DOI : https://doi.org/10.56452/7-780

ISSN: 0974-5823 Vol. 7 No. 1 January, 2022

International Journal of Mechanical Engineering

MATHEMATICAL MODELING OF COMBUSTION ANALYSIS AND PERFORMANCE CHARACTERISTICS FOR DESIGNED CATALYTIC CONVERTER.

[1]Rajlaxmi Chaudhary, [2]Dr. Mukesh Thakur, [3]Dr. S. S. K. Deepak

[1]Rungta College of Engineering & Technology, Bhilai, (C.G.), India

[2]NMDC DAV Polytechnic, Jawanga, Geedam District -South Bastar, (C.G.), India

[3]Assistant Professor, Bhilai Institute of Technology, Raipur, (C.G.), India

Abstract

At present, the level of pollution caused by vehicles are continuously increasing. Considering this problem and further work in this area, the automotive engine exhaust gases through the designed nano-coated catalytic converter reduce the concentration of pollutants. To improve it, time can be saved by reducing the number of experiments by doing numerical simulation and mathematical modeling of its design. Basically a new design of catalytic converter has introduced in this paper and combustion equation has developed for the same using mass balance equation.

In addition, the effect of nano-catalysts on catalytic converter performance has been analyzed. In this paper, a one-dimensional model has developed using a combination of chemical reaction, heat and mass transfer between the exhaust gas and the catalyst surface. The modeled equations for the converter consist of a set of coupled partial differential equations that solved by using MATLAB's "PDPE" function. The variation of CO and HC concentration along the axial length using the copper nano catalyst and the effect of varying the load has been analyzed.

Keywords: Catalytic converter; Mathematical Modeling; Numerical simulation;MATLAB

Introduction

A catalytic converter is a device which removes the harmful pollutants by converting them into less toxic pollutants. This work particularly intended to design an optimized catalytic converter to reduce the extant of Carbon Monoxide and Hydrocarbons emitted at the outlet of the four-stroke engine. The ideal Packed Bed Reactor model has the most used model to design a practical catalytic converter. In order to, theoretically design a catalytic converter both the fluid–solid and intra-particle diffusion limitation can be considered negligible. Moreover, the fluid dynamic has described simply by a plug flow approach. To describe the system, the molar balance for the i^{th} component has written by choosing as integration volume, a slice of infinitesimal depth of either volume/ length of the packed pipe or catalyst mass (Figure 1).

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Figure 1: Ideal PBR Catalytic Converter Model.

Both mass and energy balance equations for the catalytic converter model shown in Figure 1, can be derived from the general conservation equation that can be written as follows:

$$[inlet_i] - [outlet_i] = [generation_i] \quad \ldots (1)$$

Model rate kinetics and Modeling Assumption

For the complete methane oxidation following reaction take place:

CH4 + 2O2 → CO2 + 2H2O

Some major Assumptions for modeling include:

I. Heat transfer through radiation has neglected for the gas in phase.
II. Uniform gas properties assumed.
III. Axial diffusion is very small, neglected.
IV. Flow through a single channel is assumed.
V. The concentration of catalysts is constant.
VI. The heat released by the reactions is entirely transferred to inside catalytic converter through convection.
VII. Heat exchange among the substrate and the surroundings at both outlet and inlet faces is neglected.

Methodology for solving dimensionless equations

A one-dimensional model introduced for a catalytic converter which has constant gas temperature, solid temperature and gas concentration is formed using assumption where only axial gradients are considered. Dimensionless equations in with partial differential equations (PDEs), which are solved using "pdpe" function of MATLAB.

By introducing the correct terms, it is possible to obtain the following mass balance equation:

$$u\frac{\partial C_i}{\partial z} = \sum_{k=1}^{Nr} v_{ik} r_k \rho_B \quad \ldots (2)$$

Where,

$$u = \frac{\dot{V}}{a\,\varepsilon_B}, \text{ linear fluid velocity in m/s} \quad \ldots (3)$$

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Particularly C_i is the concentration of i^{th} component in the bulk phase, u the linear fluid velocity [m/s] obtained by the volumetric flow rate and the free section of the pipe, the reaction rate r given for catalyst mass units [mol/ (kg s)], catalyst bulk density ρ_B.

