Emission Characteristics and Performance of Catalytic Converter: A Review

Ashish Kumar Soni

Research Scholar, Trinity Institute of Technology and Research, RGPV Bhopal, Madhya Pradesh, India

ABSTRACT

In recent years, several strategies such as fuel treatment, engine modification, EGR and catalytic converter have been introduced to control emissions from vehicles. Catalytic converter equipment is efficient and commonly used. Catalytic converters reduce emissions of carbon monoxide, hydrocarbons, nitrogen oxides and particulate matter from internal combustion engines and allow more strict pollution standards to be met. In this study paper different methods and strategies to increase efficiency of catalytic converter is discussed. The efficiency of the catalytic converter is updated according to literature survey improvements in design, shape and content. The hexagonal monolith shape was found to have better mechanical efficiency than the square shape. Catalytic converters based on nickel have cut HC by 40 percent and CO by 35 percent. Nobel metals are toxic and costly, so we can use non-noble metals such as Cu, Ag, Au, Fe, etc.

KEYWORD: *Diesel engine, Engine performance, Emission, Catalytic Converter, IC Engine*

1. INTRODUCTION

Because of their comparatively high emissions and poor performance, internal combustion (IC) engines for automotive propulsion face significant challenges. Nonetheless, conventional forecasts suggest that IC engines, at least as components of hybrid electric power trains, will still be commonly used for a reasonably long time [1]. Major attempts are also being made by the automobile industry to further limit IC engine emissions, i.e. carbon monoxide (CO), hydrocarbon (HC), nitrogen oxides (NOx) and particulate matter (PM) [2]. To this end, after-treatment methods have been successfully introduced in spark ignition (SI) and compression ignition (CI) engines, such as three-way catalysts (TWCs)[3], diesel oxidation catalysts (DOCs)[4], selective catalytic reduction (SCR) systems[5], and diesel particulate matter filter (DPFs)[6].

1.1. Catalytic Convertor

Nowadays, automobiles are one of life essentials. This need encouraged the industry to increase the production of automobiles. Most automobiles produced are operated with fuel for which combustion is necessary. This combustion process is associated with releasing harmful emissions including carbon monoxide (CO), unburnt hydrocarbons (HC) and nitrogen oxides (NOx) which have negative effects on humans and the environment. This has led to the development of emission control units to treat exhaust gases and convert them to less harmful products. These units are called catalytic converters (Kummer, 1980 and Taylor, 1984).

1.1.1. Construction

Catalytic converters consist of honeycomb-like structures often referred to as "the monolith substrate" as shown in Figure 1.1, the catalyst which primary consists of one or more noble metals that facilitate the oxidation and reduction chemical reactions and a padding mat surrounding the substrate that helps in maintaining higher temperatures necessary for the continued operation of the converter.

The monolith substrate is typically constructed of a ceramic material namely cordierite and is shaped into a honeycomb structure to maximize the surface area to promote the chemical reaction (Heck et al. 2001, Heck and Farrauto 2001 and Shuai and Wang 2004). This honeycomb structure is loaded with the wash coat. The wash coat consists of aluminum oxide, silicon dioxide, titanium dioxide or a mixture of alumina and silica (Kummer 1980 and Ramanathan et al. 2004). The wash coat increases the surface roughness of the substrate to increase the overall surface area and act as a catalyst carrier due to its high porosity (Richardson et al. 2003).

Figure 1 Ceramic Substrate

The catalysts used are noble metals mostly palladium, rhodium and platinum. These noble metals are oxidation and reduction catalysts (Chen et al. 2004, Gandhi et al. 2003 and Kummer 1980). The oxidation reactions require enough oxygen to complete the reaction. Ceria-zirconia acts as an oxygen storage medium supply and is embedded in the wash coat as wall (Masui et al. 2000, Matsumoto, 2004 and Yao and Yao, 1984). The ceramic substrate is holding the wash coat that carries the catalyst within its porous structure. The catalytic converter assembly is placed after the exhaust manifold and downstream of the internal combustion engine of the automobile to receive the harmful exhaust gases and convert them to more environmentally friendly ones. There are two main types of catalytic converters for gasoline engine applications.

