



# CFD Modeling of the Automobile Catalytic Converter

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## Abstract:

To reduce emission level monolithic three way catalytic converter are widely been adopted in various combustion engines. Designing any catalytic converter several factors need to be considered, however, it is a very complex process involved in the optimization of different chemical and physical parameters. The catalytic performance of a converter is readily been affected by various parameters such as cell densities, length, metal coverage, composition of fuel, etc. In this article a 3D CFD analysis has been carried out using ANSYS Fluent. The performances of converter have been studied on the basis of conversion efficiency. The governing equations are solved by using FLUENT solver, which further coupled with surface reaction model. The flow characteristics across various section of the catalytic converter are visualized along with the simulation of heterogamous reaction within the converter. The results are compared with the previous experimental work of other and they present results are within acceptable limit.

**Index terms:** catalytic converter, backpressure, optimization, CFD.

## 1. INTRODUCTION

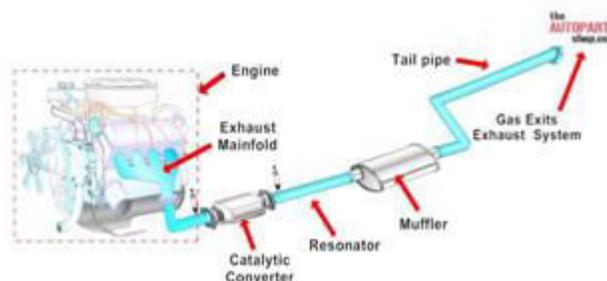
Internal Combustion engines generate undesirable emissions during the combustion process, which include, NOX CO, unburned HC, smoke etc. Apart from these unwanted gases, it produces Particulate Matter (PM) such as lead, soot. All these pollutants are harmful to environment and human health.

They are the main causes for greenhouse effect, acid rain, global warming etc. The simplest and the most effective way to reduce NOX and PM, is to go for the after treatment of exhaust. Devices developed for after treatment of exhaust emissions includes thermal converters or reactors, traps or filters for particulate matters and catalytic converters. The most effective after treatment for reducing engine emission is the catalytic converter found on most automobiles and other modern engines of medium or large size.

The catalyst and filter materials placed inside the catalytic converter increase back pressure. This increase in back pressure causes more fuel consumption, and in most cases, engine stalling might happen. The filtration efficiency and back pressure are interrelated.

If maximum filtration efficiency using very fine grid size wire meshes, is achieved, the back pressure will also be increased, which causes more fuel consumption. On the other hand, if larger grid size wire meshes are used, back pressure will be less, but filtration efficiency will also be reduced, which does not help in meeting the present emission norms. With the help of CFD analysis, it is attempted to find out the optimum solution to get maximum filtration efficiency with limited back pressure developed inside the catalytic converter. Therefore it is clear from the above discussion that the net work output per cycle from the engine is dependent on the pumping work consumed, which is directly proportional to the back pressure. To minimize

the pumping work, the backpressure must be as low as possible for obtaining the maximum output from the engine.



**Figure.1. Position of Catalytic Converter**

### 1.1 BASIC COMPONENTS

The catalytic converter assembly consists most of these components, inlet/outlet pipes/ flanges, Steel housing, insulation material, seals, inlet/outlet cones, substrate(s), coating and sensor boss. The **Substrate** is often called a "catalyst support". It is a ceramic honeycomb or a stainless steel foil honeycomb in modern catalytic converters. The ceramic substrate was invented by Rodney Bagley, Irwin Lach man and Ronald Lewis at Coming, in use to increase the amount of surface area available to support the catalyst. The washcoat is used to make converters more efficient, often as a mixture of silica and alumina. When a wash coat is added to the substrate, it forms a rough, irregular surface, which has a far greater surface area than the flat core surfaces do which then gives the substrate a larger surface area, providing more sites for active precious metal -the catalytic which is added to the wash coat (in suspension) before being applied to the substrate.

The **Catalyst** itself is most often a precious metal. Platinum is the most active catalyst and is widely used. However, because of unwanted additional reactions and/or cost, Palladium and rhodium are used as a reduction catalyst, while platinum and

palladium are used as an oxidization catalyst. Cerium, iron, manganese and nickel are also used, although each has its own limitations.

