Simulation of CRDI Vehicle and Effect of Aftertreatment Devices

Nikhil Bondre¹, Vikrant Haribhakta²

¹Department of Mechanical Engineering, College of Engineering, Pune, Maharashtra, India,
²Department of Mechanical Engineering, College of Engineering, Pune, Maharashtra, India.

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Abstract: The project aims at simulation of diesel vehicle and the effect of after treatment devices on emissions of vehicle in mathematical environment. Environmental degradation due to pollution is increasing also emission norms of vehicles are becoming more and more stringent. Newer technologies are developing to attain the target of reduction in emissions. After treatment devices like diesel oxidation catalyst (DOC) is used to oxidize CO and HC, diesel particulate filter (DPF) is used to trap particulate matter and selective catalytic reduction (SCR) is used for reduction of NOX. In this project, simulation of light-duty diesel vehicle is performed and results are validated with actual data. Simulation of above devices provided reliable results as well as variation of different parameters within the components helped to improve the efficiency of system. Based on the reduction of emission, the conversion efficiency of after treatment system is calculated. Optimization of geometrical parameters of diesel oxidation catalyst and diesel particulate filter is done to further improve the performance of system.

Keywords: Diesel Oxidation Catalyst, Diesel Particulate Filter, Selective Catalytic Reduction

1. Introduction

Diesel engines are important power systems for on-road and off-road vehicles. Heavy-duty trucks and buses are powered by a diesel engine due to its reliability, high output torque and high fuel-efficiency. Though widespread use of these engines having many advantages, they play important role in environmental pollution problems as well as severe health problems. Harmful gases produced such as CO, HC, SO and NOX, are discharged into the atmosphere. After treatment system processes the exhaust of vehicle. Light duty diesel after treatment system consists of Diesel Oxidation Catalyst (DOC), Diesel Particulate Filter (DPF), and Selective Catalytic Reduction (SCR). Performance of components have direct and indirect effect on each other. Performance characteristics of diesel oxidation catalyst and diesel particulate filter are studied here.

Simulation is faster and cost-effective way than experimental trial and error process. Simulation
for this study is carried out in GT-Suite software. Model of diesel vehicle along with after treatment system built using templates available in software.

![Diagram](https://via.placeholder.com/150)

**Figure1:** Explains the sequence of connections.

1. Method of Analysis:

1. **Driver, Vehicle and Engine Subsystem:**

For simulation purpose, NEDC drive cycle is given input to Driver template. Specifications of vehicle are of light-duty diesel vehicle. For Engine, specifications are provided as given in table. Along with these specifications, fuel consumption map, Air flow map which are functions of RPM and load are provided. Formation maps of emissions such as CO, HC, CO2, NOx and soot as functions of RPM and load are provided.

<table>
<thead>
<tr>
<th>Specification</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>EngineType</td>
<td>4-stroke</td>
</tr>
<tr>
<td>EngineDisplacement</td>
<td>2000cc</td>
</tr>
<tr>
<td>Initialspeed</td>
<td>750RPM</td>
</tr>
<tr>
<td>Minimumoperatingspeed</td>
<td>500RPM</td>
</tr>
<tr>
<td>Engine Inertia</td>
<td>0.23kg-m2</td>
</tr>
</tbody>
</table>

1. **Simulation of Diesel Oxidation Catalyst:**

![Diagram](https://via.placeholder.com/150)
**Fig 2. Diesel Oxidation Catalyst Model**

Figure 2 shows the construction of DOC model in software. ‘Inlet’ as shown in fig. 2 is exhaust gas composition given by Engine template. ‘Catalyst Brick’ as shown in fig. 2 is a template that takes values to define physical parameters of actual catalyst. Table 2 shows the values provided for simulation.

<table>
<thead>
<tr>
<th>Specification</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Frontaldiameter</td>
<td>6 inch</td>
</tr>
<tr>
<td>Length</td>
<td>6 inch</td>
</tr>
<tr>
<td>CellDensity</td>
<td>400</td>
</tr>
<tr>
<td>Channelshape</td>
<td>Square</td>
</tr>
<tr>
<td>Washcoatlayerthickness</td>
<td>0.03 mm</td>
</tr>
<tr>
<td>Substratematerial</td>
<td>Cordierite</td>
</tr>
<tr>
<td>Washcoatmaterial</td>
<td>Alumina</td>
</tr>
<tr>
<td>Initialtemperature</td>
<td>300K</td>
</tr>
</tbody>
</table>

Table 2. Parameters of Catalyst brick in DOC

Chemical reaction and Kinetics’ as shown in fig. 2 is required to specify chemical reactions and their activation energies occurring in DOC. Following chemical reactions are defined.