The dynamic terms of mass balance equation as shown in equation (2) often neglected, usually when steady-state information needed output. Therefore, to simulate the transient state of the experiment, it is necessary to introduce the time derivatives in mass balance equation of equation (1) as:

$$\frac{\partial C_i}{\partial t} = -u\frac{\partial C_i}{\partial z} + \sum_{k=1}^{Nr} v_{ik} r_k \rho_B \quad \ldots (4)$$

We can also write above equation as:

$$\frac{\partial C_i}{\partial z} = -\frac{1}{u}\frac{\partial C_i}{\partial t} + \frac{1}{u}\sum_{k=1}^{Nr} v_{ik} r_k \rho_B \quad \ldots (5)$$

The mass balance generalized equation shown in equation (5) has to be rearranged according the requirement of the present work. As discussed earlier this paper deals with the designing of catalytic converter for the reduction in Carbon Monoxide and Hydrocarbons emitted at the outlet of the four-stroke engine. Hence, equation (5) can be rearranged for governing for CO and HC separately as given by:

$$\frac{\partial C_{i,CO}}{\partial z} = -\frac{1}{u}\frac{\partial C_{i,CO}}{\partial t} + \frac{1}{u}\sum_{k=1}^{Nr} v_{ik} r_k \rho_B \quad \ldots (6)$$

$$\frac{\partial C_{i,HC}}{\partial z} = -\frac{1}{u}\frac{\partial C_{i,HC}}{\partial t} + \frac{1}{u}\sum_{k=1}^{Nr} v_{ik} r_k \rho_B \quad \ldots (7)$$

In this case, partial differential equations must be solved, thus the correct definition of the boundary conditions required. The most common Boundary Conditions adopted for ideal catalytic converter are listed as follows:

$$C_{i,CO}\,|_{z=0} = C_{i,CO,\,feed} \quad \ldots (8)$$

$$C_{i,HC}\,|_{z=0} = C_{i,HC,\,feed} \quad \ldots (9)$$

$$\frac{\partial C_{i,CO}}{\partial z}\,|_{z=L} = 0 \quad \ldots (10)$$

$$\frac{\partial C_{i,HC}}{\partial z}\,|_{z=L} = 0 \quad \ldots (11)$$

The gas concentrations are fixed at a given value, as no back-mixing possible due to the ideal condition. At the outlet of the catalytic converter, a zero derivative has assumed.

It is important to mention here, that the system temperature greatly affects the reaction rates through the temperature dependence of the kinetic constant. The well-known Arrhenius equation expresses this dependency as:

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$$k_i = k_{iref} \exp\left[\frac{E_{cat,i}}{R}\left(\frac{1}{T_{ref}} - \frac{1}{T}\right)\right] \quad \ldots (12)$$

Where k_{iref} the kinetic constant referred to a reference temperature T_{ref}, gas constant R, absolute temperature T and activation energy $E_{cat,i}$ for the reaction i. Finally reaction rate r_k of reaction k in mol/ (kg s) given by:

$$r_i = \sum_{i=1}^{Nr} k_i \times C_i \quad \ldots (13)$$

Simulation of Conventional Catalytic Converter

This section, presents simulation study of the conventional catalytic converter defined in equations (6) and (7) in the steady state for analyzing reduction capability for CO and HC. The simulation environment has been generated by the utilization of boundary conditions shown in equations (8) to (11) with the parameters defined in Table 1.