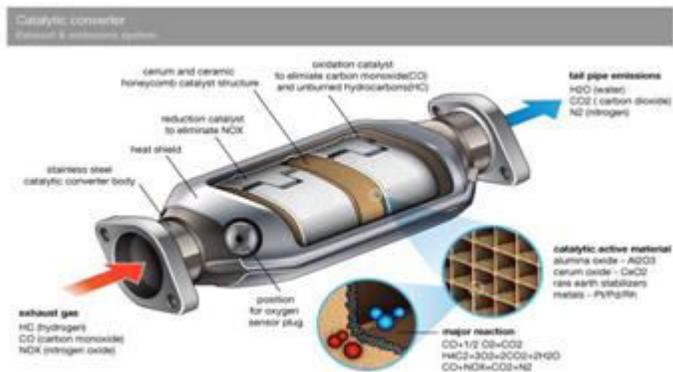


Figure.2. Basic Components

## 1.2 TYPES OF CATALYTIC CONVERTER

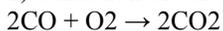
There are two main types of catalytic converter used

- 1.2.1 Two-Way or oxidation catalytic converter
- 1.2.2 Three way catalytic converter

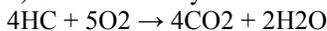
### 1.2.1 Two - way or oxidation catalytic converter

In two way catalytic converter, it will control the emission of two different toxic sources. The carbon monoxide and hydrocarbons will be converted into carbon dioxide and water.

1) Oxidation of carbon monoxide to carbon dioxide:



2) Oxidation of hydrocarbons to carbon dioxide and water:

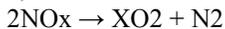


The two way catalytic converter is superseded by three-way converters because of their inability to control oxides of nitrogen.

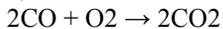
### 1.2.2 Three - way catalytic converter

The oxides of nitrogen are more toxic than carbon monoxide and hydrocarbons, to control the toxic content of nitrogen oxides effectively with the carbon monoxide and hydrocarbons, three way converters are designed and used in the automobile industries.

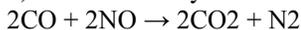
1) Reduction of nitrogen oxides to nitrogen and oxygen:



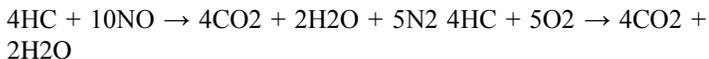
2) Oxidation of carbon monoxide to carbon dioxide:



3) Oxidation of hydrocarbons to carbon dioxide and water:



4) Reduction of nitrogen oxides by reactions involving HC and CO:



## 1.3 WORKING PRINCIPLE

A catalytic converter is a very simple device using the basic redox reactions in chemistry to help reduce the pollutants car makers. It converts around 98% of the harmful fumes produced by a car engine into less harmful gases. It is composed of a metal housing that has a ceramic honeycomb -type interior with insulating layers. This honeycomb interior has thin wall channels that are coated with a wash coat of aluminum oxide. This is very porous and increases the surface area, which allows for more reactions to take place. This is where the precious metals are

located. These metals include platinum, rhodium, and palladium. No more than 4-9 grams of these precious metals are used in a single converter. The converter utilizes simple oxidation and reduction reactions to convert toxic fumes into gases that are not nearly as harmful to the environment. Recall that oxidation is the loss of electrons and that reduction is the gaining of electrons. These precious metals listed earlier promote the transfer of electrons and in turn the conversion of toxic fumes.

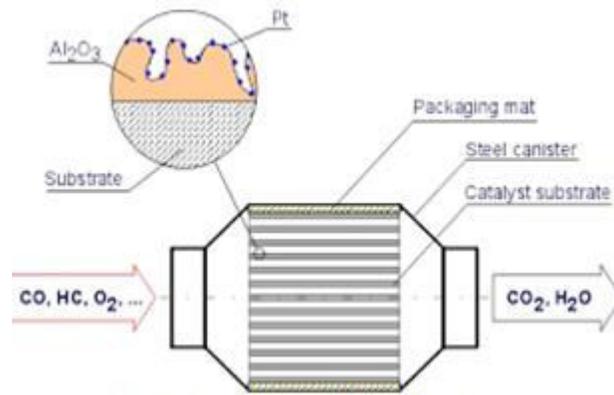


Figure.3. Basic conversion of catalytic converter

3Way converters working as two catalyst process: 1. Reduction and 2. Oxidation and a sophisticated oxygen storage/engine control system to convert three harmful gasses HC, CO and NOx. This is not an easy task: the catalyst chemistry required to clean up NOx is most effective with a rich air/ fuel bias. To operate properly, a three way converter first must convert NOx (with a rich air/ fuel bias), then HC and CO (with a lean bias).