\[
\begin{align*}
CO + 0.5O_2 & \rightarrow CO_2 \\
C_3H_6 + 4.5O_2 & \rightarrow 3CO_2 + 3H_2O \\
DF1 + 19.4O_2 & \rightarrow 13.5CO_2 + 11.8H_2O \\
H_2 + 0.5O_2 & \rightarrow H_2O \\
NO + 0.5O_2 & \rightarrow NO_2 \\
Z + DF1 & \rightarrow ZDF1 \\
ZDF1 & \rightarrow Z + DF1
\end{align*}
\]

‘DF1’ in equation (3) is used for diesel composition while ‘Z’ in equations (6) and (7) is zeolite. ‘Connector’ as shown in fig. 2 is used for connecting ‘Catalytic Brick’ to ‘Chemical Reactions and Kinetics’. Monitor is subsystem used to calculate conversion efficiency. Conversion efficiency is calculated by using mass flow rate of CO and HC at input and output of catalyst. The ‘Outlet’ is emission composition after the process in DOC that is further provided to DPF."
2. Simulation of Diesel Particulate Filter:

"Figure 3 shows the construction of DPF model in software. ‘Inlet’ as shown in fig. 3 is exhaust gas composition given by outlet of DOC. ‘Catalyst Brick’ as shown in fig. 3 is a template used for defining physical parameters of actual filter. Table 3 shows the values provided for simulation."

![Diagram of Diesel Particulate Filter Model]

**Table 3: Parameters of Catalyst brick in DPF**

<table>
<thead>
<tr>
<th>Specification</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Frontal diameter</td>
<td>6 inch</td>
</tr>
<tr>
<td>Length</td>
<td>10 inch</td>
</tr>
<tr>
<td>Cell Density</td>
<td>240/in²</td>
</tr>
<tr>
<td>Channel shape</td>
<td>Square</td>
</tr>
<tr>
<td>Substrate thickness</td>
<td>0.014 inch</td>
</tr>
<tr>
<td>Substrate material</td>
<td>Cordierite</td>
</tr>
<tr>
<td>Substrate permeability</td>
<td>8*10⁻⁷ mm²</td>
</tr>
<tr>
<td>Substrate pore diameter</td>
<td>15micron</td>
</tr>
</tbody>
</table>

Chemical Reactions and Kinetics’ as shown in fig. 3 is used to give input of chemical reactions taking place during passive regeneration. Activation energies are also provided. Following are the chemical reactions which are considered during simulation."

\[
\begin{align*}
\text{C+NO}_2 & \rightarrow \text{CO+ NO} \\
\text{C+2NO}_2 & \rightarrow \text{CO}_2+2\text{NO}
\end{align*}
\]

‘Connector’ as shown in fig. 3 is used for connecting ‘Catalytic Brick’ to ‘Chemical Reactions and Kinetics’. ‘Monitor’ as shown in fig. 3 is used to calculate soot mass retained in filter. ‘Outlet’ shown in fig. 3 is emission composition after DPF and used to give input to selective catalytic reduction."
1. Simulation of Selective Catalytic Reduction:

Figure 4 shows the construction of SCR model in software. ‘Inlet’ shown in fig. 4 is emission gas composition after the process occurred in DPF. ‘Catalyst Brick’ is template used to define physical parameters of catalyst. Values provided for simulation are given in Table 4.

**Table 4: Parameters of Catalyst brick in DPF**

<table>
<thead>
<tr>
<th>Specification</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Frontaldiameter</td>
<td>6 inch</td>
</tr>
<tr>
<td>Length</td>
<td>12 inch</td>
</tr>
<tr>
<td>CellDensity</td>
<td>400/in²</td>
</tr>
<tr>
<td>Channelshape</td>
<td>Square</td>
</tr>
<tr>
<td>Substratewallthickness</td>
<td>0.006 inch</td>
</tr>
<tr>
<td>Substratematerial</td>
<td>Cordierite</td>
</tr>
<tr>
<td>Initialwalltemperature</td>
<td>300K</td>
</tr>
</tbody>
</table>

Chemical Reactions and Kinetics’ as shown in fig. 4 is used to give input of chemical reactions taking place during reduction of NOx and their activation energies. Following are the chemical reactions used for simulation purpose.