Table 1

S. No.	Parameter	Value
1	Catalyst surface Area (a) in m^2	268 m^2
2	Catalytic converter length (L) in m	0.2 m
3	Gas Velocity (v) in cm/s	1800 cm/s
4	Catalytic Converter Porosity (ε_B) in %	60 %
5	Catalyst bulk density (ρ_B) in kg/m^3	1500 kg/m3
6	Absolute Temperature (T) in K	340 K
7	Reference Kinetic Constant k_{ref}	$6.4314e^{-7}$ mol/(kg s)
8	Reference Temperature (T) in K	340 K
9	Activation Energy $E_{cat,i}$ in J/mol	92.232×10^3 J/mol
10	Gas Constant (R) in J/(K mol)	8.3144 J/(K mol)
11	Initial Concentration of CO in % ($C_{feed,CO}$)	1.41 %
12	Initial Concentration of HC in % ($C_{feed,HC}$)	178 in PPM

Now to simulate the partial differential equations of equation (6) and (7), "pdpe" function of MATLAB version 2020 has been utilized with the boundary conditions defined in equations (8) and (9) for the parameters defined in Table 1. The obtained reduction in CO and HC after simulation for the catalyst length z ranging from 0 to 2 cm for the time span of 0 to 1000 seconds are shown in Figure (2) and (3) respectively.

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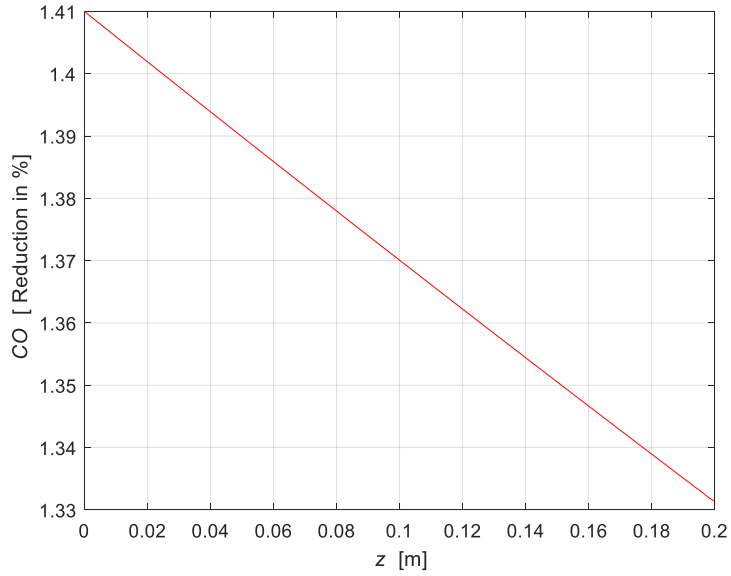

Figure (2) Change in CO concentration for different catalyst length.

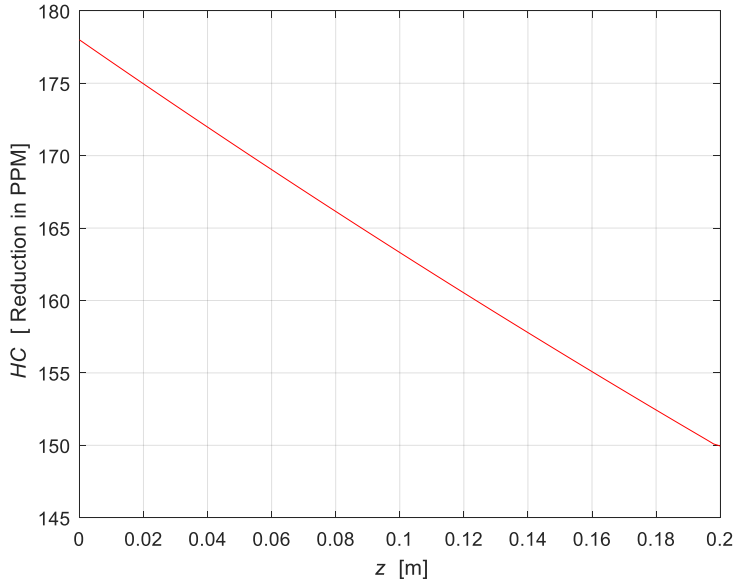

Figure (2) Change in HC concentration for different catalyst length.

Now, in order to compare the simulation results a conventional catalytic converter with the parameter listed in Table 1 has been attached to a 3 HP four stroke petrol engine and examined for various load conditions the output from the engine and the reduction obtained in CO and HC from the conventional catalytic converter.