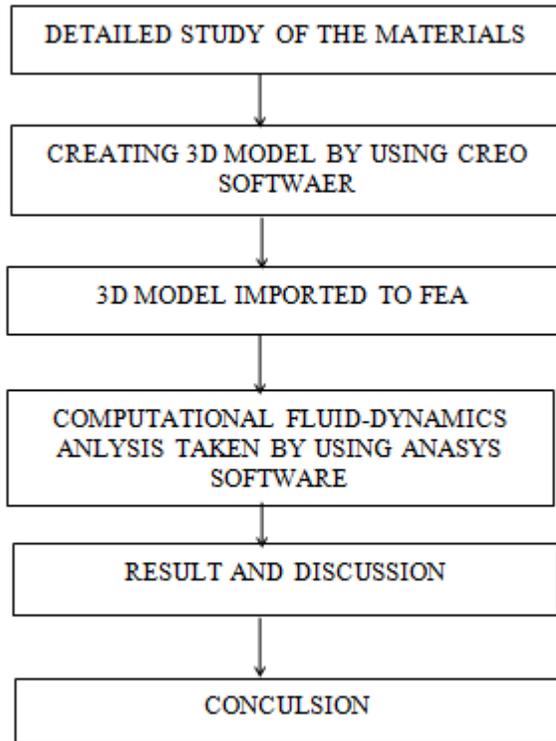
### 1.3.1 Reduction Catalyst

The reduction catalyst is the first stage of the catalytic converter. It uses platinum and rhodium to help reduce the NOx emissions. When an NO or NO<sub>2</sub> molecule contacts the catalyst, the catalyst rips the nitrogen atom out of the molecule and holds on to it, freeing the oxygen in the form of O<sub>2</sub>. The nitrogen atoms bond with other nitrogen atoms that are also stuck to the catalyst, forming N<sub>2</sub>.

## 1.4 METHODOLOGY FOLLOWED IN THE PROJECT

A comparison between the results obtained based on existing material and the results obtained from the ANSYS. Work bench has been carried out. In conventional approach conception ideas are converted into sketches or engineering drawing. With the help of this drawings the prototypes i.e. product which looks same as that of final product are made. It is launched in the market after testing of prototype which gives acceptable results. The thing is, product is launched after doing many practical testing and many trial and error procedures which consumes more time and cost too. In CAE approach some steps are same as that of conventional method. Here also ideas, concepts are converted into engineering drawing, but it is then modelled on computer. Geometric model of product is made using solid work software like CAD which enables better visualization of simple as well as complex models. These models then further used for computerized analysis by using different CAE tools (FEA/CFD software's) depending upon the application before the prototype is made to check whether the components are going to work according to its intended function. After that once

appropriate results are obtained the final practical testing is carried out.



## 1.5 OBJECTIVE

The main challenge is how to reduce the hydrocarbon (HC) emitted from vehicles during the cold start. According to vehicle driving cycle tests, approximately 80% of HC is emitted in the cold start phase due to a low temperature of the exhaust gas and monolith. Therefore, how to increase HC conversion efficiency during the cold start is the key to satisfy the stringent regulations, and the temperature inside the monolith is the most important parameter to decrease the HC emission.

## 2. MODELING

### 2.1 INTRODUCTION TO CAD/CAM

CAD/CAM is a term which means computer-aided design and computer-aided manufacturing. It is the technology concerned with the use of digital computers to perform certain functions in design and production. This technology is moving in the direction of greater integration of design and manufacturing, two activities which have traditionally been treated as distinct and separate functions in a production firm. Ultimately, CAD/CAM will provide the technology base for the computer-integrated factory of the future. Computer – aided design (CAD) can be defined as the use of computer systems to assist in the creation, modification, analysis, or optimization of a design. The computer systems consist of the hardware and software to perform the specialized design functions required by the user firm. The CAD hardware typically includes the computer, one or more graphics display terminals, keyboards, and other peripheral equipment. The CAD software consists of the computer programs to implement computer graphics on the system plus application programs to facilitate the engineering functions of the user company. Examples of these application programs include stress-strain analysis of components, dynamic response of mechanisms, heat-transfer calculations, and numerical control part

programming. Computer-aided manufacturing (CAM) can be defined as the use of computer systems to plan, manage, and control the operations of manufacturing plant through either direct or indirect computer interface with the plant's production resources.