The first type is "two-way catalytic" converters in which two chemical reactions take place; oxidation of CO to CO_2 and oxidation of unburnt HCs to CO_2 and water vapor. Two-way catalytic converters were widely used for diesel and gasoline engines and are no longer used since 1981 as they don't treat NOx emissions.

The second type is "three-way catalytic" converters (TWCC). TWCC incorporate three chemical reactions; two oxidation reactions (similar to "two-way catalytic converters ") and a reduction reaction in which NOx are converted to O_2 and N_2 (Diesel Net 2004; Kummer 1980; Pontikakis et al. 2004).
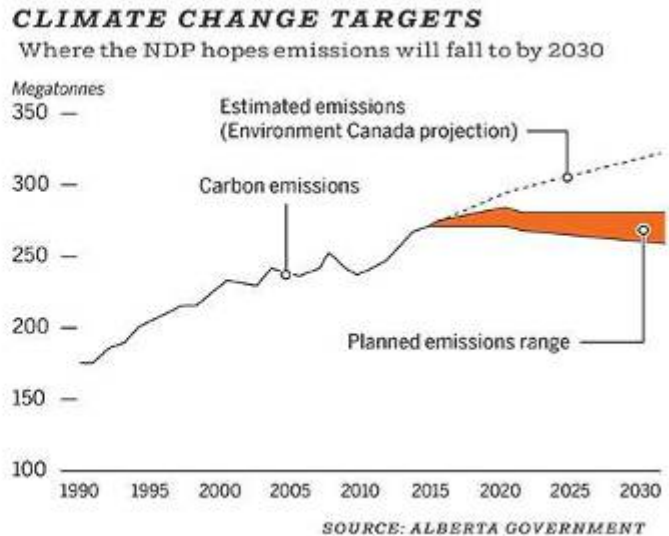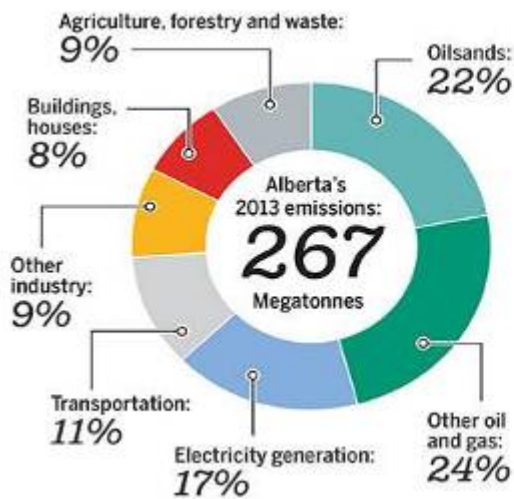