In order to analyze the comparative efficiency of the simulation study of this work a comparison has been performed by generating simulated value for the catalytic converter output by using equations (6) and (7) for the values of engine output COWOCC and HCWOCC respectively along with engine load range of 5 to 12 kg. The comparative values of practical and simulation along with the percentage difference for CO and HC are given in Table 2 and Table 3 respectively.

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Table 2

Load in (Kg)	COWOCC in %	COWCC in %	SCOWCC in %	Percentage Error
5	1.41	1.33	1.33	0.000
6	1.36	1.27	1.28	0.787
7	1.3	1.21	1.22	0.826
8	1.25	1.17	1.18	0.855
9	1.11	1.08	1.04	3.704
10	1.08	0.952	0.95	0.210
11	0.971	0.885	0.91	2.825
12	0.885	0.793	0.83	4.666

Table 3

Load in (Kg)	HCWOCC in PPM	HCWCC in PPM	SHCWCC in PPM	Percentage Error
5	178	150	150	0.000
6	178	149	149	0.000
7	177	147	148	0.680
8	172	143	144	0.699
9	171	140	144	2.857
10	166	138	139	0.725
11	163	133	137	3.008
12	150	129	127	1.550

From Table (2) and Table (3) it has clearly observable, that the maximum percentage error obtained between practical and simulation values for COWCC and SCOWCC is 4.666% and for HCWCC and SHCWCC is 2.85%, which is very small and hence the simulation developed for this work to mimic the mathematical characteristics of conventional catalytic converter has very closed to practical and hence can be used for the development of optimized catalytic converter for this work.

Development of New Proposed Catalytic Converter

In order to achieve more reduction on CO and HC as compared to the conventional catalytic converter defined in previous section, this work proposes a new Catalytic Converter. The new proposed catalytic converter utilizes pores formation and coating of Copper Nano material to achieve higher reduction in CO and HC with less area and length. A physical model of the new proposed catalytic converter has developed as per the parameters then practically tested for different load conditions by attaching it with the same four-stroke petrol engine used in the analysis shown in previous section. The resultant values of the CO in % and the HC in PPM obtained from the new proposed catalytic converter.

From, obtained result, we have analyzed that the physically developed new proposed catalytic converter offers significant higher reduction in the CO and HC as compared to the conventional catalytic converter. This higher reduction has the result of increase in reaction rate due to utilization of copper

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Nano material coating in the new proposed catalytic converter design. Hence, the next task of this section has to be estimate the extant of increase in reaction rate offered by the new proposed catalytic converter, which will lead us towards the more compact and optimized catalytic converter for future work.

In order to estimate the increase in reaction rate the mathematical model defined in the equations (6) and (7) are again simulated for the catalyst parameters along with the boundary conditions defined in equations (8) to (11). The aim has to be obtain the increase in reaction rate which can provide the readings obtained for COWNCCC and HCWNCC, with various load conditions by taking COWOCC and HCWOCC as input to the catalytic converter simulation. To achieve this goal initially the Load has taken as 5 kg, COWOCC as 1.41 and the desired COWNCCC taken as 1.31 for CO analysis, HCWOCC as 178 and HCWNCCC taken as 130 for HC analysis. The variations in COWNCCC and HCWNCCC with respect to increase in reaction rate shown in Figure (3) and Figure (4) respectively.