## 3. DESIGN PROCESS

The process of designing is characterized by six identifiable steps or phase

1. Recognition of need
2. Definition of problem
3. Analysis and optimization
4. Evaluation
5. Presentation
6. Synthesis

### 3.1 APPLICATION OF COMPUTER FOR DESIGN

The various design-related tasks which are performed by a modern computer-aided design system can be grouped into four functional areas:

1. Geometric modelling
2. Engineering analysis
3. Design review and evaluation

#### 3.1.1 GEOMETRIC MODELLING

In computer-aided design, geometric modeling is concerned with the computer- compatible mathematical description of the geometry of an object. The mathematical description allows the image of the object to be displayed and manipulated on a graphics terminal through signals from the CPU of the CAD system. The software that provides geometric modeling capabilities must be designed for efficient use both by the computer and the human designer.

There are several different methods of representing the object in geometric modeling. The basic form uses wire frames to represent the object. Wire frame geometric modeling is classified into three types, depending on the capabilities of the interactive computer graphics system.

#### 3.1.2 ENGINEERING ANALYSIS

CAD/CAM systems often include or can be interfaced to engineering analysis software which can be called to operate on the current design model. Examples of this type are

1. Analysis of mass properties
2. Finite element analysis

The analysis may involve stress –strain calculations, heat-transfer computations, or the use of differential equations to describe the dynamic behavior of the system being designed.

#### 3.1.3 INTRODUCTION TO CREO

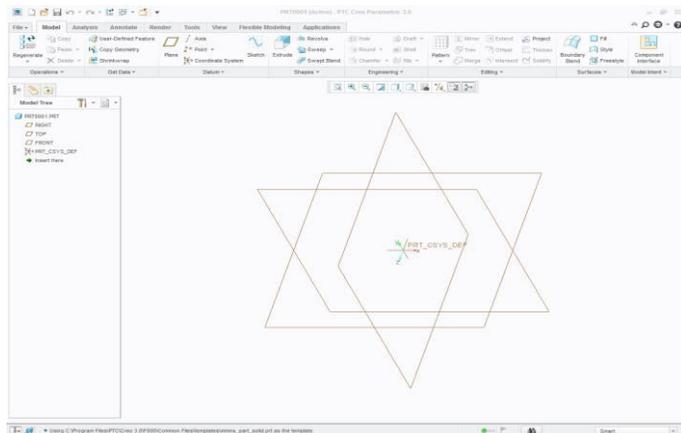
Creo is a family or suite of Computer-aided design (CAD) apps supporting product design for discrete manufacturers and is developed by PTC. The suite consists of apps, each delivering a distinct set of capabilities for a user role within product development..Creo runs on Microsoft Windows and provides apps for 3D CAD parametric feature solid modeling, 3D direct modeling, 2D orthographic views, Finite Element Analysis and simulation, schematic design, technical illustrations, and viewing and visualization. PTC began developing Creo in 2009, and announced it using the code name Project Lightning at Planet PTC Live, in Las Vegas, in June 2010. In October 2010, PTC

unveiled the product name for Project Lightning to be Creo. PTC released Creo 1.0 in June 2011. Creo apps are available in English, German, Russian, French, Italian, Spanish, Japanese, Korean, Chinese Simplified, and Chinese Traditional. The extent of localization varies from full translation of the product (including Help) to user interface only. Creo is part of a broader product development system developed by PTC. It connects to PTC's other solutions that aid product development, including Wind-chill for Product Life cycle Management (PLM), Math cad for engineering calculations and Arbor text for enterprise publishing software.

