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Catalytic Converter Simulation for Pressure and Velocity Measurement

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Abstract: Chemicals produced by automobiles, such as low-level ozone and photochemical smog, were a major contributor to the pollution. Nitrogen oxides, carbonized hydrocarbons, and carbon monoxide are some of these hazardous gases that are harmful to both the environment and people. By transforming hazardous smoke into less hazardous gases, a catalytic converter purges the air of harmful substances. Typically, automobiles use catalytic converters that are simulated in this present work using ANSYS (Fluent). It is noted that the catalytic converter depends on its length, density, output pressure, and inlet velocity. Comparing the results to models of other catalytic converters, three planes, each with two oxidation and reduction blocks, produce better outcomes. This catalytic converter simulation transforms three toxic gases into less hazardous gases and works efficiently, in contrast to conventional catalytic converter models that only transform two dangerous gases.

Keywords: ANSYS Fluent; Air pollution; Catalytic Converter; Harmful gases; Platinum; Palladium; Rhodium.

1. INTRODUCTION

A catalytic converter is a tool that transforms harmful smoke into less harmful gases and makes the environment clean from harmful gases [1]. Catalytic converters are used more in dynamo-electric-machine, dumpers, drilling machine engines, and boats. These converters are used on the franklin stove for clean air [2]. The catalytic converter is mainly used in vehicles. It is placed near the engine of the vehicle. The exhaust or harmful gases are produced from the air and burned gases from the engine [3]. These harmful gases are carbon monoxide, hydrocarbons & nitrogen oxides which are very dangerous to the natural environment [4]. The catalytic converter basic diagram is given in Fig. 1 [5].



Fig. 1. Basic diagram of catalytic converter. Reproduce from ref. [5]. Copyright 2016 MDPI.

Equation (1) illustrates that the dioxygen chemically reacts with the two molecules of the very dangerous pollutant carbon monoxide. It produces carbon dioxide, a gas that is not particularly toxic. And equation (2) demonstrates the chemical reaction between the two molecules of nitric oxide and the two molecules of carbon monoxide. As a result, nitrogen and carbon dioxide are produced [6].

$$O_2 + 2CO \rightarrow 2CO_2 \tag{1}$$

$$2NO + 2CO \rightarrow N_2 + 2CO_2 \tag{2}$$

Another pollutant nitrogen oxides, the most dangerous molecules of gas and very harmful to the environment,

are generated by nitrogen and oxygen as shown in equation (3).

$$N_2 + O_2 \rightarrow NO_x \tag{3}$$

Equation (4) shows that the molecules of hydrocarbons react with oxygen molecules, and these two are converted into less harmful carbon dioxide and water vapor. In this way, both oxidizing and reduction blocks convert harmful gases into less harmful gases and make the environment clean

$$HC + O_2 \rightarrow H_2O + CO_2 \tag{4}$$



Fig. 2. Internal structure of catalytic converter. Reproduce from ref. [9]. Copyright 2021 MDPI.

In many of the world's biggest cities, the air quality had already become so horrible that a fix was required as early as the 1940s and 1950s. The pollutants released from motor vehicles, such as photochemical smog and low-level ozone, were a significant effect of this pollution [7]. Despite some initial opposition from the

automotive industry, catalytic converters were installed in vehicles in the middle of the 1970s, initially in California, to tackle this issue and improve air quality. The use of catalytic converters has gradually increased around the world [8]. The internal structure of the catalytic converter is given in Fig. 2 [9].

