International Journal of Engineering Sciences 2023 15(4) 148 - 158

INTERNATIONAL JOURNAL OF ENGINEERING SCIENCES

Simulation of CRDI Vehicle and Effect of Aftertreatment Devices

Nikhil Bondre[1], Vikrant Haribhakta[2]

[1]Department of Mechanical Engineering, College of Engineering, Pune, Maharashtra,India,

[2]Department of Mechanical Engineering, College of Engineering, Pune,Maharashtra, India.

(Received 2 November 2022; Accepted 10 January 2023)

DOI: https://doi.org/10.36224/ijes.150403

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

*Corresponding author
Email address: nikhilbondre09@gmail.com (Nikhil Dilip Bondre)
ISSN 0976 – 6693.

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.

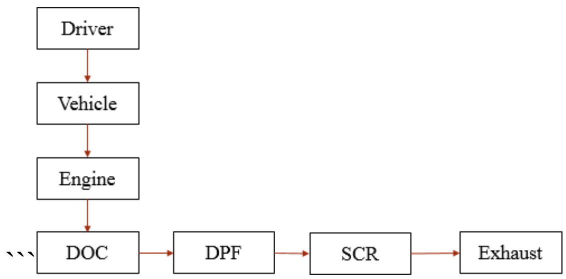


Figure1: Explains the sequence of connections.

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.

Table1.Engine specifications

Specification	**Value**
EngineType	4-stroke
EngineDisplacement	2000cc
Initialspeed	750RPM
Minimumoperatingspeed	500RPM
Engine Inertia	0.23kg-m2

1. Simulation of Diesel Oxidation Catalyst:

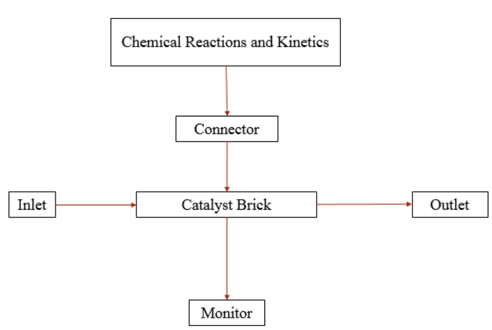


Fig 2.Diesel Oxidation Catalyst Model

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 2.Parameters of Catalyst brickin DOC

Specification	**Value**
Frontaldiameter	6 inch
Length	6 inch
CellDensity	400
Channelshape	Square
Washcoatlayerthickness	0.03 mm
Substratematerial	Cordierite
Washcoatmaterial	Alumina
Initialtemperature	300K

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..

CO+0.5O2-—>CO2 (1)

C3H6+4.5O2-—>3CO2+3H2O (2)

DF1+19.4O2 -—>13.5CO2+11.8H2O (3)

H2+0.50O2-—>H2O (4)

NO+.5O2-—>NO2 (5)

Z+DF1-—>ZDF1 (6)

ZDF1-—>Z+DF1 (7)

'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:

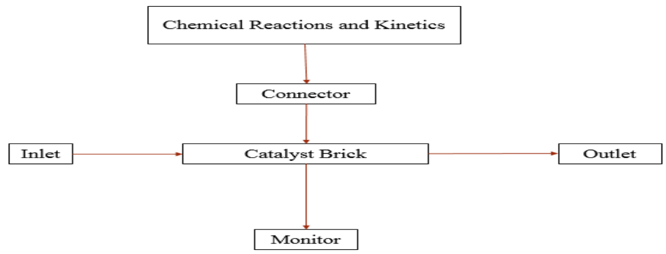


Fig.3: Diesel Particulate Filter Model

"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.".

Table 3:.Parameters of Catalyst brick in DPF

Specification	**Value**
Frontaldiameter	6 inch
Length	10 inch
CellDensity	240/in^2
Channelshape	Square
Substratethickness	0.014 inch
Substratematerial	Cordierite
Substratepermeability	8*10^{-7} mm^2
Substrateporediameter	15micron

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."

$C + NO_2 \longrightarrow CO + NO$ (1)

$C + 2NO_2 \longrightarrow CO_2 + 2NO$ (2)

'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:

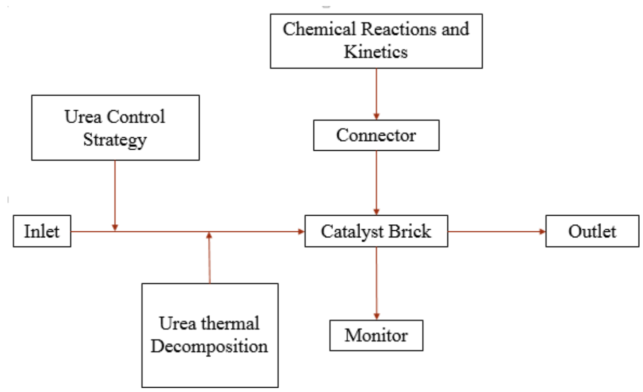


Fig.4: Selective Catalytic Reduction Model

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

Specification	**Value**
Frontaldiameter	6 inch
Length	12 inch
CellDensity	400/in^2
Channelshape	Square
Substratewallthickness	0.006 inch
Substratematerial	Cordierite
Initialwalltemperature	300K

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.