\[
\text{NH}_3 + Z \rightarrow \text{NH}_3 - Z \\
\text{2NH}_3 - Z + 1.5\text{O}_2 \rightarrow \text{N}_2 + 3\text{H}_2\text{O} + 2Z \\
\text{NO} + 0.5\text{O}_2 \rightarrow \text{NO}_2 \\
\text{2NH}_3 - Z + \text{NO} + \text{NO}_2 \rightarrow 2\text{N}_2 + 3\text{H}_2\text{O} + 2Z
\] (1) (2) (3) (4)
4NH3-Z+3NO2 —>3.5N2 +6H2O +4Z  
2NH3-Z+2NO2 —>N2+N2O +3H2O +2Z  
Urea—>NH3+HNCO  
HNCO+H2O—>NH3+CO2  

Z' used in equations above represent Zeolite which is site element used for purpose of increasing surface area to facilitate increased reaction rate. ‘Urea control strategy’ shown in fig. 4 is a subsystem used to reduce ammonia slip. This subsystem takes input of NOx from inlet of ‘Catalyst Brick’ and of ammonia slip from outlet of ‘Catalyst Brick’. Based on input values, injection rate of urea is decided considering stoichiometric ratio of chemical reaction. ‘Urea thermal decomposition’ shown in fig. 4 is used for chemical decomposition of urea after injection. Chemical reactions that given input are as

AdBlue—>0.1262urea+0.8738H2O  
Urea—>NH3+HNCO  
HNCO+H2O—> NH3 +CO2  

‘Monitor’ shown in fig. 4 monitors the reduction of NOx into N2 and H2O. Also, ammonia slip with respect to time can be measured. ‘Outlet’ shown in fig. 4 is output of exhaust after passing through aftertreatment system and is emitted to environment. Effect of aftertreatment system i.e. oxidation of CO and HC, trapping of soot and reduction of NOx is measured at this end. Composition of CO, HC, CO2, NOx, and H2O at output gives the conversion efficiency of system.

3. Results and Discussion

At first, simulation was carried out by using only DOC in the system to check for the effectiveness in oxidation. CO and HC are measured at input and output of DOC and conversion efficiency calculated. Results were recorded for first 200 sec. Of drive cycle.

Fig.5: DOC-Input and output COmole fraction

![Graph showing DOC-Input and output COmole fraction](image-url)
In fig. 5 and fig. 6, input and output mole fraction of CO and HC are shown respectively. The conversion rate increases after certain time because after that time light-off temperature is reached. Light-off temperature is temperature at which conversion becomes equal to 50%. And the time at which catalyst becomes active is called light-off time. From fig. 7 it can be seen that 50 sec is light-off time for HC while 58 sec is for CO. Geometrical parameters of DOC varied to check effectiveness of catalyst at constant volume. Length and front diameter varied such as to keep constant volume and average conversion efficiency is calculated and following results are obtained.
As we can see in fig. 8 and 9, for diameter of 8 inches average conversion efficiency is highest keeping constant volume of catalyst. After simulation of DOC, only DPF is connected to record soot mass retained in filter.

Fig. 8 DOC – Average conversión efficiency vs diameter for CO

Fig. 9 DOC – Average conversión efficiency vs diameter for HC

Fig. 10 Soot mass retained in DPF

Fig. 10 indicates the cumulative soot mass retained in DPF for specifications as shown in table 2. For DPF, cell density is important parameter which affects soot mass retained as well as pressure drop of exhaust gas. The cell density of DPF varied to find relation with soot mass retained and pressure drop.\(^n\)
As shown in fig. 11 and fig. 12, we can conclude that as cell density increases trapped soot mass increases but pressure drop also increases. Though soot mass retained increases, the rate of increase decreases as cell density increases. Also, increased pressure drop deteriorates engine performance. Hence, cell density should be optimum.

Fig. 11 Variation of average soot mass retained vs cell density in per inch².

Fig. 12 Variation of average pressure drop vs cell density in per inch².

Fig. 13 Input and Output Mass flow rate of CO in After treatment System.
"Fig. 13, fig. 14, and fig. 15 shows input and output mass flow rate of CO, HC, and NOx passing through DOC, DPF, and SCR. Hence, diesel engine, light-duty vehicle having aftertreatment system is constructed in GT-Suite software. Simulation is carried out and results are validated with actual data. So, from simulation of aftertreatment system, we can conclude that DOC, DPF, and SCR can be used for reduction of emissions to meet permissible levels of emissions defined by emission norms. Conversion efficiency for DOC calculated. Effect of geometrical parameters on the performance of DOC and DPF is explained above."

4. References:

8. Cozzolini, Alessandro, ”Advanced DOC-DPF Model to Predict Soot Accumulation and Pressure Drop in Diesel Particulate Filters”, Graduate Theses, Dissertations, and Problem Reports