Figure 2 Global GHG productions

1.2. Placement of catalytic converter

Catalytic converters require temperature of 800 degrees Fahrenheit (426 °C) to efficiently convert harmful exhaust gases into inert gases, such as carbon dioxide and water vapor. Therefore, the first catalytic converters were placed close to the engine to ensure fast heating. However, such placing caused several problems, such as vapor lock. It occurred several minutes after the engine is shut off, as the heat from the catalytic converter influences fuel in the fuel lines, which makes it first boil and then aerate. This condition of fuel results in non-start condition, which lasts until the engine and fuel in the lines cool down. As an alternative, catalytic converters were moved to a third of the way back from the engine, and were then placed underneath the vehicle.
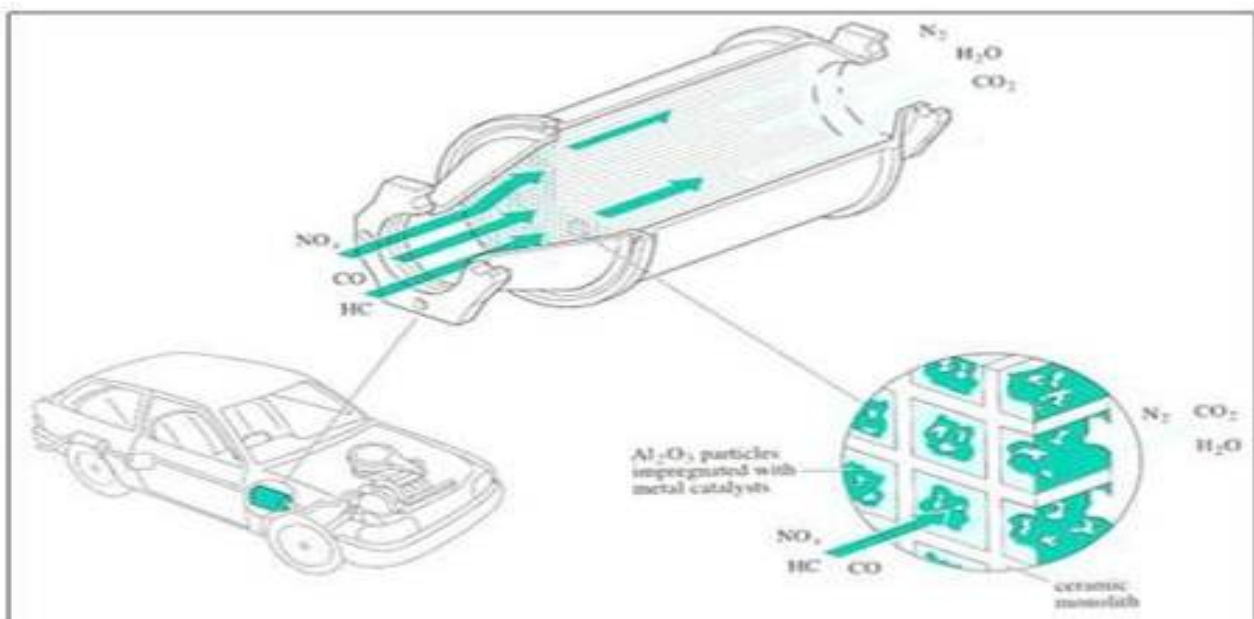

Figure 3 Placement of a catalytic converter

1.2.1. Types of catalytic converter

A. Two-way catalytic converter:
A 2-way (or "oxidation", sometimes called an "oxi-cat") catalytic converter has two simultaneous tasks:
I. Oxidation of carbon monoxide to carbon dioxide: $2 CO + O_2 \rightarrow 2 CO$
II. Oxidation of hydrocarbons (unburnt and partially burned fuel) to carbon dioxide and water: $C_xH_{2x+2} + [(3x+1)/2] O_2 \rightarrow x CO_2 + (x+1) H_2O$ (a combustion reaction).

This type of catalytic converter is widely used on diesel engines to reduce hydrocarbon and carbon monoxide emissions. They were also used on gasoline engines in American- and Canadian-market automobiles until 1981. Because of their inability to control oxides of nitrogen, they were superseded by three-way converters. [5]

B. Three-way catalytic converter:
Three-way catalytic converters (TWC) have the additional advantage of controlling the emission of nitric oxide (NO) and nitrogen dioxide (NO_2) (both together abbreviated with NO_x and not to be confused with nitrous oxide (N_2O)), which are precursors to acid rain and smog.

Since 1981, "three-way" (oxidation-reduction) catalytic converters have been used in vehicle emission control systems in the United States and Canada; many other countries have also adopted stringent vehicle emission regulations that in effect require three-way converters on gasoline-powered vehicles. The reduction and oxidation catalysts are typically contained in a common housing; however, in some instances, they may be housed separately. A three-way catalytic converter has three simultaneous tasks:

Reduction of nitrogen oxides to nitrogen (N_2)
➢ $2 CO + 2 NO \rightarrow 2 CO_2 + N_2$
➢ hydrocarbon $+ NO \rightarrow CO_2 + H_2O(vapor) + N_2$
➢ $2 H_2 + 2 NO \rightarrow 2 H_2O(vapor) + N_2$

Oxidation of carbon monoxide to carbon dioxide
➢ $2 CO + O_2 \rightarrow 2 CO_2$

Oxidation of unburnt hydrocarbons (HC) to carbon dioxide and water, in addition to the above NO reaction
➢ hydrocarbon $+ O_2 \rightarrow H_2O(vapor) + CO_2$

These three reactions occur most efficiently when the catalytic converter receives exhaust from an engine running slightly above the stoichiometric point. For gasoline combustion, this ratio is between 14.6 and 14.8 parts air to one part fuel, by weight. The ratio for auto gas (or liquefied petroleum gas LPG), natural gas, and ethanol fuels are slightly different for each, requiring modified fuel system settings when using those fuels. In general, engines fitted with 3-way catalytic converters are equipped with a computerized loop feedback fuel injection system using one or more oxygen sensors though early in the deployment of three-way converters, carburetors equipped with feedback mixture control were used.