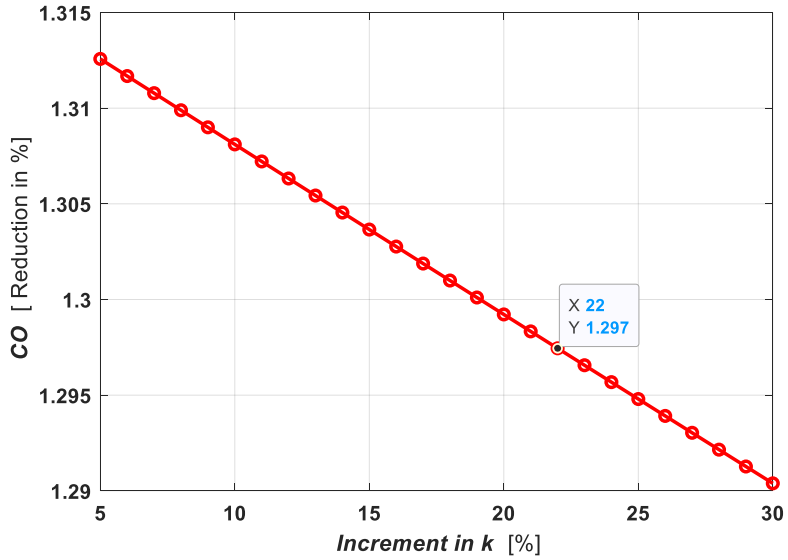

Figure (3) Variation in CO with respect to increase in reaction rate for new proposed catalytic converter.

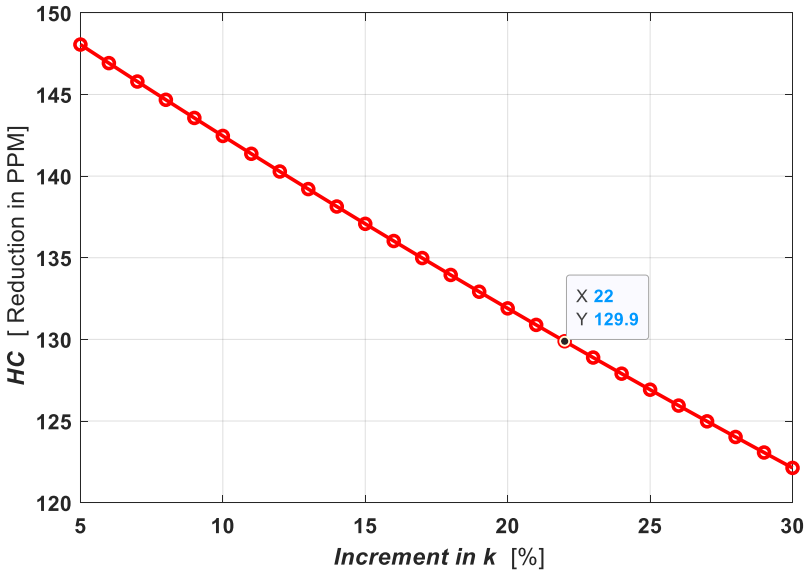

Figure (4) Variation in HC with respect to increase in reaction rate for new proposed catalytic converter.

DOI : https://doi.org/10.56452/7-780

From the plots of Figure (3) and (4), which shows obtained variations in CO and HC by increase in the reaction rate, we can easily estimate that the desired value of increase reaction rate for both the cases of CO and HC equal to 22%. The new proposed catalytic converter provides **22%** of average increase in reaction rate as compared to the conventional catalytic converter.

Development of Final Optimized Catalytic Converter

This subsection propose a final optimized catalytic converter to achieve more reduction on CO and HC as compared to the new proposed catalytic converter developed in previous section. The main aim has to be develop a compact catalytic converter that can provide higher reduction on CO and HC as compared to the new proposed catalytic converter with smaller length and less catalyst surface area. In order to achieve this aim the increment in reaction rate of 22% has set for the proposed final optimized catalytic converter as the main reaction rate. The final optimized catalytic converter also uses copper Nano material coating similar to the new proposed catalytic converter. However, to make the more compact now the porosity should be increased. For the proposed final optimized catalytic converter, the porosity has increased to 13.33 % by utilization of more coating and pores in the design. With the reaction rate increment of 22 % and porosity of 68 instead of 60 along with the other parameters, the length and area of the proposed final catalytic converter has estimated which can provide higher reduction rate in CO and HC as compared to the new proposed catalytic converter.

The plot of variations in CO and HC after simulating equations (6) and (7) for the above mentioned parameters with respect to change in catalyst length are shown in Figure (5) and (6).

