CFD Analysis of Catalytic Converter to reduce Particulate

Matter and To Achieve light off Temperature early with more Surface Area of the Monolithic Structure.

> A Project Report Submitted in partial fulfilment For the award of the Degree of Bachelor of Technology In the Department of Mechanical Engineering



(Academic Session: 2017-2021)

Submitted by:		
M. Jyothi Swaroop	(16ME8003)	
Clan Aby Philip	(17ME8014)	
Deepanjan Jha	(17ME8070)	
B. Lokesh Naga Sai	(17ME8101)	
Sougata Sarkar	(17ME8126)	

Project Guide:

Prof. Biswajith Halder

Department of Mechanical Engineering National Institute of Technology, Durgapur

DEPARTMENT OF MECHANICAL ENGINEERING NATIONAL INSTITUTE OF TECHNOLOGY DURGAPUR, INDIA.

CERTIFICATE

This is to certify that the project entitled "CFD Analysis of Catalytic Converter to reduce Particulate Matter and To Achieve light off Temperature with more Surface Area of the Monolithic Structure", submitted jointly by M. Jyothi Swaroop, Deepanjan Jha, Clan Aby Philip, B. Lokesh Naga Sai, Sougata Sarkar of Mechanical Engineering Department, National Institute of Technology Durgapur, in partial fulfilment of the requirement for award of the degree in Bachelor of Technology in Mechanical Engineering is a bonafide record of work carried out by them under my guidance during the academic year 2020-2021.

> (Biswajith Halder) Professor Department of Mechanical Engineering National Institute of Technology Durgapur.

DECLARATION

We, hereby declare that the discussion entitled 'CFD Analysis of Catalytic Converter to reduce Particulate Matter and To Achieve light off Temperature with more Surface Area of the Monolithic Structure.' being submitted by us towards the partial fulfilment of the degree of bachelor of technology, in the department of Mechanical Engineering is a project work carried by us under the supervision of Prof.Biswajith halder and have not been submitted anywhere else.

Date:_____

M. Jyothi Swaroop	(16ME8003)
Clan Aby Philip	(17ME8014)
Deepanjan Jha	(17ME8070)
B. Lokesh Naga Sai	(17ME8101)
Sougata Sarkar	(17ME8126)

ACKNOWLEDGEMENT

We like to share our sincere gratitude to all those who help us in completion of the project. During the work we faced many challenges due to our lack of knowledge and experience but these people help us to get over from all the difficulties and in final completion of our idea to a shaped sculpture.

We would like to thank Prof.Biswajith halder for his guidance and governance, because of which our team was able to learn the minute aspects of the project work and about the related topic.

In the last we would like to thank the management of National Institute of Technology, Durgapur for providing us such an opportunity to learn from these experiences.

We are also thankful to all the staffs and faculty members of the mechanical engineering department of National Institute of Technology, Durgapur, for their help and support towards the project and our team.

We are also thankful to our whole class and most of all to our parents who inspired us face all the challenges and win all the hurdles in our life.

Thank you all,

M. Jyothi Swaroop	(16ME8003)
Clan Aby Philip	(17ME8014)
Deepanjan Jha	(17ME8070)
B. Lokesh Naga Sai	(17ME8101)
Sougata Sarkar	(17ME8126)

ABSTRACT

A catalytic converter is an exhaust emission control device that reduces toxic gases and pollutants in exhaust gas from an internal combustion engine into less-toxic pollutants by catalyzing a redox reaction (an oxidation and a reduction reaction). Catalytic converters are usually used with internal combustion engines fueled by either gasoline or diesel—including leanburn engines as well as kerosene heaters and stoves. One problem is that they only really work at high temperatures (over 300°C/600°F or so), when the engine has had chance to warm up. Early types of catalytic converters typically took about 10–15 minutes to warm up, so they were completely ineffective for the first few kilometres/miles of a journey (or any part of a very short journey). Modern converters warm up in only 2–3 minutes; even so, significant emissions can still occur during this time.

Monolithic honeycomb structure coated with Noble metals as catalysts are used for this purpose. Noble metals cause a redox reaction and put a check on the emission of toxic elements. Thus, increases in contact time with noble metals, lesser the emission. Hence the larger surface area is preferred in the monolithic structure of catalytic converter for coating Noble metals

So, the objective of our project is based on finding solution to the emission released before light off temperature. The researchers had worked on it by increasing the surface area of the monolith and resulting it closer to the light off temperature during preheating. Through CFD analysis with appropriate conditions, it was found that monolith structures play a major role in influencing results.