Three-way converters are effective when the engine is operated within a narrow band of air-fuel ratios near the stoichiometric point, such that the exhaust gas composition oscillates between rich (excess fuel) and lean (excess oxygen). Conversion efficiency falls very rapidly when the engine is operated outside of this band. Under lean engine operation, the exhaust contains excess oxygen, and the reduction of NO_x is not favored. Under rich conditions, the excess fuel consumes all of the available oxygen prior to the catalyst, leaving only oxygen stored in the catalyst available for the oxidation function.[4]

Closed-loop engine control systems are necessary for effective operation of three-way catalytic converters because of the continuous balancing required for effective NO_x reduction and HC oxidation. The control system must prevent the NO_x reduction catalyst from becoming fully oxidized, yet replenish the oxygen storage material so that its function as an oxidation catalyst is maintained.

Three-way catalytic converters can store oxygen from the exhaust gas stream, usually when the air–fuel ratio goes lean. When sufficient oxygen is not available from the exhaust stream, the stored oxygen is released and consumed. A lack of sufficient oxygen occurs either when oxygen derived from NO_x reduction is unavailable or when certain maneuvers such as hard acceleration enrich the mixture beyond the ability of the converter to supply oxygen.

1.3. Basic conversion of catalytic converter

3- Way converters working as two-catalyst process:
➢ Reduction
➢ Oxidation
➢ A sophisticated oxygen storage/engine control system to convert three harmful gasses- HC, CO and NO_x.

This is not an easy task: the catalyst chemistry required to clean up NO_x is most effective with a rich air/ fuel bias. To operate properly, a three- way converter first must convert NO_x (with a rich air/ fuel bias), then HC and CO (with a lean bias).
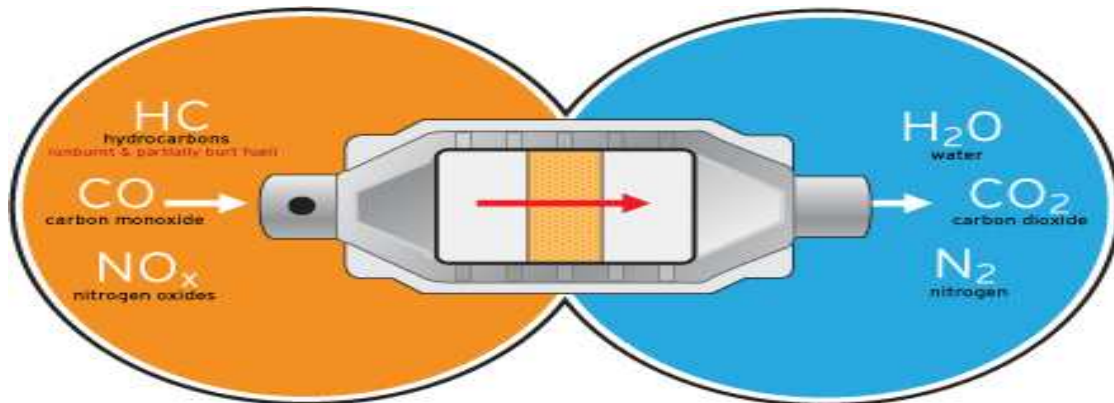
Figure 4 Basic Conversion of Catalytic Converter

1.4. Danger Pollutants
Without the redox process to filter and change the nitrogen oxides, carbon monoxides, and hydrocarbons into less harmful chemicals, the air quality (especially in large cities) would reach a harmful level to the human being.

➤ **Nitrogen oxides**- these compounds are in the same family as nitrogen dioxide, nitric acid, nitrous oxide, nitrates, and nitric oxide. When NOx is released into the air, it reacts with organic compounds in the air and sunlight, the result is smog. Smog is a pollutant and has adverse effects on children's lungs.