**RELEASE HISTORY**

**Version Release date**

- Creo 1.06 January 2011
- Creo 2.0 27 March 2012
- Creo 3.0 17 June 2014
- Creo 4.0 15 December 2016



**Figure. 3.1** Creo Parametric Work Bench

**4. ANALYSIS**

**4.1 INTRODUCTION TO FEM**

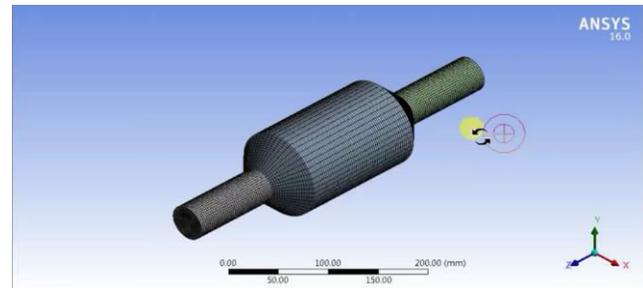
In mathematics, the finite element method (FEM) is a numerical technique for finding approximate solutions to boundary value problems for partial differential equations. It uses variation methods (the calculus of variations) to minimize an error function and produce a stable solution. Analogous to the idea that connecting many tiny straight lines can approximate a larger circle, FEM encompasses all the methods for connecting many simple element equations over many small sub domains, named finite elements, to approximate a more complex equation over a larger domain.

**The subdivision of a whole domain into simpler parts has several advantages:**

- Accurate representation of complex geometry
- Inclusion of dissimilar material properties
- Easy representation of the total solution
- Capture of local effects.

FEM is best understood from its practical application, known as finite element analysis (FEA). FEA as applied in engineering is a computational tool for performing engineering analysis. It includes the use of mesh generation techniques for dividing a

complex problem into small elements, as well as the use of software program coded with FEM algorithm. In applying FEA, the complex problem is usually a physical system with the underlying physics such as the Euler-Bernoulli beam equation, the heat equation, or the Navier-Stokes equations expressed in either PDE or integral equations, while the divided small elements of the complex problem represent different areas in the physical system. FEA is a good choice for analyzing problems over complicated domains (like cars and oil pipelines), when the domain changes (as during a solid state reaction with a moving boundary), when the desired precision varies over the entire domain, or when the solution lacks smoothness. For instance, in a frontal crash simulation it is possible to increase prediction accuracy in "important" areas like the front of the car and reduce it in its rear (thus reducing cost of the simulation). Another example would be in numerical weather prediction, where it is more important to have accurate predictions over developing highly nonlinear phenomena (such as tropical cyclones in the atmosphere, or eddies in the ocean) rather than relatively calm areas.



**Figure.4.1** Meshing

FEM mesh created by an analyst prior to finding a solution to a magnetic problem using FEM software. Colours indicate that the analyst has set material properties for each zone, in this case a conducting wire coil in orange; a ferromagnetic component (perhaps iron) in light blue; and air in grey. Although the geometry may seem simple, it would be very challenging to calculate the magnetic field for this setup without FEM software, using equations alone. FEM solution to the problem at left, involving a cylindrically shaped magnetic shield. The ferromagnetic cylindrical part is shielding the area inside the cylinder by diverting the magnetic field created by the coil (rectangular area on the right). The colour represents the amplitude of the magnetic flux density, as indicated by the scale in the inset legend, red being high amplitude. The area inside the cylinder is low amplitude (dark blue, with widely spaced lines of magnetic flux), which suggests that the shield is performing as it was designed to. Finite element analysis (FEA) involves solution of engineering problems using computers. Engineering structures that have complex geometry and loads, are either very difficult to analyze or have no theoretical solution. However, in FEA, a structure of this type can be easily analyzed. Commercial FEA programs, written so that a user can solve a complex engineering problem without knowing the governing equations or the mathematics, the user is required only to know the geometry of the structure and its boundary conditions. FEA software provides a complete solution including deflections, stresses and reactions.

**FEA is divided in 3 steps**

**Pre-processing**

Using a CAD program, the structure is modeled. A model consists of several elements that collectively represent the entire

structure. The geometry of the structure, the constraints, loads and mechanical properties of the structure are defined. Thus, in pre-processing, the entire structure is completely defined by the geometric model. The structure represented by nodes and elements is called mesh.