TABLE OF CONTENTS:

Certificate Declaration Acknowledgement Abstract	
Chapter no.	page no.
1.Introduction:	7
1.1. Historical Background	7
1.2. Modern Day Development	8
1.3. Construction	9
1.4. Types	11
1.5. Installation	13
1.6. Benefits of installing catalytic converter	13
1.7. Disadvantages of removing catalytic converter	14
2. Design and material selection	16
2.1. Design calculations	16
2.2. material selection	18
3. selection of catalysts and adsorbents	19
3.1.Catalyst and its selection3.2.Adsorbent and its selection	19 20
4. Ceramic monolith structure	23
4.1.Modelling	23
4.2.design of proposed ceramic model	24
5. Results	27
6. Conclusions	37
7.References.	38

1. INTRODUCTION

Air pollution has been a major concern around the world. Climate change and lethal diseases being byproducts of this. Countries around the world are into achieving net zero emissions in order to preserve global average temperature increment below 1.5 degree Celsius before Industrial era. Kyoto Protocol, Paris agreement are some of the efforts.

India being one of the most polluted countries in the world, it was found out that the vehicular emission is the major contributor for its highly polluted environment. Transition from BS-IV to BS-VI and scrappage policy were the steps taken by the Government.

These factors made us choose the project regarding improving the efficiency of catalytic converters. Catalytic converters detoxify the air pollutants (CO, NO_x etc.) to less harmful gases (H₂O, CO₂ etc.). But these work only in high temperatures and significant amount of pollution occur during this pre-ignition period.

The project is about how an alternate solution can be achieved for before effects of light-off temperature emissions and to attain it quickly. Increasing the surface area, modifying the mesh pattern, using electric preheaters, using activated charcoal as the material were among the ideas proposed and by CFD analysis the feasibility of the ideas was analyzed.

Within the limitations and constraints in research, a feasible result was achieved which can be implemented for a better performance in catalytic converters which will also play a high impactful role in reducing air pollution in the environment.

1.1. HISTORICAL BACKGROUND:

Catalytic converter prototypes were first designed in France at the end of the 19th century, when only a few thousand "oil cars" were on the roads; it was constituted of an inert material coated with platinum, iridium, and palladium, sealed into a double metallic cylinder.

A few decades later, a catalytic converter was patented by Eugene Houdry, a French mechanical engineer and expert in catalytic oil refining, who moved to the United States in 1930. When the results of early studies of smog in Los Angeles were published, Houdry became concerned about the role of smokestack exhaust and automobile exhaust in air pollution and founded a company called Oxy-Catalyst. Houdry first developed catalytic converters for smokestacks called "cats" for short, and later developed catalytic converters for warehouse forklifts that used low grade, unleaded gasoline. In the mid-1950s, he began research to develop catalytic converters for gasoline engines used on cars. He was awarded United States Patent for his work.

Catalytic converters were further developed by a series of engineers including carl D. Keith, John J. Mooney, Antonio Eleazar, and Phillip Messina at Engelhard Corporation, creating the first production catalytic converter in 1973.

The first widespread introduction of catalytic converters was in the United States automobile market. To comply with the U.S Environmental protection agency 's new regulation of exhaust emissions, most gasoline-powered vehicles starting with the 1975 model year are equipped with catalytic converters. These "two-way" converters combined oxygen with carbon monoxide (CO) and unburned hydrocarbons (C_nH_n) to produce carbon dioxide (CO₂) and water (H_2O). These stringent emission control regulations forced the removal of the antiknock agent tetraethyl lead from automotive gasoline, to reduce lead in the air. Lead is a catalyst poison and would effectively destroy a catalytic converter by coating the catalyst's surface. Requiring the removal of lead allowed the use of catalytic converters to meet the other emission standards in the regulations.

1.2. MODERN DAY DEVELOPMENTS:

First improvement in catalytic converter was it was developed based on catalyst materials consisting of metal oxides such as Titanium dioxide (TiO2) and cobalt oxide (CoO) with wire mesh substrate. Both of the catalyst materials are inexpensive in comparison with conventional catalysts such as platinum or palladium. Another improvement is upon grafting Cerium Oxide to MnFeOy (CeO2/MnFeOy) and using this as a catalyst in the catalytic converter. By doing this the oxygen release was improved as compared to the oxygen release when we use CeO2/Fe2O3 or CeO2/Mn2O3 as a catalyst. The oxygen storage capacity (OSC) was also improved by using MnFeOy (CeO2/MnFeOy) as a catalyst. Next improvement was when a device was implemented that could combine all the catalyst functions into one catalyst. This was named as three way catalyst (TWC). It comprises of platinum or palladium to catalyse oxidation reaction and rhodium for reduction of the NOx.

Next improvement was using non-noble based catalytic converter instead of noble based catalytic converter because in the latter case the operating temperature is very high compared to the non-noble material and also in noble material based catalytic converter the cost is high and noble materials are rarely available into earth's crust. Another significant improvement was formation of a synthetic material based on the chemistry of iron silicate which acts as a catalyst for converting nitrogen oxides into nitrogen & oxide and also combining carbon monoxide & oxygen to convert them into carbon dioxide, which in result will improve to reduce the harmful emissions and this is also cheaper to manufacture.