➤ **Carbon monoxide**- this form of CO_2 is a harmful variant of a naturally occurring gas. Odorless and colorless, this gas does not have many useful functions in everyday processes.

➤ **Hydrocarbons**- inhaling hydrocarbons from gasoline, household cleaners, propellants, kerosene and other fuels can cause death in children. Further complications can be central nervous system impairments and cardiovascular problems.
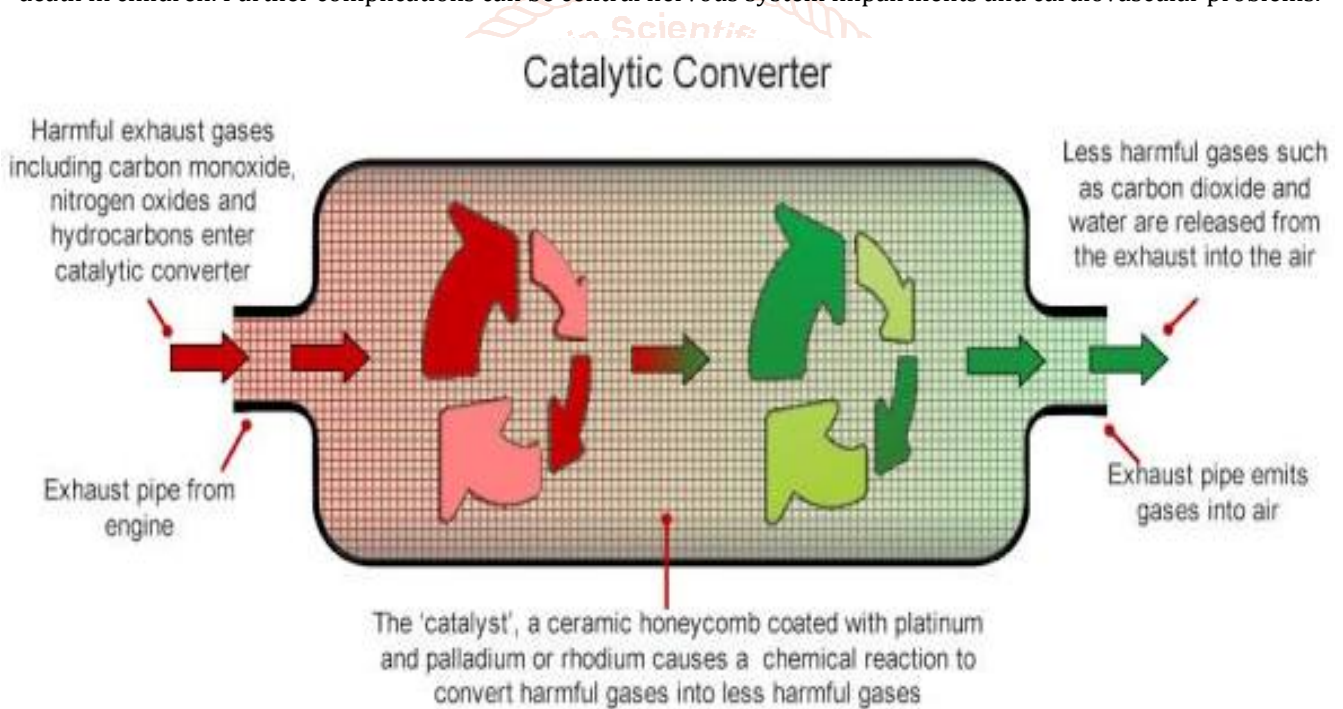

Figure 5 Working of Catalytic Converter

1.5. Methodology to reduce emissions
Emission control is one of the biggest challenges in today's automotive industry. Emission control can be achieved either by controlling combustion or by treating the exhaust gas. The latter is comparatively easier since there is less or no need to modify the engine itself. One such after treatment method is the use of catalytic converter. However, the 3-way converter is expensive due to use of both platinum and palladium/rhodium. One of the alternatives is the use of selective catalytic reduction, i.e., reduction of a particular mission based on the type of the engine used. The flow distribution across the monolith frontal area depends on the geometry of a specific design of inlet diffuser

As global automotive emission standards become more stringent, several efforts have been taken to determine the source of emissions and development of new technologies for controlling regulated and non-regulated emissions. An Automotive catalytic converter usually consists of a round, or oval shaped, monolith reactor encased in a metallic shell, and connected to the exhaust system through inlet and outlet cones.