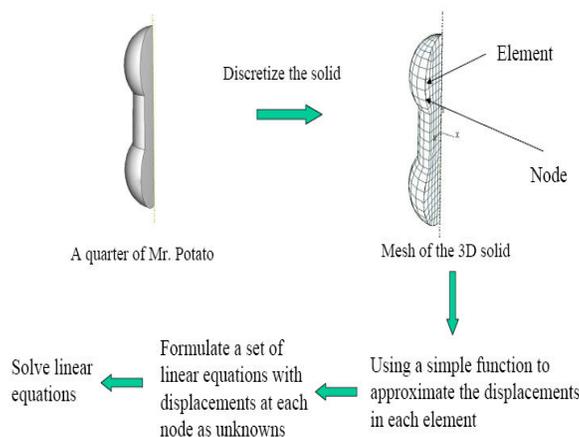
**Solution**

This phase can be performed in the Model Solution task of the simulation application, or in an equivalent external finite element solver. Model Solution can solve for linear and nonlinear static, dynamics, buckling, heat transfer, and potential flow analysis problems.

**Post-processing**

CAD program is utilized to manipulate the data for generating deflected shape of the structure, creating stress plots, animation. Graphical representation of the results is useful in understanding behavior of the structure.

**4.1.1 HOW FEA WORKS**



**Figure.4.2 How FEA works**

**5. COMPUTATIONAL FLUID DYNAMICS**

Computational Fluid Dynamics (CFD) is the simulation of fluids engineering systems using modeling (mathematical physical problem formulation) and numerical methods (discretization methods, solvers, numerical parameters, and grid generations, etc.) Firstly, we have a fluid problem. To solve this problem, we should know the physical properties of fluid by using Fluid Mechanics. Then we can use mathematical equations to describe these physical properties. This is Navier-Stokes Equation and it is the governing equation of CFD. As the Navier-Stokes Equation is analytical, human can understand it and solve them on a piece of paper. But if we want to solve this equation by computer, we have to translate it to the discretized form. The translators are numerical discretization methods, such as Finite Difference, Finite Element, Finite Volume methods. Consequently, we also need to divide our whole problem domain into many small parts because our discretization is based on them. Then, we can write programs to solve them. The typical languages are Fortran and C. Normally the programs are run on workstations or supercomputers. At the end, we can get our simulation results. We can compare and analyze the simulation results with experiments and the real problem. If the results are not sufficient to solve the problem, we have to repeat the process until find satisfied solution. This is the process of CFD.

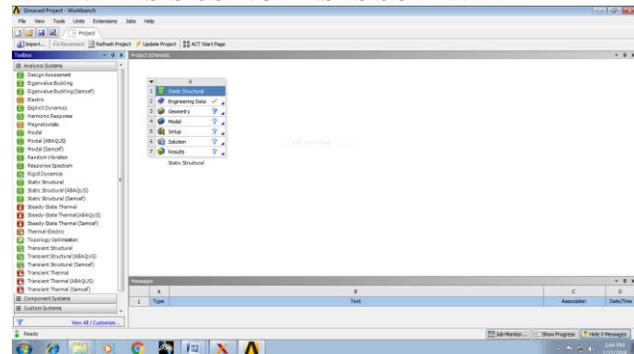
**5.1 IMPORTANCE OF COMPUTATIONAL FLUID DYNAMICS**

There are three methods in study of Fluid: theory analysis, experiment and simulation (CFD). As a new method, CFD has many advantages compared to experiments.

**Table. 1. Comparison of Simulation and Experiment**

	Simulation(CFD)	Experiment
Cost	Cheap	Expensive
Time	Short	Long
Scale	Any	Small/Middle
Information	All	Measured Point
Repeatable	Yes	Some
Safety	Yes	Some Dangerous

