the SCR catalyst were the ammonia and nitrogen dioxide is mixed together due to the chemical reaction the exhaust gas along with the other emission NO_x is converted into Nitrogen + Water.

The ammonia sprayed in the exhaust chamber would not be completely mixed with the exhaust gas. We are trying to introduce the mixture plates of 2 numbers which is similar to the baffle plates with and without holes.

Experimental setup has been arranged and the reading are recorded and tabulated and the same is been used in CFD simulation.

4. EXPERIMENTAL RESULTS

Experimental value taken at 750 ºC

T	p	h	s	C_p	ɥ	k
750	0.47	782.3	7.62	1.03	0.36	0.052

Table: 4.1 Experimental values taken at 750 ºC

Values at the inlet and outlet for base case without mixer

	Inlet (kPa)	Outlet (kPa)
Model without mixer	117	107

Table: 4.2 Values at Inlet and Outlet without mixer

Pressure Drop or Back Pressure of each chamber for mixer with hole

	Pressure (kPa)
Inlet chamber	0.0896
Mixer chamber	134
Perforation pipe	7.32

Table: 4.3 Pressure Drop in Each Chamber with Hole

Pressure Drop or Back Pressure of each chamber for mixer without hole

	Pressure (kPa)
Inlet chamber	0.0932
Mixer chamber	152
Perforation pipe	5.28

Table: 4.4 Pressure Drop in Each Chamber without Hole

5. NUMERICAL SIMULATION

Model

The model is as shown it consists of mixing element which contains two baffle plates each consists of eight blades arranged in circumferentially and the distance between the two baffles is 75mm. The mixer reduces the velocity of the exiting air and consequently reducing the amount of noise produced. The mixer element is placed at the inlet of the exhaust system. .

Model of Mixing Element

The model consists of perforated pipe with each perforation diameter 10mm and the substrate has the length and diameter of 250mm and 397mm respectively. For case-3 the 10mm hole is created in the baffle plates.

CFD codes are structured around the numerical algorithms that can tackle fluid flow problems. In order to provide easy access to their solving power all commercial CFD packages include sophisticated user interfaces to input problem parameters and to examine the results. Hence all the codes contain three main elements like pre-processor, solver and post-processor.

MIXER PART (WITHOUT HOLE)

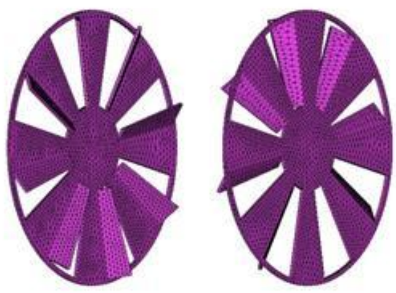

Fig 5.1 Mixer Plate without Hole

MIXER PART (WITH HOLE)

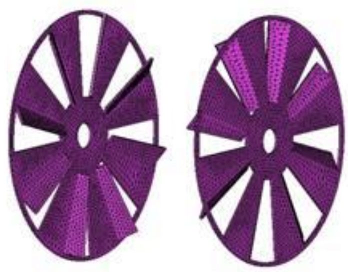

Fig 5.2 Mixer Plate with Hole

Boundary conditions at inlet at the inlet

Mass flow rate	2000 kg/hr
Inlet velocity	129.6 m/s
Inlet temperature	723 k
Density	0.5458 Kg / m^3
Turbulent Kinetic Energy	0.05 m^2/s^2
Turbulent Length Scale	0.01 m

Table: 5.1 Boundary condition

Material Properties

Fluid	**Air**
Molecular Viscosity	3.4280e-05 kg/ms
Molecular Weight	28.97
Conductivity	0.02637 W/ m K
C_p	1006 J/ Kg K

Table: 5.2 Material Properties

At the outlet

Pressure	101325 Pa
Turbulent Kinetic Energy	0.05 m2/s2
Turbulent Length Scale	0.01m

Table: 5.3 Properties at Outlet

Boundary conditions at Back Pressure

Mixer without hole = 3.28 kPa
Mixer with hole = 3.08 kPa

6. CFD SIMULATION RESULTS AND DISCUSSIONS

The figure below shows the gamma distribution plot here we see the distribution of the fluid in the substrate. From the plots it shows that in the both the cases the distribution of the flow is satisfactory.