1.3. CONSTRUCTION:

The catalytic converter's construction is as follows:

 The catalyst support or substrate For automotive catalytic converters, the core is usually a ceramic monolith that has a honeycomb structure (commonly square, not hexagonal). (Prior to the mid 1980s, the catalyst material was deposited on a packed bed of alumina pellets in early GM applications.) Metallic foil monoliths made of Kanthal (FeCrAl) are used in applications where particularly high heat resistance is required. The substrate is structured to produce a large surface area. The cordierite ceramic substrate is used in most catalytic converter



Cutaway of a metal-core converter



Ceramic-core converter

2. The washcoat. A washcoat is a carrier for the catalytic materials and is used to disperse the materials over a large surface area. Aluminium oxide, Titanium Dioxide, Silicon Oxide, or a mixture of Silica and Alumina can be used. The catalytic materials are suspended in the washcoat prior to applying to the core. Washcoat materials are selected to form a rough, irregular surface, which increases the surface area compared to the smooth surface of the bare substrate.

3. Ceria or ceria-zirconia. These oxides are mainly added as oxygen storage promoters.

4. The catalyst itself is most often a mix of precious metals, mostly from the platinum group. Platinum is the most active catalyst and is widely used, but is not suitable for all applications because of unwanted additional reactions and high cost. Palladium and rhodium are two other precious metals used. Rhodium is used as a Reduction catalyst, palladium is used as an oxidation catalyst, and platinum is used both for reduction and oxidation. Cerium, Iron, Manganese, and Nickel are also used, although each has limitations. Nickel is not used because of its reaction with carbon monoxide into toxic Nickel Tetracarbonyl. Copper can be used everywhere.

Upon failure, a catalytic converter can be recycled into Scrap. The precious metal inside the converter, including platinum, palladium, and rhodium, are extracted.

PLACEMENT OF CATALYTIC CONVERTER

-Catalytic converters require a temperature of 800 degrees Fahrenheit (426 °C) to operate effectively. Therefore, they are placed as close to the engine as possible, or one or more smaller catalytic converters (known as "pre-cats") are placed immediately after the exhaust manifold.

1.4. <u>TYPES:</u>

1.Two-way

A 2-way (or "oxidation", sometimes called an "oxi-cat") catalytic converter has two simultaneous tasks:

1.Oxidation of Carbon Monoxide to Carbon Dioxide: 2 CO + $O_2 \rightarrow$ 2 CO₂

2. 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 threeway converters.

2.Three-way

Three-way catalytic converters have the additional advantage of controlling the emission of nitric oxide(NO) and nitrogen dioxide(NO₂) (both together abbreviated with NOx and not to be confused with nitrous oxide(N₂O)), which are precursors to acid rain and smog.

The reduction and oxidation catalysts are typically contained in a common housing; however, in some instances, they may be housed separately. A threeway catalytic converter has three simultaneous tasks

Reduction of nitrogen oxides to nitrogen (N₂)

- $C + NO_2 \rightarrow CO_2 + 2NO$
- $CO + NO \rightarrow CO_2 + \frac{1}{2}N_2$
- $2CO + NO_2 \rightarrow 2CO_2 + \frac{1}{2}N_2$
- $H_2 + NO \rightarrow H_2O + \frac{1}{2}N_2$

Oxidation of carbon, hydrocarbons, and carbon monoxide to carbon dioxide(CO_2)

• $C + O_2 \rightarrow CO_2$

•
$$\operatorname{CO} + \frac{1}{2} \operatorname{O}_2 \rightarrow \operatorname{CO}_2$$

• $aC_xH_y + bO_2 \rightarrow c CO_2 + d H_20$ a, b, c, d, x, y $\epsilon \mathbb{Z}$

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 autogas (or Liquified Petroleum gas LPG), natural gas, and ethanol fuels can vary significantly for each, notably so with oxygenated or alcohol based fuels, with e85 requiring approximately 34% more fuel, requiring modified fuel system tuning and components when using those fuels. In general, engines fitted with 3-way catalytic converters are equipped with a computerized closed-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.

Closed-loop engine control systems are necessary for effective operation of three-way catalytic converters because of the continuous balancing required for effective NOx reduction and HC oxidation. The control system is intended to prevent the NOx 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 NOx reduction is unavailable or when certain maneuvers such as hard acceleration enrich the mixture beyond the ability of the converter to supply oxygen.

Unwanted reactions

Unwanted reactions result in the formation of hydrogen sulpide and ammonia, which poison catalysts. Nickel or manganese are sometimes added to the washcoat to control of hydrogen-sulfide emissions. Sulfur-free or low-sulfur fuels eliminate or minimize problems with hydrogen sulfide.

1.5. Installation:

Many vehicles have a close-coupled catalytic converter located near the engine's exhaust manifold. The converter heats up quickly, due to its exposure to the very hot exhaust gases, enabling it to reduce undesirable emissions during the engine warm-up period. This is achieved by burning off the excess hydrocarbons which result from the extra-rich mixture required for a cold start.