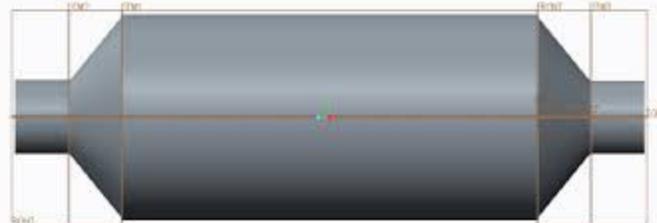
**5.2 ANALYSIS USING ANSYS SOFTWARE**



**Figure.5.2 ANSYS of work bench**

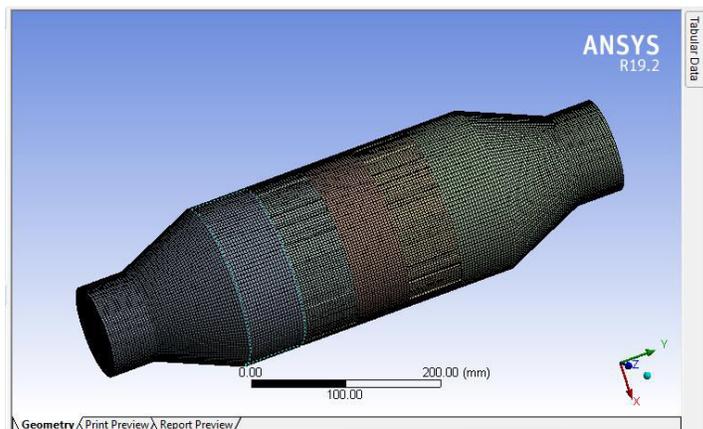
**6. REPORTS OF CATALYTIC CONVERTER**

**6.1 DESIGN OF CATALYTIC**



**Figure.6.1 Catalytic Geometrical Concentration**

**6.2 MESHING OF PROPELLER GEOMETRY**



**Figure.6.2 Meshing**

## 7. RESULT AND CONCLUSION

### 7.1 ANALYZING PRESSURE

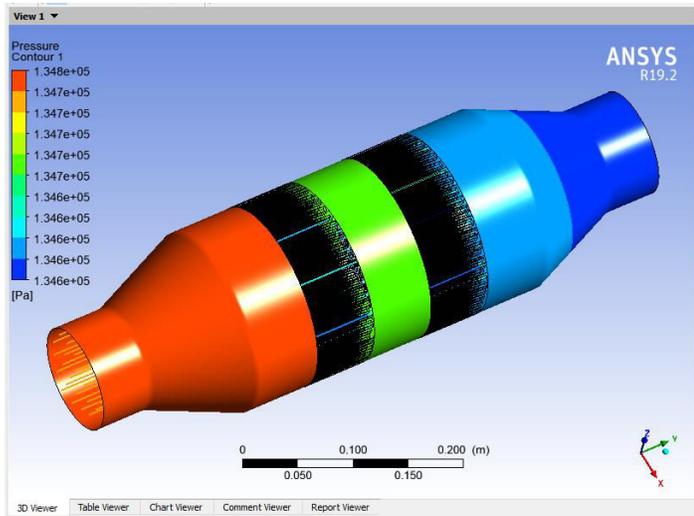
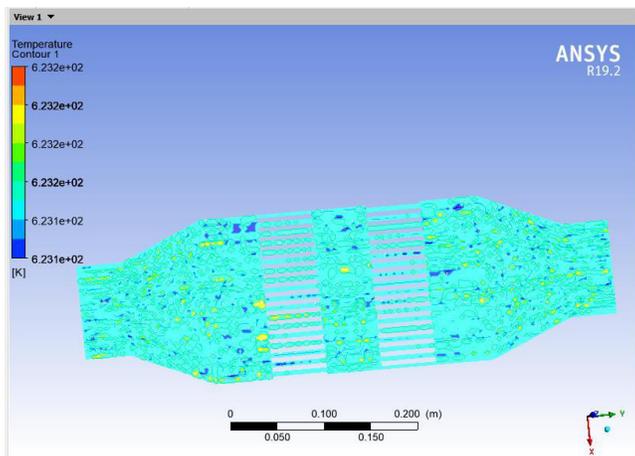


Figure.7.1 Pressure Diagram

### 7.2 ANALYZING TEMPERATURE



## 8. CONCLUSION

1. According to the type of engine, the discharge of emissions into the atmosphere through an exhaust pipe is different. We can reduce the emissions by the use of catalytic converter. Even the catalytic converter is used, itself causing the problem of increasing the back pressure.

2. The emissions and the back pressure are identified at different speeds. The back pressure exerted by the catalytic converter during the working condition causes the decrease in the volumetric efficiency and it leads to increasing fuel consumption.

3. So here the back pressure is reduced by using the air box, by which atmospheric air enters into the exhaust emissions will increase the performance of the engine as well as performance and durability of the catalytic converter.

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