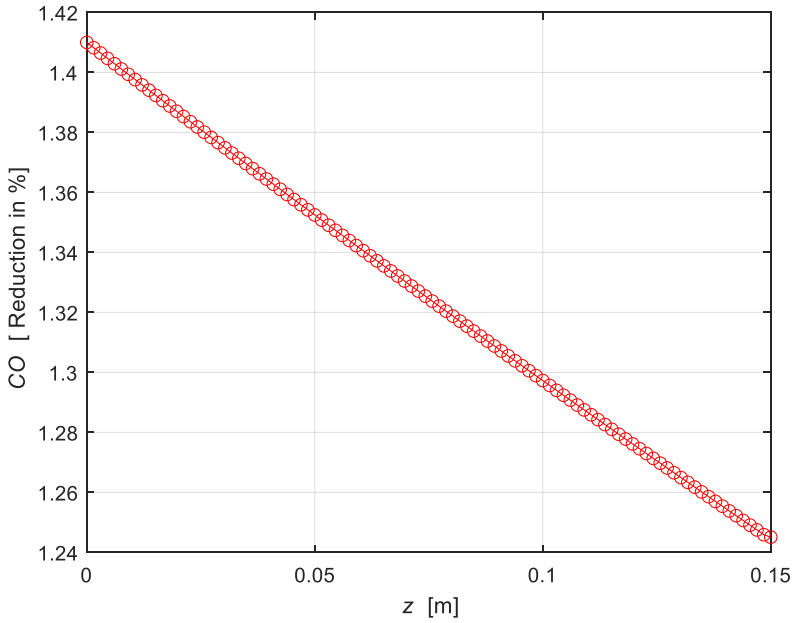

Figure (5) Variation in CO with respect to change in length of final optimized catalytic converter.

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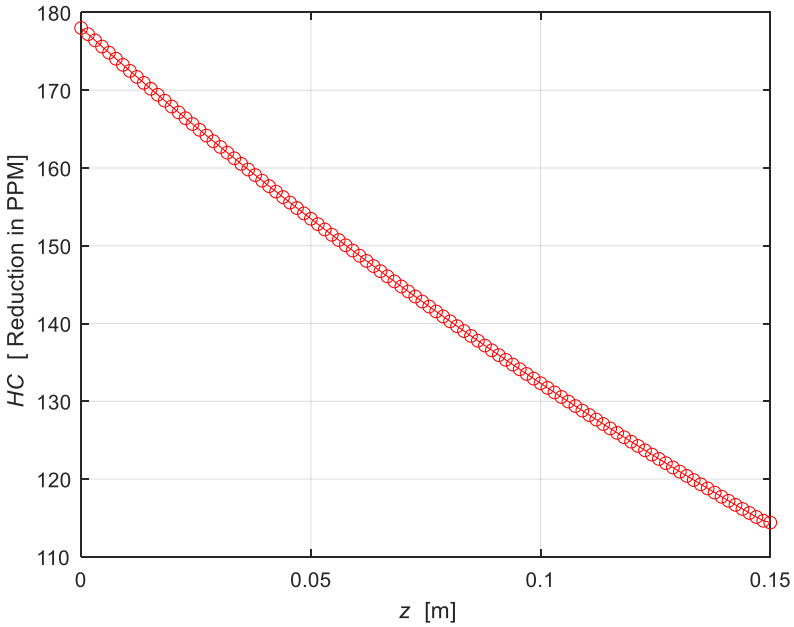
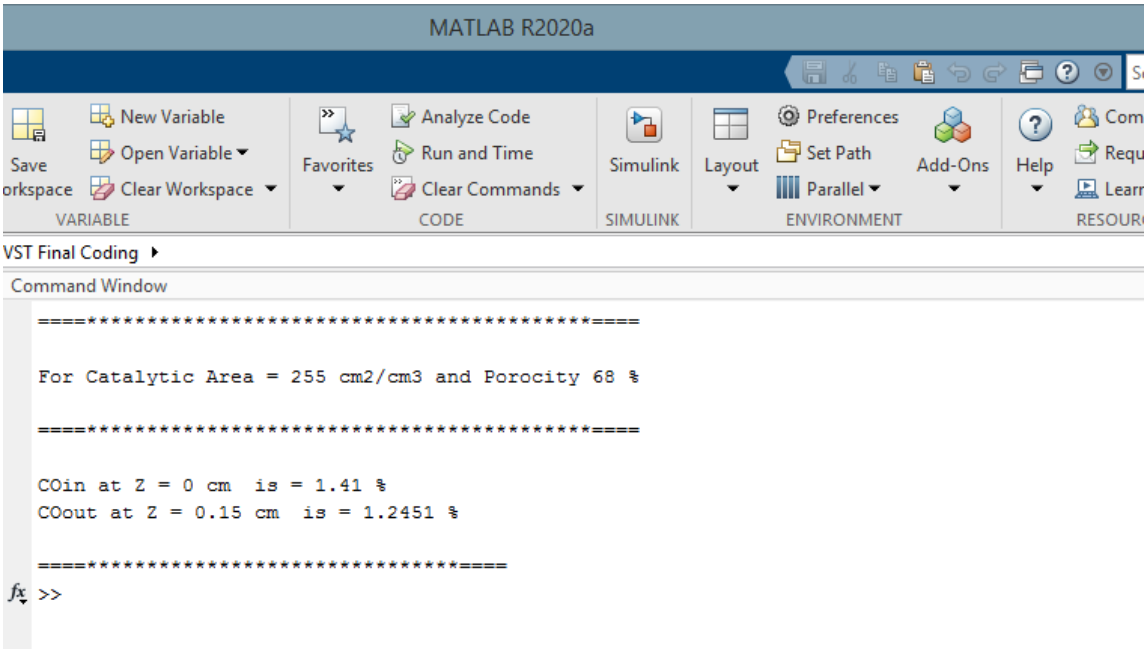