When catalytic converters were first introduced most vehicles used carburetors that provided a relatively rich air-fuel ratio. Oxygen (O_2) levels in the exhaust stream were therefore generally insufficient for the catalytic reaction to occur efficiently. Most designs of the time therefore included secondary air injection, which injected air into the exhaust stream. This increased the available oxygen, allowing the catalyst to function as intended.

Some three way catalytic converter systems have air injection systems with air injected between the first (NOx) and second (HC and CO oxidation) stages of the converter. As in two-way converters, this injected air provides oxygen for the oxidation reactions. An upstream air injection point, ahead of the catalytic converter, is also sometimes present to provide additional oxygen only during the engine warm up period. This causes unburned fuel to ignite in the exhaust tract, thereby preventing it reaching the catalytic converter at all. This technique reduces the engine runtime needed for the catalytic converter to reach its "light-off" or operating temperature.

1.6. Benefits of installing catalytic converter:

- The catalytic converter's sole purpose is to reduce the amount of harmful pollution produced by the combustion of hydrocarbon-based fossil fuels in cars.
- Catalytic converters decrease hydrocarbon emissions by about 87 percent, carbon monoxide by 85 percent and nitrous oxide by 62 percent during the expected life of a vehicle.
- Initially, automakers believed the catalytic converter would make cars prohibitively expensive. On the contrary, catalytic converters only add about two percent to the cost of a vehicle. In 1985, the Environmental Protection Agency estimated that catalytic converters saved at least 10 times more in health costs than the price of a catalytic converter

Disadvantages of installing catalytic converter-

- They are very expensive to get/replace. In addition, because carbon dioxide is a product of the reaction that takes place inside catalytic converters, widespread use of catalytic converters has also contributed to increased atmosphere levels of carbon dioxide.
- Bad catalytic converter can cause Sluggish engine performance, Reduced acceleration, Dark exhaust smoke, The smell of sulfur or rotten eggs from the exhaust, Excessive heat under the vehicle
- Catalytic converter issues can lead to increased exhaust emissions and a decrease in engine performance. As a result, the catalytic converter becomes less effective, less chemical conversions take place and the exhaust output contains more harmful gases

1.7. Disadvantages of removing catalytic converter:

- Releases toxic fumes in the atmosphere. It has been explained above how the catalytic converter works and helps your vehicle emit cleaner gases. It can clean or convert up to 90 percent of harmful gases into less toxic substances. Removing it will cause more harmful pollutants released in the air. It does not only cause harm to the environment, it could also harm you. If for some reason these toxic fumes like carbon monoxide reached your car cabin and you are driving or parked with your windows down, inhaling it is harmful and can be life threatening
- Some vehicles experience more fuel consumption. Some car owners are experiencing more fuel consumption after removing their catalytic converters. The explanation for this is because their vehicle's O2 sensors readings are not correct which cause it to require more usage of fuel. Removing it can also lead to consuming more oil and this too will be added to your expenses.
- Its loud noise can be annoying. Without the muffling effect of a catalytic converter, the loud noise coming from your car when you drive can be very apparent especially when you rev up the engine. Conversations inside your car might be affected and you won't be able to enjoy a long, quiet ride anymore. The loud noise can also create a problem if your neighbours or the people from your street start to complain about it.

• You may experience losing your low-end torque. If you are into off roads and adventures, then removing your catalytic converter won't be beneficial for you since you may experience low-end torque loss.

Advantages of uninstalling catalytic converter-

- A significant increase of horsepower. Vehicles with a removed catalytic converter have experienced a significant increase of horsepower. This has been made possible because the catalytic converter creates a considerable source of back-pressure on the engine. This is because it limits the impact of the exiting gases and when it is removed, these gases can leave the engine and pass through the exhaust at a faster rate and at a larger quantity. Without the catalyst's limiting effects, the engine can now operate and use its optimum horsepower.
- You will have more fuel options. Catalytic converter requires the vehicle to only use unleaded gasoline. This is because the lead found in conventional gasoline can be harmful to some inner catalyst materials and keeps it from doing its job efficiently. Removing catalytic converters can give you access to more fuel options. You can choose to use those high-performance fuels that are widely sold in the market today.
- Lower engine operating temperature is achieved. Without the catalytic converter, the vehicle's engine workload is decreased since the exhaust's exit from it can be done at a faster rate. This results in a relatively reduced engine operating temperature. With the engine working under lesser load and using lesser effort, you can expect that it will also generate less friction that can help reduce the wear and tear of your vehicle and its parts over time.

2.DESIGN AND MATERIAL SELECTION.

2.1. Design calculations

Criteria for selection of converter is the minimum pressure drop and chotic gas flow distribution

Modelling of the converter -

The objective of this study was to determine the effect of geometry of the on the pressure drop and heat-mass flow distribution. CFD analysis enabled to observe the pressure drop in each of these shapes and sizes.