NH3+Z—>NH3-Z (1)

2NH3-Z+1.5O2 —>N2+3H2O +2Z (2)

NO+0.5O2—>NO2 (3)

2NH3-Z+NO +NO2—>2N2 +3H2O+ 2Z (4)

$$4NH_3\text{-}Z+3NO_2 \longrightarrow 3.5N_2 +6H_2O +4Z \quad (5)$$

$$2NH_3\text{-}Z+2NO_2 \longrightarrow N_2+N_2O +3H_2O +2Z \quad (6)$$

$$Urea \longrightarrow NH_3+HNCO \quad (7)$$

$$HNCO+H_2O \longrightarrow NH_3+CO_2 \quad (8)$$

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

$$AdBlue \longrightarrow 0.1262urea+0.8738H_2O \quad (1)$$

$$Urea \longrightarrow NH_3+HNCO \quad (2)$$

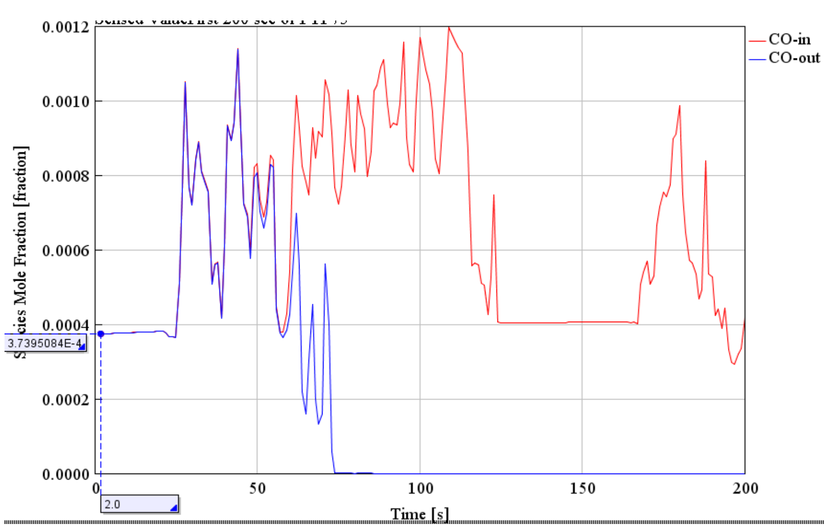
$$HNCO+H_2O \longrightarrow NH_3 +CO_2$$

'Monitor' shown in fig. 4 monitors the reduction of NOx into N_2 and H_2O. 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, CO_2, NOx, and H_2O at output gives the conversion efficiency of system. (3)

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



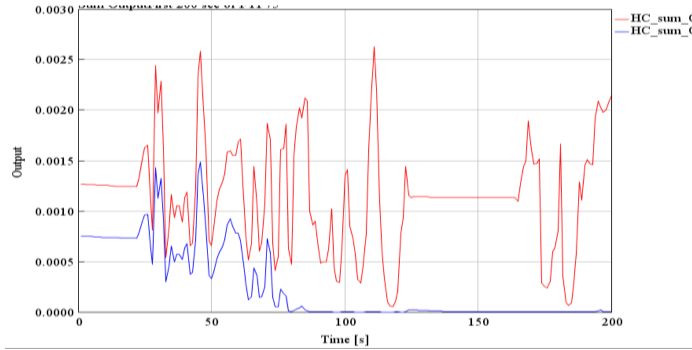


Fig.6: DOC–Input and output HC molefraction

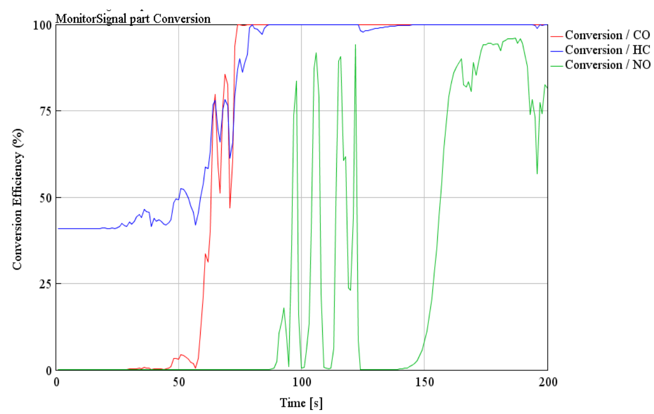
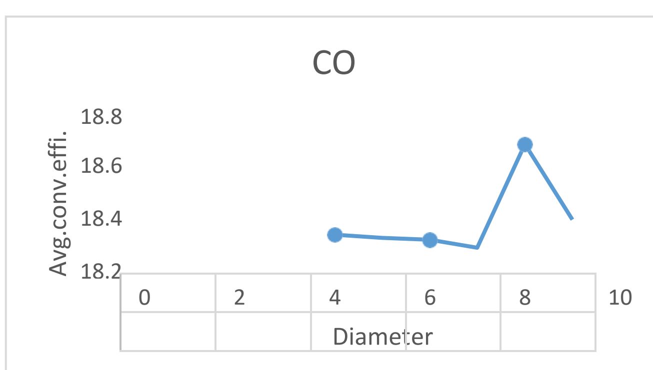