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UNIFORMITY INDEX CONTOURS

With Hole

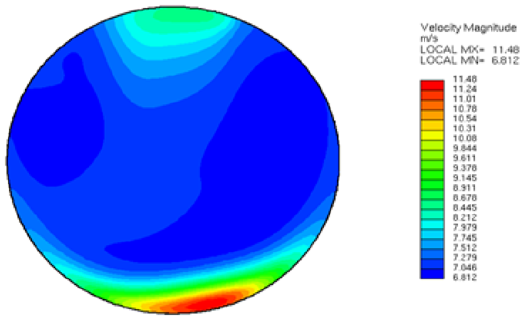


Fig 6.1 Gamma Distribution with Hole

This shows that velocity magnitude is slightly more thus more uniform mixing.

Without Hole

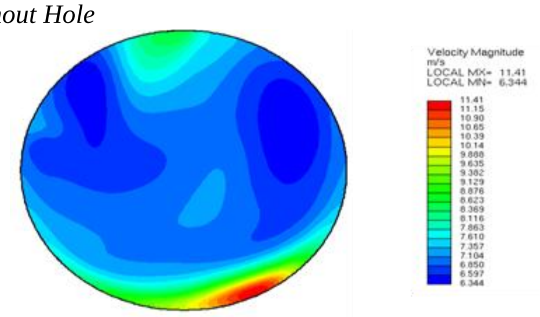


Figure 6.2 Gamma Distributions without Hole

This shows that velocity magnitude is slightly less thus less uniform mixing.

TOTAL PRESSURE AT DIFFERENT SECTIONS

Pressure Drop or Back Pressure of each chamber for mixer with hole

	Pressure (kPa)
Inlet chamber	0.1
Mixer chamber	138
Perforation pipe	7.46
Substrate	3.08
Substrate Downstream Chamber	1.49

Table: 6.1 Pressure Drop of Each Chamber with Hole

Pressure Drop or Back Pressure of each chamber for mixer without hole

	Pressure (kPa)
Inlet chamber	0.1
Mixer chamber	154
Perforation pipe	5.58
Substrate	3.28
Substrate downstream chamber	1.34

Table: 6.2 Pressure Drop of Each Chamber without Hole

Velocity Deviations

Velocity deviations at mid section of the substrate of the three case as shown in the table.

	Mixer with hole	Mixer without hole
Maximum value	11.51	11.47
Minimum value	6.8	6.33
Average value	7.4	7.226
Gamma	0.967	0.967

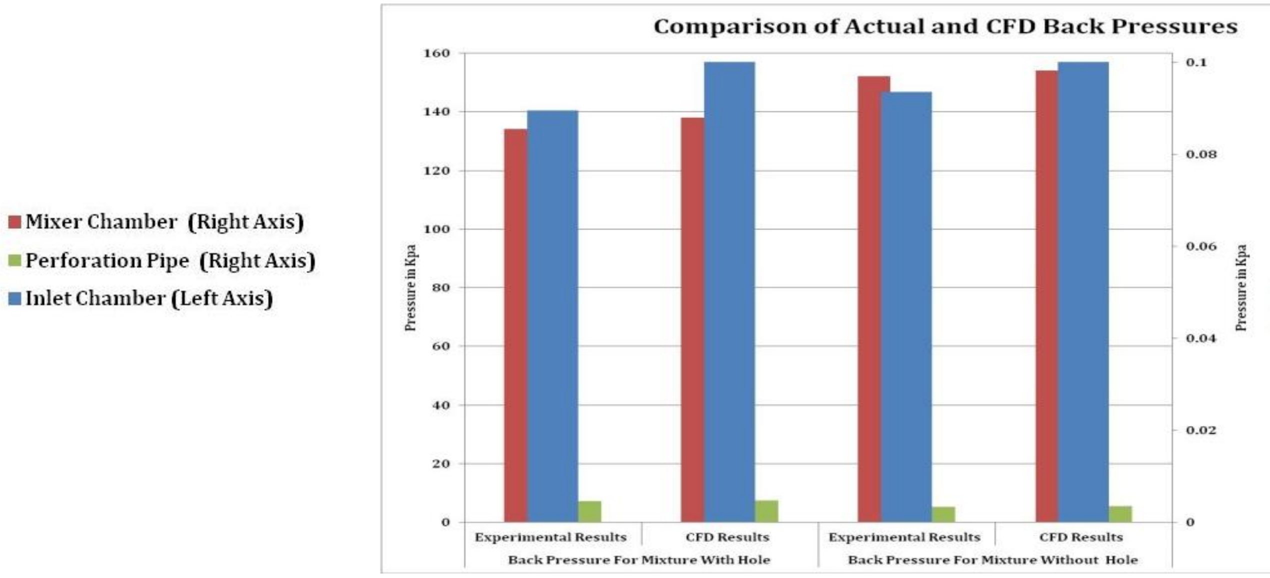
Table: 6.3 Velocity Deviation At with and without Hole