The catalytic converter chamber was designed while considering the engine specifications which are as follows:

Engine type	Briggs & Stratton 10 HP
Swept Volume	305cc
Engine Speed (N)	2800
Bore Diameter (d)	0.08178 m
	0.05701
Stroke (L)	0.05/91

Volume flow rate

Space Velocity = -----

Catalyst volume

For single cylinder let us assume Space velocity = 63,915 hr⁻¹ Volume flow rate of exhaust gases = swept volume x No. of intake strokes per hour = $305 \times 10^{-6} \times (3800/2) \times 60$ = $34.77 \text{ m}^3/\text{hr.}$ Volume flow rate 34.77Catalyst volume = -------Space velocity 63915= $543.94 \text{ cc} \approx 544 \text{ cc.}$

Shell Dimensions:

For L=2D. Volume = Area × Length. Volume of catalyst = 544 cc.

Volume =
$$\frac{\Pi}{4} D^2 L$$

= $\frac{\Pi}{4} D^2 (2.5 D)$
544 cc = $\frac{\Pi}{4} D^2 (2.5 D)$

Therefore, D = 65.2 mm and L = 2.5 D = 2.5(65.2) = 163 mm.

Considerations for the catalytic converter design based on the above obtained results,

Thickness of the pipe = 1.5mm Length of the inlet pipe = 85.8mm Length of the outlet pipe = 57mm Angle between the inlet and the diffuser = ° Length of the diffuser = 63.613mm Length of the core region = 163mm Length of the nozzle = 63.653mm Angle between the outlet and the nozzle = 30° Diameter of the inlet pipe=42mm Diameter of the outlet pipe = 42mm



Converter geometry

DESIGN FINALIZATION BASED ON NURBS CRITERIA NURBS

Non-uniform rational basis splines are used to generate a curve using the given constrained tangents [5]. Using the same concept here, the 90° step was discretized and semi polygonal structure was developed. This structure was then converted to a smooth curve. This was done using iterative method. Volumetric error of 5.67% was seen, which does not affect the functionality.



Initial Design

Final Design

2.2. material selection:

S. No	Component	Material
1.	Inlet pipe	SUS 409 L
2.	Inlet clam shell	SUS 409 L
3.	Converter shell	SUS 409 L
4.	Outlet clam shell	SUS 409 L
5.	Outlet pipe	SUS 409 L
6.	Zeolite and catalyst converter shell	Ceramic monolith
7.	Inlet and outlet flanges	FE410

Reason for choosing SUS 409L

-JIS **SUS 409L** Stainless Steel Sheets have excellent resistance to exhaust gas and atmospheric corrosion.

- The nominal 11% chromium (Cr) content offers improved corrosion resistance over carbon steel.

- The composition of Type 409 is balanced with a titanium (Ti) addition and low-carbon levels to avoid austenite formation making the alloy essentially non-hardenable when exposed to annealing temperatures and when welding.

- The titanium additions not only stabilize the steels to prevent hardening during welding, but also prevent the formation of chromium carbides. Welds and weld heat affected zones perform nearly as well as the base metal in corrosion resistance and forming.

So, these benefits are achieved by choosing SUS 409L

3. selection of catalysts and adsorbents

3.1.Catalyst and its selection

a substance that enables a chemical reaction to proceed at a usually faster rate or under different conditions (as at a lower temperature) than otherwise possible. an agent that provokes or speeds significant change or action

General considerations while choosing a catalyst

- The catalyst used in the converter is mostly a precious metal such as platinum, palladium and rhodium
- Platinum is used as a reduction catalyst and as an oxidation catalyst. Although platinum is a very active catalyst and widely used, it is very expensive and not suitable for all applications.
- Rhodium is used as a reduction catalyst, while palladium is used as an oxidation catalyst.

We thought of alternative catalyst because There are several types of problems associated with precious metal based catalytic converter.

These factors encourage for the possible application of non noble metal based material:

- The use of platinum, palladium and rhodium are very expensive because of scarcity of these metals.
- Rhodium and palladium is the big contributors to smog.
- Copper is low cost catalyst composition and has superior durability than platinum and palladium.
- Catalysts only work at fairly high temperatures
- All are very expensive, have very limited supply sources, and limited future availability.

So, in place of platinum-palladium, Rhodium catalyst we use copper -nickel catalyst which promotes both oxidation and reduction reaction(Redox reactions)

• Aluminium oxide(Aluminia) is the best ceramic material used for most catalytic converters because it withstands higher temperatures , it remains chemically neutral and low thermal expansion.

Some often use cerium oxide which promotes water gas shift reaction during the redox reaction

As we concentrate more on the light-off temperature we are not elaborating our discussions on the catalyst used.

2.2. Adsorbent and its material selection

Adsorption-the process by which a solid holds molecules of a gas or liquid or solute as a thin film.

Adsorption is caused by London Dispersion Forces, a type of Van der Waals Force which exists between molecules. The force acts in a similar way to gravitational forces between planets.

Adsorbent-a substance that adsorbs another.

The adsorbent used in the catalytic converter plays an important role in capturing chaotic emissions such as unburnt hydrocarbons(HC), oxides of carbon (COx), oxides of nitrogen (NOx), oxides of sulphur(SOx), and solid particulate matter.