Fig.7: DOC – Conversion efficiency graph for CO,HC andNOx

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.



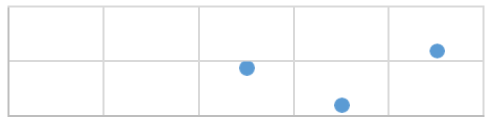


Fig.8 DOC –Average conversión efficiency vs diameter for CO

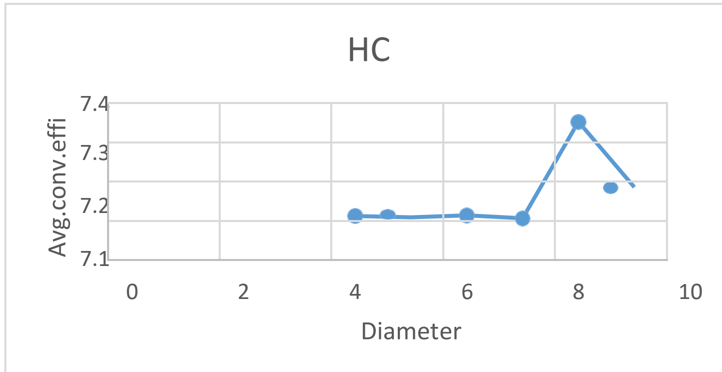


Fig.9 DOC –Average conversión efficiency vs diameter for HC

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.

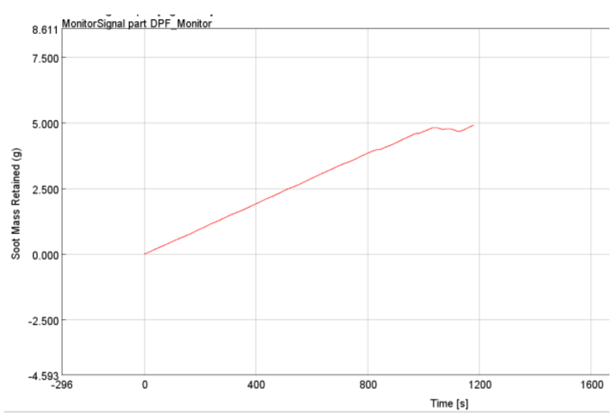


Fig.10 Soot mass retained in DPF

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."

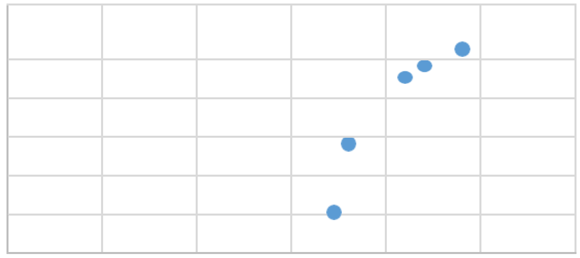


Fig.11 Variation of average soot mass retained vs cell density in per inch2

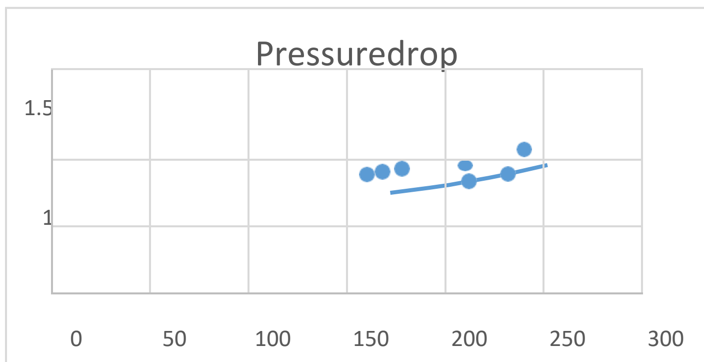


Fig.12 Variation of average pressure drop vs cell density in per inch 2.

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.