7. COMPARISON OF BACK PRESSURE BETWEEN WITH AND WITHOUT MIXERS.

By analysing the experimental and CFD results obtained it is found that the mixer without hole produces more back pressure when compared to the mixer with hole. The back pressure produced by mixer without hole is 152 kPa and the back pressure produced by mixer with hole is 134 kPa. In the previous segments it is noted that the distribution of flow is almost same for both the mixer configurations. So the deciding factor for finding the better or more efficient mixer configuration is by comparing the back pressure produced by them. Thus it can be concluded by analysing the experimental and CFD results that the mixer with hole is more efficient because it produces less back pressure when compared to the mixer without hole.

8. COMPARISON OF BACK PRESSURE OF EXPERIMENTAL AND CFD SIMULATION

In this part we are going to compare the Chamber Pressure results from actual Experiment and the result obtained from CFD simulation. From the above graphs we can see that the CFD chamber pressure closely matches the experimental chamber pressure within a margin of **±10%** deviation. This basically is due to the assumptions that were assumed before the simulations. This deviation can further be reduced by altering the boundary condition and material properties, so that they closely match the actual conditions and properties.



9. CONCLUSION

In order to enhance the mixing and evaporation of UWS (urea water solution) droplets, a mixer element is used in SCR systems which make the fluid to get distributed uniformly throughout the substrate and make most of the fluid to come in contact with the catalyst surface for reactions to take place. In this study two types of mixing elements are designed and analyzed using CFD. A base case without mixer element is considered just to get the back pressure in order to compare that for the cases with mixer elements. For analysis two cases with a mixer element are considered. Both cases have two baffle plates each consists of 8 blades arranged circumferentially. The blades are tilted to 45 deg. to change the direction of the fluid. First case is done with a mixer element which produced higher back pressure. In order to reduce the back pressure and enhance the velocity distribution second case with a hole in the mixer elements is considered.

The first factor considered is the Gamma Distribution or the Uniformity Index which is a measure of distribution of the flow through the substrate that makes sure that most of the fluid is contacting the catalyst surface for the better utilization of the catalyst in reactions. Uniformity Index of a value 1 indicates uniform distribution of the flow and less than one indicates deviation of flow from uniform flow. In both the cases considered here the gamma value is 0.96 which shows the satisfactory flow distribution in the porous media. Also it can be observed from the turbulent kinetic energy plots that the turbulence created for the case with mixer hole is more which enhances the mixing of the fluid thereby enhancing the distribution.

The second factor considered is Back Pressure or the Pressure Drop which has direct influence on the engine performance. The high back pressure from the exhaust system due to more components reduces the engine performance. Therefore an attempt is made here to reduce the back pressure in the second case by making a hole in the mixer element without compromising in the velocity distribution which is another factor considered.

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