Adsorption Material selection:

The key characteristic parameters for the selection of adsorbents were the following:

- Disintegration Temperature of the adsorbent
- Desorption temperature
- Limiting Reaction (Saturation Pressure)
- Back Pressure
- Number of active spots remaining after the process
- Commercial Availability and feasibility

Based on these parameters we evaluated **Activated Carbon**, **BEA Zeolite**, **ZSM5** because of its higher affinity towards adsorbing carbonous materials, its higher disintegration and desorption temperature and also its availability.

• adsorption catalyst serves our purpose When the temperature is less than light off temperature during cold start when engine is at idling rpm then the temperature remains lower than 350'C and our catalysts does not performs catalytic reaction and this adsorption catalyst adsorbs harmful CO and HC.

The following are the material properties ZSM-5 :

- Empirical formula $Na_nAl_nSi_{96-n}O_{192}$ ·16 H₂O 19<n<96.
- The crystallographic unit cell of ZSM-5 has 96 T sites (Si or Al), 192 O sites, and a number of compensating cations depending on the Si/Al ratio, which ranges from 12 to infinity.
- ZSM 5 of any pore size can adsorb hydrocarbons and to some extent other carbon based emissions it has a pore size ranging from 4.6 Angstroms to 5.4 Angstroms.
- No deterioration up to temperature of 1100°C
- The limiting factor is calculated to be 1.75*
- Desorption starts at a temperature way above the Light off temperature of the commercial available catalytic converters.
- Inexpensive and available in varied sizes, powder, extrusions.

The Limiting factor for a adsorption-desorption cycle must be in the range of 1.5 - 2.0

Flow of gases in the converter during the process of adsorption

-exhaust gases from the engine passes through the adsorption catalyst .

-if the temperature below than the light-off temperature HC and Co are adsorbed

-then it passes through the ceramic monolith structure passes coated with catalysts

-then exhaust gases with harmful CO,HC and NOx are reduced .

So finally our catalytic converter consists of

- A Non precious metal (copper& nickel) to be act as catalyst for oxidation and reaction respectively in the form coating to the wire mesh or perforated copper plates.
- A ceramic monolith substrate is coated with catalyst along with wash coats which enables the durability of the coated catalyst
- Adsorption catalyst(zeolite ,activated charcoal)

 monolith surface structure serves as a support to our oxidation and reduction catalysts

BLOCK DIAGRAM



4. Ceramic monolith structure

This study is based on the idea that greater the surface area of a monolithic substrate, lesser the emission and a higher conversion efficiency obtained. For this objective, in this work, an attempt was made to investigate the use of advanced fractal curve based monolithic structure for the catalytic converter. Further, comparison was done between the conventional and proposed design using simulation software packages in terms of pressure drop, uniformity in flow.

4.1. Modelling-

There are a variety of curves in nature which possess different kinds of geometry and features. A fractal is generally a rough or fragmented geometric shape that can be subdivided into parts, each of which is a reduced-size copy of the whole. This property is called self-similarity and are governed by various algorithms.

They possess various other properties like self-repeating space-filling, symmetry and maximum area occupancy in a given volume.

Ceramic monolith, ceramic foam, steel wire meshes, ceramic silicon fibre, porous ceramic honey comb are the few types of filter materials Reasons considered while selection of filter materials

- Thermal stability during regeneration.
- Good mechanical properties.
- Long durability.
- Easy availability and less cost
- high corrosion resistance
- high adhesion of active substances
- high melting temperature
- easiness in shaping.

Hilbert curve, which is a type of fractal curve, the area to the square made by it remains unchanged with an increase in the iteration values, thus when making a higher iteration curve then the effective length increases but the edge length remains the same. So the advantage is without increasing the size of the square it can incorporate an infinite length of the curve and as the length increases the effective current path also increases thus generating more area to collect power. Different methodologies are used to generate fractal curves. Some of the prominent methods are the L- system, space folding algorithm and the tabledriven algorithm

4.2. design of proposed ceramic model:

computer aided design (CAD) software does not have provision for the direct modelling of fractal curve model and manual sketching of fractal curve for higher iteration was drawn manually in the CAD Software

the view of our proposed model(3D model)





generally we use honeycomb structure as the trivial structure in most of the catalytic converters

the view of the honey comb structure(3D model)





2-D models



(a) Honeycomb model

(b) proposed model

The width of the filter materials be 1.5mm(Assumption).

5.RESULTS

<u>comparing results of the proposed model with the general honey comb</u> <u>structure :</u>

The procedures/phases we need to discuss before comparing results

Phase-1: Design phase

-generally in this phase we refer to many things and devise a methodology to start preparing/constructing the model which is the basic requirement and it will become like a system on which our observation is going to be concentrated.