The stainless steel body shows point 1 of Fig. 2 engineered to last for a long time [10]. The ribbed shell reduces expansion and distortion while also generating chambers that shield the cushioning mat from direct exhaust gas contact. Free-following monolithic from point 2 of Figure. 2 substrates are the converter backbone. The conversion process can occur here because of the proprietary combination of precious metals and the wash coat [11]. Coatings are designed to withstand high temperatures and provide optimal catalytic activity with OBD (On-Board Diagnostics) systems. The converter substrate is shielded by the cushioning mat catalyst in point 3 of Fig. 2; it also holds the ceramic catalyst in place and permits body heat expansion. The vehicle undercarriage is shielded from the heat produced by the chemical reactions occurring in the converter by the OE-Matching Head Shields from point 4 of Fig. 2. On an OBDII (on-board diagnostics II) vehicle, sensor ports for O_2 (oxygen) are situated before and after the catalytic converter and are a crucial component of the emissions control system [12]. They are employed to gauge the converter condition and keep an eye on how much oxygen is present in the exhaust gas. Using this information, along with information from the mass air flow, MAP (manifold absolute pressure), and engine data, the PCM (Pulse code modulation) may change the fuel controls. Raw exhaust gases can be chemically treated in tanks with catalysts or precious metals that are placed on the substrate [13]. The most popular metals are platinum (Pt), palladium (Pd), and rhodium (Rh). A typical car catalytic converter serves similar functions to a muffler [14]. Its job is to lessen the number of gases that the engine emits as a result of the burning and combustion of fuel. When combined with a car muffler, this lessens exhaust noise. And the car makes a louder noise when the catalytic converter isn't there [15]. When the catalytic converter is removed, some car models noticeably gain more power and the engine can perform to its full potential since the gas leaves the exhaust more quickly. The unit's capacity to produce a source of back pressure on the engine makes this benefit possible. Exhaust gases are regulated as they depart the car system via restrictions. Though there is certainly a need for improvement, the catalytic converter significantly decreases pollutants [16]. One of its main flaws is that it can only function at a moderately high temperature. The catalytic converter does very little to minimize pollution in the exhaust while your automobile is cold. Moving the catalytic converter closer to the engine is a simple solution to this problem [17]. This implies that the converter is exposed to much higher temperatures, which may shorten its lifespan while also implying that the converter absorbs more exhaust gases and warms up more quickly. To keep the converter at a safe temperature, it is often placed behind the front passenger seat. The catalytic converter can be preheated to reduce emissions [18]. The easiest method

to preheat the converter is with electric resistance heaters. Unfortunately, the majority of cars use 12-volt electrical systems, which are not strong enough to quickly heat the catalytic converter [17]. Most people wouldn't start their automobile until the catalytic converter had warmed up for a while. Large, high-voltage battery packs can supply enough power in hybrid cars to quickly heat the catalytic converter. Diesel engine catalytic converters are less effective at reducing NO_x [19]. Diesel engines run more comfortably than gasoline ones, which, among other things, helps converters work more effectively when they warm up [20]. Some of the most well-known environmental car experts have come up with a creative solution to this problem. Before the converter, they inject a urea solution into the exhaust pipe, which evaporates and reacts chemically with the exhaust to reduce NO_x. Urea, commonly known as carbamide, is an organic molecule made up of carbon, nitrogen, oxygen, and hydrogen. It can be detected in the urine of mammals and amphibians. When urea and NO_x interact to generate nitrogen and water vapor, more than 90% of the NO_x is eliminated from the atmosphere [21].

G. Sathish Sharma et al. (2022) investigated the design and approval of a catalytic converter made with additives to control controlled and unregulated emissions from a gasoline-fueled spark-ignition engine. The unique design has a 10.4% bigger surface area, 1.29 times higher cell density, more uniform flow, greater pressure drops, and a lower exit velocity than a traditionally shaped substrate, according to computational fluid dynamics (CFD). The insulated catalytic converter was shown to be the most effective solution to address the cold start emissions, with a conversion efficiency that is 75% greater than a traditional TWC (three-way catalytic converter), according to the results of the cold start study [22]. AS Blinov et al. (2021) investigated the simulation of NO_x reduction in an SCR system using mathematics. Systems for converting nitrogen oxide (NO_x) in exhaust gases into safe N₂ are called selective catalytic reduction aftertreatment systems. Numerical modeling is used throughout the design phase of SCR (selective catalytic reduction) systems to speed up the process and cut expenses [23]. YJ Kim et al. (2019) investigated the computational fluid dynamics study on the uniformity and characteristics of exhaust gas in the diesel particulate filter/diesel oxidation catalyst of a ship diesel reduction system. Ship laws on harmful emissions tighten as air pollution worsens due to the rise in diesel vessel operations. As a result, constructing a diesel exhaust after-treatment system for ships is necessary, and the treatment efficiency increases with the exhaust treatment system's flow uniformity [24]. Patil et al. (2019) investigated using commercial CFD code, a numerical study of fluid flow, and pressure drop analysis of a catalytic converter. A catalytic converter is now required for all vehicles to achieve low emissions. Understanding fluid flow and improving the design are the goals of this study of the post-treatment device. To design the catalytic converter, it is crucial to understand the pressure drop occurring inside the converter" [25]. AM Leman et al. (2019) investigated the review of toxic gas simulation in vehicle exhaust with a modified catalytic converter. The velocity for the exhaust emission gas using CFD