Mainly, NOx, CO, and unburned hydrocarbons (HC). Significant effort has been invested into the design of a converter that will lead to maximum use of the catalyst volume. It is known that this maximum utilization of the catalyst volume would be achieved by having a uniform flow distribution through the monolith substrate. Therefore, most modern catalytic converters have long, tapered inlet and outlet headers to smooth the flow between sections of different cross-sectional areas. This tapered header provides

a uniform flow distribution across the monolith inlet face. A no uniform flow across the substrate leads to uneven residence time distribution and non-uniform poison accumulation during the catalyst aging.

2. LITERATURE REVIEW

Engine exhaust gas treatment has been a major concern for decades. In the thirties, automobile manufacturers realized the need to treat the products of the combustion process that occurred within the internal combustion engines (Farrauto and Heck, 1999). The initial solution for this challenge was the utilization of pellet catalytic converters. These pellets were the major component of the catalytic converters in the 1970s. The pellets were spherical particles with diameter ranging from 2.5 mm to 5 mm and made of gamma-alumina. The pellets were enclosed in a steel shell to form the catalytic converter and loaded with noble metals and stabilizers for the exhaust treatment .This catalytic converter technology had many disadvantages. Due to the shape of the pellets, a large pressure drop occurred across the converter which directly affected the performance of the engine. Moreover, the risk of losing the catalyst was higher due to particle wear (Diesel Net, 1998). These disadvantages encouraged scientists and engineers to develop monolithic catalytic converter which are being used today.

CFD simulations have been the most commonly used tool to evaluate the performance of the catalytic converter for the last three decades because they offer a great advantage in terms of time and cost efficiency. Researchers used CFD to predict the fluid behavior, thermal characteristics and conversion efficiency of the monolith substrates.

2.1. Previous work

For analysing the catalytic convertor the various researches have been study some of these are explained here.

Yugal Kishore et.al.2017 carried out a 3D CFD analysis on three way monolithic converter on the basis of it various conclusions have been drawn. The rates of conversion of NO, CO, C3H6 are the function of temperature. On increasing temperature the rate of surface reaction with the catalyst first increases and then become stable.

S. P. Venkatesanet.al 2017 has study on emission control of catalytic convertor by using copper oxide. The main aim of this work is to fabricate system, where the level of intensity of toxic gases is controlled through chemical reaction to more agreeable level. This system acts itself as an exhaust system; hence there is no needs to fit separate the silencer. The whole assembly is fitted in the exhaust pipe from engine. In this work, catalytic converter with copper oxide as a catalyst, by replacing noble catalysts such as platinum, palladium and rhodium is fabricated and fitted in the engine exhaust.

Vladimir Lozhkinet.al 2017 The purpose of investigation was the development of mathematic model of catalysis process in the mode of heat rejection ("discharge") of phase change storage device and substantiation of high efficiency of cleaning from harmful substances and possibility of device arrangement in the engine compartment of a bus instead of noise suppressor using calculation method proceeding from experimental data of converter operation in the city cycle.

Jeong and Kim 2016 numerically simulated the cold start of a vehicle when the catalytic converter is placed closer to the engine exhaust manifold. They considered a 3D, transient compressible reacting flow in the warm-up to investigate the effect of the warm-up period on the thermal behavior of the main catalyst and the emissions. They also examined the effect of the flow distribution as well as the catalyst loading on the temperature distribution and the emission performance. They concluded that flow maldistribution and large pressure drops occurred more significantly in the warm-up period of the catalyst systems. Moreover, during the warm-up stage, the velocity and temperature distributions have similar patterns due to the dominance of heat transfer by convection of the incoming exhaust gas. The catalyst did not contribute in the conversion of the exhaust gas during the warm-up process due to lower temperatures at the middle regions. Furthermore, when the space velocity was very large, concentrating the precious metal in the entrance will have no effect on the conversion efficiency which suggested taking the flow distribution into consideration when loading the precious metal within the warm-up catalytic converter to ensure higher conversion efficiencies.