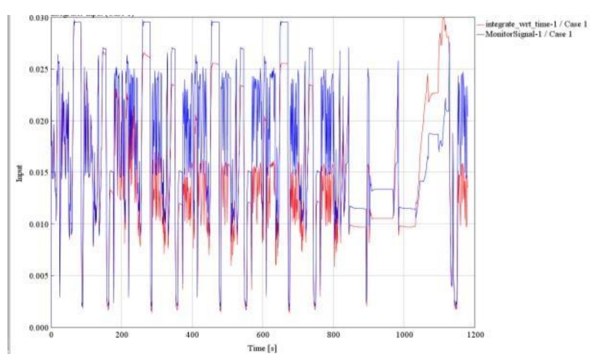


Fig.13 Input and Output Mass flow rate of CO in After treatment System.

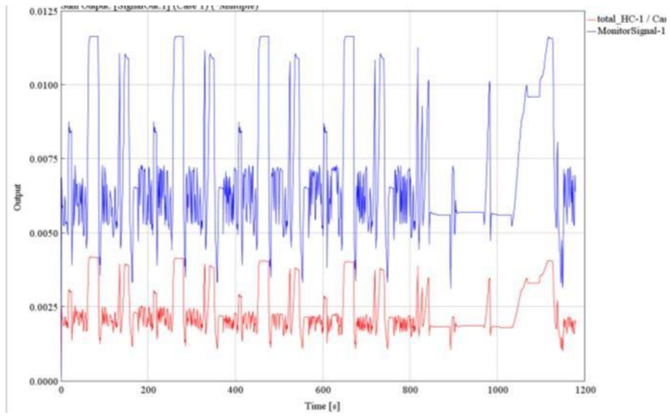


Fig.14 Inputand Output Massflow rate of HC in after treatment

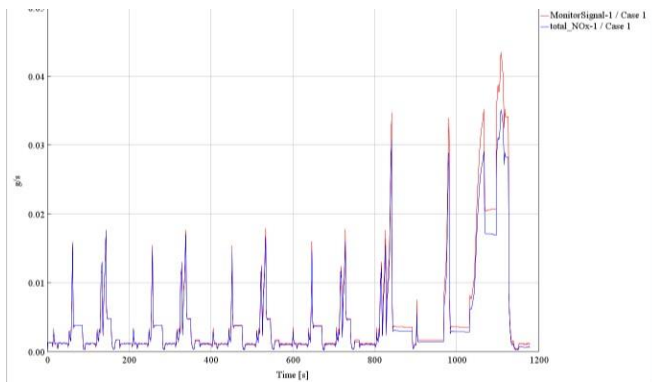


Fig.15 Input and Output Mass flow rate of NOx in After treatment System

"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:

1. Bagavathy, S.S., Ramesh, A., "Parametric Investigations on the Performance of Diesel Oxidation Catalyst in a Light Duty Diesel Engine", SAE Technical Paper 2019-26-0299, 2019
2. Syed Wahiduzzaman, Weiyong Tang, Seth Wenzel, "Integrated Aftertreatment System Modelling Using GT-POWER", 10th DOE Crosscut Workshop on Lean Emissions Reduction Simulation, May 1st-3rd, 2007
3. Archit Srinivasacharya Ayodhya, Kumar Gottekere Narayanappa, "An overview of after-treatment systems for diesel engines", Springer-Verlag GmbH Germany, part of Springer Nature 2018
4. April Russell & William S. Epling, "Diesel Oxidation Catalysts, Catalysis Reviews", Science and Engineering, 53:4, 337-423

5. G. Cerrelli, P. Ferreri, “Conventional and electrically heated diesel oxidation catalyst modeling in gt-suite”, GT-Conference 2018, Frankfurt
6. Massimiliano Sosio, Michael Grill, “Diesel exhaust system aftertreatment modelling with the perspective on hybrid vehicle strategies”, GT-User Conference – Frankfurt
7. Xinying Zhao, Kun Luo, “The Use of MATLAB and GT-SUITE in Simulation and Optimization of the Diesel Exhaust After-treatment System”, 2018 International Conference on Security, Pattern Analysis, and Cybernetics (SPAC)
8. Cozzolini, Alessandro, "Advanced DOC-DPF Model to Predict Soot Accumulation and Pressure Drop in Diesel Particulate Filters", Graduate Theses, Dissertations, and Problem Reports
9. Mahadevan, B.S., Johnson, J.H., and Shahbakti, M., “Development of a catalyzed diesel particulate filter multi-zone model for simulation of axial and radial substrate temperature and particulate matter distribution”, Journal of Emission Control Science Technology
10. Fan Su, Brandon W. Gordon and Henry Hong, “Simulation of a Diesel Engine Aftertreatment System Using Singularly Perturbed Sliding Manifold”, 16th IEEE International Conference on Control Applications Part of IEEE Multi-conference on Systems and Control Singapore