Phase-2: Analysis phase

-Here we use some analysis software that fits our required work or that fulfil our target and we obtain some results in this phase which was not the ultimate result but we go on iterate these results by changing some of the instructions and dimensions or some conditions to ultimately achieve our required output

Phase-3: Manufacturing phase

-Here we manufacture a product based on our design and analysis phase and this phase is very crucial as it represents our basic model

Phase-4: testing phase

-Here the important task is to note down our results which is also called as experimental results or real time results and here the conditions are entirely different when compared to the analysis phase results also called theoretical results .we encounter some errors .So, mostly we try to reduce this errors as possible.

BOUNDARY CONDITIONS(for analysis)-

The inlet velocity will be 22.6 m/s

Inlet temperature is 300°C.

Assuming the inlet and outlet boundaries are static and there is no slip between the flow gases and the surfaces and surface has no roughness .

Results and discussion-

After modelling, volume of honeycomb model and proposed fractal curve model was calculated using CAD software . Contact surface area of both the models and fluid domain area are summarized below. The proposed fractal curve model had higher surface area. Greater the surface area more quantity of catalyst could be coated to increases the redox reaction in catalytic converter. Proposed fractal curve model structure is having 10% of surface area more than honeycomb. New model occupies more area in given volume than honeycomb. Due to this greater surface area of the proposed fractal curve model, effects on pressure, velocity and flow distribution also varied. This will significantly reduce the weight of the catalytic converter also. Hence it possesses greater volumetric efficiency. The new model has lesser volume so weight of the component reduced and material cost also reduced.

properties	Honeycomb	Proposed	Increment/decrement
	model	model	
Mass	0.07kg	0.04kg	-42.85%
Surface area of	0.11m ²	0.121m ²	10%
the monolith			
Density	2200kg/m ³	2200kg/m ³	

Comparison of pressure contours:

The pressure contour of both conventional honeycomb and proposed fractal curve are shown below. From the contours, it is observed that the proposed model possess higher pressure drop compared to honeycomb.

Greater pressure drop than the conventional honey model, it could produce lesser noise and less damage to monolithic structure .

The maximum, minimum and weighted average pressure of both models is summarised in Table.

Pressure contour distribution for both models is almost same, where the pressure gets increase from inlet to outlet. Though there is significance

difference in static pressure, on average scale the pressure variation is not significance



(a)



(b)

Pressure contour of (a) honeycomb and (b) the proposed fractal curve model

(a) Honey comb model		(b) proposed model	
maximum	minimum	maximum	minimum
5.97 x 10 ⁶ pa	2.99 x 10 ⁶ pa	4.38 x 10 ⁶ pa	1.31 x 10 ⁶ pa

Comparison of velocity contours:

Velocity plots were analysed and compared between both models. The velocity contour plots for both models are shown below. The rise in velocity was recorded in both the monolithic structures. The minimum velocity rise was recorded in newly developed structure when compared with result of conventional honeycomb structure. From the velocity plot of simulation, it can be concluded that newly developed model possess does not have significant change in velocity of flow. Maximum, minimum and weighted average velocity is summarised in Table.



(a)



Velocity contour of (a) honeycomb and (b) the proposed fractal curve model Comparison of velocity contour between both structures

(a) Honey comb model		(b) proposed model	
maximum	minimum	maximum	minimum
45.12 m/s	18.05 m/s	48.42 m/s	24.2 m/s

Comparison of flow distribution contours

Flow distribution over both the monolithic substrate was analysed with help of stream line plots. Through which we could find out which monolithic substrate possess less disturbance in flow. This parameter will influence the light off temperature of the catalyst. Greater the uniform flow quickly can achieve the light off temperature. The flow distribution results of both honeycomb and proposed fractal curve model is shown



Flow distribution lines of the general honeycomb monolith structure



Flow distribution lines of the proposed monolith structure

More disturbances are observed in conventional honeycomb structure while comparing with the newly developed structure. This result shows that newly developed structure will have fewer disturbances due to which it can have higher conversion efficiency than conventional honeycomb . The above results imply that the newly developed model has higher uniform flow when it is compared with conventional honeycomb. From which it can be concluded that the proposed fractal curve structure will achieve quicker light off temperature for the catalyst. Quickly achieved light off temperature of catalyst lead to a quicker response of catalyst with exhaust gas so we could have a lesser emission while comparing with conventional honeycomb structured monolithic.

Results of catalytic converter model:

1. Pressure contour

2.pressure contours from inlet to outlet:

3.velocity streamlines:

4.static pressure variation graph

5.Mass flow rate

6.velocity magnitude

the above results help us in modifying our model by which ultimately we get the required model with less errors

The special shaped catalytic beads allow the exhaust gas to flow freely without making any obstruction or blocking. Since the partial flow technology is used, it helps to limit the back pressure to the minimum level resulting in better engine performance and fuel saving. The process of regeneration of PM through DOC is continuous. Even if the automatic regeneration is saturated with the collected soot over a period of time, the system will not fail as it happens in wall flow filter, rather all the exhaust gases can flow straight to the other end of the neighboring catalytic bead, similar to flow through substrate. It is estimated that, with the existing volume of catalyst and steel wire meshes, the cleaning may be required for every 10,000 Kilometers of engine run, for efficient fuel consumption. As the catalytic beads are very hard, no wear and tear of catalyst can take place, and hence long life of catalyst is assured. This also ensures no chance of washout catalytic materials coming out along with the exhaust gas adding further pollution to the environment. This after treatment technology for PM reduction is cost effective and robust which needs no interaction with the engine management system and is totally independent.