fluctuates between 5.78 m/s. This result shows that the four different types of manifolds provide a total pressure drop of around 14.6 Pa, 12.2 Pa, 10.8 Pa, and 14.3×10^3 Pa, with the catalyst producing a pressure drop of roughly 10×10³ Pa [26]. CI Priyadarsini et al. (2019) investigated the CFD technique analysis of catalytic converter performance with an air box. At the same time, shear stresses are very low and barely noticeable in the substrate region, where the fluid velocity changes as it passes through the porous substrate due to friction developed across the converter wall, the velocity of gases has been rapid there, averaging 2.42 m/s for Set-B and 2.38 m/s for Set-A. A low-pressure drop of 974.755 Pa, shows that Set-C performed 13.28 percent better than Set-B. This is because the air in the air box restricts the backflow of gases, lowering back pressure by 5.25 percent and temperature by 9.78 percent in Set-C compared to Set-B [27]. SM Kumar and S Satish (2018) investigated that the activated carbon 20 is used in a numerical investigation of the pressure drop of a catalytic converter to capture CO_2 emissions. 4.3×10^3 Pa of pressure drop is attained. The SCR catalytic converter for diesel engines, numerical simulation of the internal flow field, and structural optimal design. According to calculations, the pressure loss at the catalytic converter's ideal design point is 7.9121×10^5 Pa [28].

I Cornejo et al. (2018) investigated an innovative method for simulating turbulent flows in car catalytic converters. In this study, a novel method for forecasting turbulent flows inside catalytic converters is presented. It accounts for the decay and ignition of turbulence at the monolith entrance and exit zones, respectively. A monolith substrate, which is the main component of the converter, is typically depicted as a homogeneous porous media due to computational restrictions. Such simplification removes any contact between the flow and the solid as it enters and exits the substrate. The effective viscosity and kinetic energy inside and after the monolith show significant changes when the results are compared to converter models that are frequently employed [29]. C.P. Om Ariara Guhan et al. (2015) investigated to reduce IC engine emissions, the flow homogeneity inside an oval substrate under the body has been numerically optimized. When the flow inlet plane is moved 10, 20, and 30 mm respectively, away from the geometrical center along the direction of the longer axis, a significant improvement in flow uniformity is seen. A significant improvement is seen at a rotation angle of 20° when the inlet plane is rotated once more using geometry that has been changed by 30 mm. When the second shift is carried out based on the second rotation, the flow homogeneity is at its best [30]. FD Denia et al. (2012) investigated using nonconforming finite element meshes and transfer matrices and acoustic modeling of exhaust devices. In the numerical modeling of the acoustic behavior related to exhaust devices in the breathing system of internal combustion engines, such as catalytic converters, particle filters, perforated mufflers, and charge air coolers, transfer matrices are frequently taken into account. For the inlet/outlet and tapering ducts, which can have multidimensional acoustic fields, finite element discretization is still used. In this instance, the capillary tubes only contain plane waves, whereas the remaining

catalytic subcomponents allow for three-dimensional propagation [31]. In this research paper, I have used ANSYS Fluent to determine the values of velocity and pressure.

In simulation research work, the temperature of the catalytic converter is 278.6 K. This catalytic converter simulation transforms three harmful gases into less risky gases, in contrast to existing catalytic converter models that only transform two risky gases. It runs more efficiently than other converters as a result.

2. ANSYS SIMULATION

An effective program for real-time simulations is ANSYS. Many researchers have used ANSYS software for the simulation before fabrication [32–43]. The catalytic converter is simulated using ANSYS fluid flow (fluent) to assess velocity and pressure in this work. A catalytic converter body can grow up to 4.0448×10^{-2} m in size. The converter defeature size is 1.0112×10^{-4} m. The ANSYS Workbench design modeler creates curves with a minimum radius of 2.0224×10^{-4} m, as shown in Fig. 3.



Fig. 3. geometry of catalytic converter.



Fig. 4. Geometry of catalytic converter.

The catalytic converter's initial speed is 22.6 m/s. The ANSYS engineering data source chooses material attributes for real-time simulation. The table provides the characteristics catalytic converter material and dimensions. The catalytic converter material composition includes various data such as the catalytic converter length, the viscosity of $1.789 \times 10^{-5} \text{ N-S/m}^2$, and outlet pressure of 0 Pa. Gases entering the catalytic converter have an intake velocity of 20 m/s. The converter has a volume of 1.4514 x10⁶ mm³ and a density of 1.225 kg/m³. The catalytic converter features also include a thickness of 38 mm and a surface area of 89322 m². The catalytic converter geometry and element size have been perfectly matched for accurate modeling. The coarse relevance center, medium smoothing, and coarse span angle center are included in the mesh setup. There are 38255 nodes and 57158 total elements in the mesh

geometry. The basic diagram of catalytic converter with meshing from Fig. 4.