Shamim et al. 2015 developed a numerical simulation to predict the performance of the three-way catalytic converter. The model incorporates heat conservation and chemical reaction sub model with oxygen storage mechanism and it showed that the conversion efficiency was improved when operating under rich oxygen content.

Groppi&Tronconi, 2014 investigated the heat and mass transfer for a monolith with equilateral triangular channels. They implemented 3-D modeling to approach the analysis in which they assumed a fully developed laminar flow and equal thermal and mass diffusivity. Their analysis concluded lower heat and mass transfer for the triangular channels due to the acute corners of the triangles compared to square and circular channels which resulted in reaching operating temperatures and lower gas heating rates for the coefficients of heat and mass transfer.

Chakravarty et al., 2013 utilizing multi-dimensional channel model. It was recorded that the ignition behavior can be dramatically affected by flow recirculation at the inlet of the substrate which lead to high flow maldistribution especially at lower exhaust temperatures. The study concluded that flow no uniformity effects were more significant with increasing flow temperature. In addition, the pressure drop distribution remained constant and was dependent on the recirculation pattern at the front face of the monolith.

Agrawal et al., 2013 developed a planar two-dimensional model to study the interactions between flow, reactions and thermal effects of the catalytic converter. They utilized a full-scale model consisting of 85 channels and a reduced-scale model consisting of 21 channels. They investigate the effect of the friction coefficient for the channels on the flow distribution. They investigated the effect of the flow distribution on the conversion of carbon monoxide. They concluded that the flow tends to be non-uniformly distributed with the flow expansion within the inlet diffuser. Moreover, the higher the pressure drop across the channels the more uniform flow distribution is obtained. The

implementation of the reduced-scale model yielded matching results to the full-scale model. Furthermore, the conversion efficiency of the catalytic converter decreased as the flow mal-destitution was increased and the reactions taking place within the monolith did not have any effect on the flow distribution.

Hayes et al., 2012 found that the flow distribution for reacting and non-reacting condition is a function of the catalytic converter properties like cell density, diffuser angle and aspect ratio of the monolith. In addition, the mass flow rate highly influenced the distribution. Moreover, faster light-off behaviorwas obtained with higher monolith cell densities. Dual monolith configurations with high cell density cores and low cell density at the periphery showed the worst flow uniformity.

Amirnordin et al., 2011 adopted a sub-scale model to predict the pressure drop of different sizes of the square and hexagonal cell shapes of the catalytic converter. They used the model to investigate the effect of the channel design on the performance of the catalytic converter. They tested various combination of wall thickness and cell density in their study and the developed model showed better results than the single channel model utilized commonly in the literature. They concluded that the hexagonal cells are dynamically more efficient as they offer lower pressure drop compared to the square cells.

Liu et al. 2007 performed an experimental and a numerical study on the reverse flow catalytic converter for a natural gas/diesel dual engine. The simulation involved a 1-dimensional single channel model to monolith substrate. They concluded that the conversion efficiency of CO and HC was improved for the reverse flow catalytic converter for low inlet temperature and light engine load only when the catalytic converter initial temperature is high enough given that the converter initial temperatures was varied from 694 K to 919 K.

Guojiang& Song, 2005 utilized a 2D symmetrical transient model to study the effect of the flow and temperature distribution on the performance of the catalytic converter and introduced a honeycomb spherical at the exit of the inlet pipe to redistribute the flow across the inlet face of the monolith and investigated the flow distribution. The arc improved the flow distribution with a small increase in pressure drop which can be reduced by manipulating the opening area of the arc and cross section area of the pipe.

Chen et al. 2004 utilized a 3D CFD flow modeling and a heterogeneous reaction model of the catalytic converter. They calculated the pressure and the velocity field with incorporating the flow resistance within the monolith substrate. They concluded that the flow field is influenced by the monolith substrate resistance for a specific geometry and Reynolds number. Moreover, the flow uniformity at the front face increased with increasing cell density of the monolith and decreased when increasing the flow Reynolds number.