Figure (6) Variation in HC with respect to change in length of final optimized catalytic converter.

After several iterations the optimized value of area and length for the final optimized catalytic converter for the CO and HC reduction has obtained and shown in MATLAB command window is shown in Figure (7).



(a) For CO

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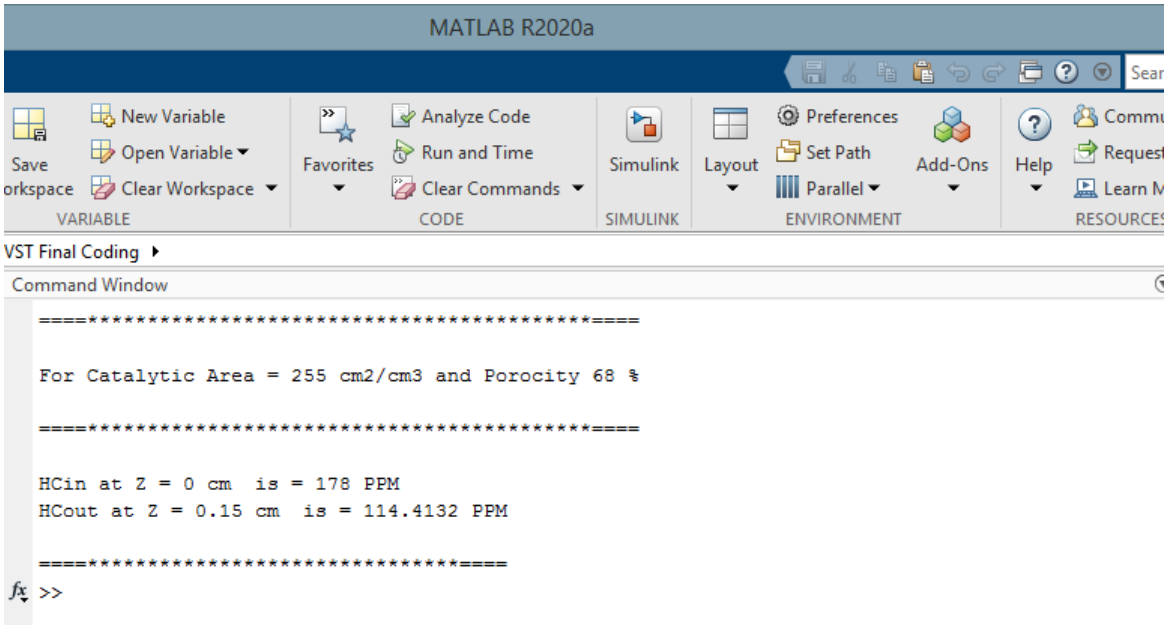