6.CONCLUSION

In this work an attempt to understand the effect of the fractal curve based monolithic structure for monolithic wash coat in catalytic convertor to achieve the light-off temperature as early as possible. From the detailed study of surface area, velocity distribution, pressure contour, flow distribution and pressure drop on both conventional honeycomb structure and proposed model the following conclusions are obtained.

i. Newly developed model has 10% greater surface area than honeycomb structure so it could be coated with more quantity of catalyst.

ii. The volume of the proposed model is lesser volume when compared with honeycomb structure. This will result in high performance to weight ratio in the catalytic converter.

iii. Performance of Fractal curve model in terms of pressure drop and velocity of flow is almost the same for both fractal and honeycomb model.

iv. Flow distribution results suggest that lesser disturbance of flow occur in the newly developed model so it will have greater conversion efficiency and have more uniform flow and less light off temperature while comparing with honeycomb

so, the newly developed model has higher uniform flow when it is compared with conventional honeycomb. From which it can be concluded that the proposed fractal curve structure will achieve quicker light off temperature for the catalyst

In future, this proposed fractal curve manufacturing feasibilities and its performance in the experimental setup can be studied.

*selected Possible combinations of catalysts available for reduction of chaotic gases mass fraction

1.Adsorption catalyst (ZSM-5 or activated charcoal)

2.Ceramic monolith substrate coated with copper and nickel

By the above considerations we have achieved the results and may vary while considering other conditions

7. references:

[1] Jiang L, Wanga LW, Wang RZ, Roskilly AP. Performance analysis on a novel self-adaptive sorption system to reduce nitrogen oxides emission of diesel engine: Applied Thermal Engineering; 2017; 127:1077–1085.

[2] Sagar D, Chaitanya SV. Comparision between EGR & SCR technologies. In: International Conference on Ideas, Impact and Innovation in Mechanical Engineering, pp. 856-861; 2017.

[3] Chivate A, Dengale P. Design, analysis & testing of catalytic converter for emission reduction & backpressure optimisation. In: IRF International Conference, pp. 28-32; 2017.

[4] Maheshappa H, Pravin VK, Umesh KS, Veena PH. Design analysis of catalytic converter to reduce particulate matter and achieve limited back pressure in diesel engine by CFD. International Journal of Engineering Research and Applications; 2013; 3(1): 998-1004.

[5] Bagus Irawan RM, Purwanto P, Hadianto H. Optimum design of manganesecoated copper catalytic converter to reduce carbon monoxdie emissions on gasoline motor. Procedia Environmental Sciences;2015; 23: 86-92.

[6] M.B. Beardsley et al., (1999). —Thermal BarrierCoatings for Low Emission, High Efficiency Diesel Engine Applications II. SAE Technical Paper 1999-01-2255

[7] C. Lahousse, B. Kern, H. Hadrane and L. Faillon "Backpressure Characteristics of Modern Three-way Catalysts, Benefit on Engine Performance" SAE Paper No. 2006-01-1062, 2006 SAE World Congress, Detroit, Michigan ,April 3-6
[8]Ozhan C, Fuster D, Costa PD. Multi-scale flow simulation of automotive catalytic converters. Chemical Engineering Science; 2016; 116: 161–171.
[9] Martin AP, Will NS, Bordet A, Cornet P. Effect of flow distribution on emissions performance of catalytic converters. SAE Technical Paper: 980936; 1998.

[10] Pandhare A, Atul Padalkar S. Experimental and simulation study of design engine for lower exhaust emissions. SAE Technical Paper: 26-0136; 2013.
[11] Pandhare A, Lal A, Vanarse P, Jadhav N, Yemul K. CFD analysis of flow through muffler to select optimum muffler model for CI engine. International Journal of Latest Trends in Engineering and Technology; 2014; 4(1): 12-19.
[12] Lai MC, Lee T, Kim JY, Cheng CY, Li P, Chui G. Numerical and experimental characterizations of automotive catalytic converter internal flows. Journal of Fluids and Structures; 1992; 6(4): 451-470.

[13] Hayes RE, Fadic A, Mmbaga J, Najafi A. CFD modelling of the automotive catalytic converter. Catalysis Today; 2012; 188: 94-105.

[14] Family F, Vicsek T. Dynamics of fractal surfaces. 1st ed. Singapore: World Scientific Publishing Co Pte Ltd; 1991.

[15] Peitgen HO, Jürgens H, Saupe D. Chaos and fractals. 2nd ed. New York: New Frontiers of Science, Springer; 2004