Three hazardous gases are changed into less harmful gases via a catalytic converter. The entrance velocity in the simulation varies between 22.6 m/s, 20 m/s, 18 m/s, and many other numbers. When gases react chemically, a pressure outlet appears. Pressure values range from 0 Pa to 1 Pa. The values of pressure and velocity are used to display the simulation's result.

3. RESULTS AND DISCUSSIONS

For catalytic converter simulation, the catalytic converter is designed with an inlet, outlet, and substrate. The velocity inlet is measured in and from the outlet section. Three input variables, thickness, length, and catalytic converter, are used in the simulation of the catalytic converter. A catalytic converter simulation observes the reduction of hazardous gases in the environment. The catalytic converter produces results with velocity and pressure-like characteristics with a crisp value of 288.16 k, 38 mm of thickness, and 98 mm of length. ANSYS fluid fluency created a geometry of the catalytic. Catalytic converter with dimensions of 9838 mm for realtime simulation. The calculation of the velocity contour mapping is given in Fig. 5.



Fig. 5. Velocity contour.

At a pressure of 0 Pa, the catalytic converter's starting speed is 22.6 m/s. The catalytic converter results are also computed using the ANSYS fluid flow software to verify simulation findings. We have found the resultant values of pressure and velocity for the catalytic converter and compared these values with previous findings. The values of pressure and velocity of the catalytic converter in this study are 4.921×10^1 ms⁻¹ and 7.373×10^5 Pa respectively, through ANSYS (Fluent). The harmful gas molecules enter from the converter with inlet velocity and after being processed in the substrate convert into less harmful gas molecules by exerting pressure at the outlet (exit) of the catalytic converter. The relationship between pressure and catalytic converter velocity is inverse. The simulation's results and those from the conventional formulation agree pretty well. Using ANSYS simulation software, the previous researchers AM Leman et al. (2019), CI Priyadarsini et al. (2019), and SM Kumar & S Satish (2017) discovered the pressure and velocity results of 10.8×10^3 Pa and 5.78 ms⁻ 1 , 9.5×10⁻⁴ Pa and 2.38 m/s, and 7.9121×10⁵ Pa and 3.93 m/s, respectively. Results for pressure and velocity are 7.373×10^5 Pa and 4.9×10^1 m/s, respectively, in this paper.

This essay makes it abundantly evident how well the findings of this study agree with earlier studies. The results of the pressure contour mapping are given in Fig. 6.



Fig. 6. Pressure contour.



Fig. 7. Graph between pressure and velocity.

The relationship between pressure and velocity in the catalytic converter is inverse to each other. The velocity of the catalytic converter increases gradually from inlet to outlet and pressure drops. So we conclude that velocity and pressure have an inverse relation. The graph between pressure and velocity is illustrated in Fig. 7.

The vertical values and percentage values in the circular graph show the pressure and velocity respectively. The black color in vertical values shows the maximum pressure of 4.9 Pa at the inlet side of the catalytic converter. The orange color in vertical values shows the minimum pressure of 1.5 Pa at the outlet side of the catalytic converter. So that we have concluded that the pressure drops from black color to orange color. The black color in the circular graph shows the minimum value of the velocity of 4.8% at the inlet side of the catalytic converter. The orange color shows the maximum value of 15.4% of velocity at the outlet side of the catalytic converter. We have examined that the velocity of the catalytic converter gradually increases from black to orange color in a circular graph. Thus, the pressure and velocity have an inverse relation to each other. The values of pressure and velocity are illustrated in Fig. 8.

4. CONCLUSION



Fig. 8 Circular graph plotted between pressure and velocity.

This study provides a clear procedure for using ANSYS Fluent to examine the catalytic converter pressure and velocity. The velocity at the intake is 4.9×10^1 m/s, while the pressure at the outflow is 7.3×10^5 Pa. According to our findings of the study, velocity and catalytic converter pressure are inversely related. For the same input conditions, ANSYS (Fluent) also generates the contour mapping in the results. The comparison of results with the simulation of other catalytic converters is more improved with three planes which include two blocks, oxidation, and reduction blocks, respectively. The simulation of this catalytic converter is used to convert three harmful gases into less harmful gases, while other catalytic converter simulations are only used to convert two harmful gases. Therefore, it works more efficiently in comparison to other converters. Our results clearly show excellent agreement with the results of previous research.

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