(b) For HC

After getting final values of optimized length as 0.15 m or 1.5 cm and the optimized areas as 255 cm^2, the final task has to obtained the different values of reduced CO and HC for various load conditions of the engine and perform a comparative analysis against the previous catalytic converters. The resultant values of the CO in % and the HC in PPM obtained after simulation of final optimized catalytic converter with parameters along with the length L = 0.15 m and Area a = 255 cm^2 shown in Table 4 and Table 5 respectively.

Table 4

Load in (Kg)	COWOCC in %	COWCC in %	COWNCCC in %	COWFOCC in %
5	1.41	1.33	1.29	1.24
6	1.36	1.27	1.23	1.20
7	1.3	1.21	1.17	1.14
8	1.25	1.17	1.14	1.10
9	1.11	1.08	1.04	0.98
10	1.08	0.952	0.922	0.91
11	0.971	0.885	0.845	0.82
12	0.885	0.793	0.701	0.68

DOI : https://doi.org/10.56452/7-780

Table 5

Load in (Kg)	HCWOCC in PPM	HCWCC in PPM	HCWNCCC in PPM	HCWFOCC in PPM
5	178	150	130	114.41
6	178	149	129	114.41
7	177	147	127	113.77
8	172	143	123	110.55
9	171	140	120	109.91
10	166	138	118	106.69
11	163	133	114	104.77
12	150	129	110	96.41

From, Table 4 and Table 5, we can easily analyze that in the simulation environment performed in MATLAB the final optimized catalytic converter offers significant higher reduction in the CO and HC as compared to the conventional and new proposed catalytic converters.

Conclusion

For reducing the harmful effect of exhaust pollution hear a newly designed nano coated catalytic converter has been introduced and for that the combustion equation has been developed using mass balance equation. The result of nano-catalysts on the catalytic converter performance was analyzed and for that one-dimensional model was developed using combination of chemical reaction, the heat & mass transfer between the exhaust gas and the catalytic surface. The modeled equations for the converter comprised of a set of coupled partial differential equations which are solved using "pdpe" function of MATLAB.

Then from developed mathematical modeling and by using numerical simulation Comparison results are carried out for various load and also the new proposed designed and conventional with simulating technic. Result shows that about 22% reaction rate is increased, that's why gases pollutant concentration in exhaust gas has 20-30% decreased.

Nomenclature

a = Catalyst surface in m^2

C_i = Concentration of component i in the bulk phase in mol/m^3

L = Catalytic converter length in m

N_r = Number of reactions (dimensionless)

r_k = Reaction rate of reaction k in mol/ (kg s)

t = Time in seconds

V = volume of catalytic converter in m^3

$\dot{V}$ = Fluid flowrate in m^3/s

w_{cat} = Catalyst mass in kg

z = Catalytic converter length coordinate in m

ε_B = Catalytic Converter Porosity (dimensionless)

ρ_B = Catalyst bulk density in kg/m^3

$v_{i,k}$ = Stoichiometric coefficient of component i in reaction k (dimensionless)

COWOCC = Engine output: CO Without Catalytic Converter.
COWCC = Catalytic Converter output: CO With Catalytic Converter.
HCWOCC = Engine output: HC Without Catalytic Converter.
HCWCC = Catalytic Converter output: HC With Catalytic Converter.
SCOWCC = Simulated Catalytic Converter output: Simulated CO With Catalytic Converter.

SHCWCC = Simulated Catalytic Converter output: Simulated HC With Catalytic Converter.

COWNCCC = Catalytic Converter output: CO With New Proposed Catalytic Converter.

HCWNCCC = Catalytic Converter output: HC With New Proposed Catalytic Converter.

COWFOCC = Catalytic Converter output: CO With Final Optimized Catalytic Converter.

HCWFOCC = Catalytic Converter output: HC With Final Optimized Catalytic Converter.

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