Chen and Schirmer 2003 employed a semi-empirical 0-D steady state catalyst model and a 1-D transient plug flow model to optimize the design of the catalytic converter for internal combustion engines. They utilized CFD simulations and modeled the monolith substrate as a porous medium with empirically calculated viscous and inertial resistances. They solved the flow field over a perforated plate as an inlet condition to the monolith substrate. They concluded that the assumption of the perforated plate was reasonable as a surface of pressure discontinuity. Moreover, they observed higher flow uniformity with installation of a perforated plate at the front face of the monolith substrate.

Cho et al, 1998 studied the flow distribution for steady and transient flow conditions. They investigated the flow distribution at the exit of the first monolith of a two-brick system under the assumption that the flow through each channel does not interfere with the flow in adjacent channels. Steady tests yield more flow maldistribution than the transient tests and the configuration of the exhaust manifold has a significant influence on the flow distribution within the monolith.

Holmgren et al. 1997 investigated the effect of shaping the inlet face of the monolith on the flow distribution utilizing the flat, parabolic and conical shapes. They implemented a 3D, isothermal, incompressible and axisymmetric model to predict the flow field in the exhaust pipes and a 1D laminar flow model was used to model the monolith and the study concluded that using parabolic and conical monolith inlet face increases the efficiency and the utilization of the catalyst hence the conversion efficiency and reduces the pressure drop due to the shorter channels at the periphery.

Lai et.al 1991 and 1992 studied the effect of the exhaust manifold geometry on the flow distribution as bent pipes tend to distort the flow and increase the flow maldistribution. They utilized 3D simulations with incorporation of the brick resistance to the simulation to obtain accurate predictions. They concluded that the flow becomes more uniformly distributed when the inlet pipe is shorter in length and the bending angle is smaller. Moreover, they investigated the effect of brick properties on the flow distribution concluding that the higher the brick resistance the more uniform the flow distribution is observed.

Bella et al. 1991 utilized 3D simulations to model the flow inside the exhaust manifold and concluded that with the existence of the inlet diffuser, the flow became significantly more uniformly distributed. Complimentary conclusion reached by **Chen and Schirmer 2003**; **Hayes et al. 2012** who implemented 0D steady state catalyst model, 1D transient plug model and 2D model to further investigate the design of the inlet diffuser. They stated that with increasing the inlet diffuser angle, the flow tends to be non-uniformly distributed and that effect is more severe when increasing the volume flow rate. **Hayes et al. 2012** in investigating the effect of the diffuser angle on the flow uniformity index which is an indication on the variation of the local velocity from the average velocity at the upstream face of the monolith.

3. CONCLUSIONS
The above-mentioned researchers had studied various aspects of catalytic converter and various methods to implement in catalytic converter to reduce emission rate in various catalytic converter. In some research works, the study was focused on to reduce emissions in catalytic converter. However, there was no work found which considered cumulative an attempt a work in the field of

geometry changes in catalytic converter in terms of emission reduction.

Yugal Kishore et.al 2017: in the simulation analysis work titled "CFD ANALYSIS OF THREE WAY MONOLITHIC CATALYTIC CONVERTER USING ANSYS "carried out a 3D CFD analysis on three way monolithic converter on the basis of it various conclusions have been drawn. The rates of conversion of NO, CO, C_3H_6 are the function of temperature. On increasing temperature the rate of surface reaction with the catalyst first increases and then become stable and obtained the following results**:**

➤ The rates of conversion of NO, CO, C_3H_6 are the function of temperature.
➤ On increasing temperature the rate of surface reaction with the catalyst first increases and then become stable.
➤ The present proposed model has higher NOx conversion rate as compared to other species.
➤ Increasing mass flow rate the pressure drop increases linearly.
➤ On increasing flow velocity pressure drop across the substrate and converter drastically increases.
➤ Cell density of substrate plays crucial role in flow uniformity.
➤ At high Reynolds number i.e. above 40000 due to turbulence flow uniformity affects and the turbulence can be seen across the radial region and the outlet.
➤ Porosity of substrate extensively gets affected at high temperature and the rate of species conversion decreases.

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