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Research Article

Nanoparticles Based Catalytic Converter Model Analysis and Redesign for Enhanced Fluid Dynamics

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Abstract

The catalytic converter serves a crucial function in mitigating vehicle emissions by effectively limiting the release of dangerous pollutants into the atmosphere. Nevertheless, the inclusion of a catalytic converter inside the exhaust system has a discernible effect on the emission of exhaust gases from internal combustion engines. The proposed design aims to enhance the fluid flow rate in the nanoparticles based catalytic converter by improving upon the existing monolith design, surpassing the capabilities of conventional designs. The conventional and enhanced models are designed using computer-aided design (CAD) software and subsequently evaluated using the ANSYS software, specifically employing the FLUENT solver. The flow results are shown, including a comparison between the conventional design and the newly enhanced design. The proposed design incorporating shape modification offers enhanced fluid flow capabilities compared to the standard approach.

Keywords

Nanoparticles, Engine, Exhaust gas, Catalytic converter, Computer-aided design, ANSYS, FLUENT

Introduction

The utilization of internal combustion engines in automobiles leads to the emission of detrimental exhaust gases as a direct consequence of the combustion process. Consequently, the ensuing air pollution has become a significant contemporary issue. Numerous studies are currently being conducted across various domains with the aim of minimizing air pollutants emitted by internal combustion engines. These efforts involve enhancing fuel quality, optimizing vehicle aerodynamics, implementing electronic fuel injection systems, improving heat transfer within engines and their components, refining vehicle tire tread design, and utilizing catalytic converters, among other strategies [1-4]. The catalytic converter is utilized as a final measure in the implementation of emission control strategies, typically integrated into the exhaust system of a vehicle. Contemporary cars have exhibited enhanced fuel efficiency, superior gasoline quality, and several other advancements in comparison to their counterparts utilized in the preceding decade. Nevertheless, the combustion of fuels inevitably results in the release of substantial quantities of exhaust gases. Consequently, numerous researchers are currently engaged in the development of enhanced catalytic converters and the exploration of novel materials that exhibit superior capabilities in terms of pollutant absorption and conversion rates. The utilization of monoliths in catalytic converters has prompted researchers to explore alternative materials for the present ceramic-based monoliths [5-8]. The implementation of catalytic converters has significantly enhanced the regulation of vehicle emissions and has now become a compulsory component in most compact passenger vehicles.

Catalytic convertors

The catalytic converter is a device utilized for controlling exhaust emissions, which facilitates the conversion of harmful gases and pollutants emitted by internal combustion engines into less harmful substances through the process of catalyzing a redox reaction including both oxidation and reduction reactions.

Automotive catalytic converters often employ a ceramic monolith as its core, which exhibits a honeycomb structure, commonly characterized by a square rather than hexagonal configuration. In earlier General Motors applications, particularly prior to the mid-1980s, the catalyst material was often put on a packed bed of pellets [9, 10]. Metallic foil monoliths composed of Kanthal (FeCrAl) are employed in scenarios necessitating exceptional thermal endurance. The substrate is designed in such a way as to maximize its surface area.

A wash coat serves as a medium for the catalytic substances, facilitating their dispersion across a substantial surface area. Aluminium oxide, titanium dioxide, silicon dioxide, or a composite of silica and alumina are viable options for utilization. The materials of interest in this study are ceria and ceria-zirconia. The primary purpose of including these oxides is to serve as promoters for oxygen storage [11]. The catalyst typically consists of a combination of noble metals. Platinum, being the most active catalyst, finds extensive utilization in various applications. However, its suitability is limited due to the occurrence of undesired secondary reactions and its relatively high cost. Palladium and rhodium are more examples of precious metals that are utilized. Rhodium serves as a catalyst for reduction reactions, whereas palladium functions as a catalyst for oxidation reactions. Platinum, on the other hand, has catalytic activity for both reduction and oxidation processes [11].

2-way catalytic converter

The 2-way catalytic converter, often known as an "oxidation" or "oxi-cat" converter, is responsible for performing two concurrent functions:

The process of oxidizing carbon monoxide (CO) to carbon dioxide (CO_2) can be represented by the chemical equation (Equation 1).

$$2CO + O_2 \rightarrow 2\ CO_2 \quad (1)$$

The process of oxidizing hydrocarbons, which includes unburnt and partially burned fuel, results in the formation of CO_2 and water (H_2O). This reaction can be represented by the equation (Equation 2).

$$C_xH_{2x+2+[(3x+1)/2]}O_2 \rightarrow xCO_2 + (x+1)H_2O$$

The given chemical equation represents a combustion reaction in which oxygen (O_2) reacts with a compound to produce CO_2 and H_2O.

3-way catalytic converter

3-way catalytic converters possess the supplementary benefit of regulating the discharge of nitric oxide (NO) and nitrogen dioxide (NO_2).

A three-way catalytic converter is responsible for performing three concurrent functions: The process of converting nitrogen oxides into nitrogen (N_2) gas. Two molecules of carbon monoxide react with two molecules of nitric oxide. In the given chemical reaction, two molecules of CO_2 combine with one molecule of N_2 gas. Additionally, a hydrocarbon reacts with a molecule of NO. CO_2, H_2O, and N_2 gas. The chemical equation represents the reaction between two molecules of hydrogen (H_2) gas and two molecules of NO. The chemical equation represents the reaction between two molecules of H_2O and one molecule of N_2 gas.

The process of converting CO into CO_2 by oxidation. The chemical equation provided is as follows 2 CO molecules react with one O_2 molecule to produce two CO_2 molecules.

The process of oxidizing unburnt hydrocarbons to CO_2 and H_2O, together with the aforementioned reaction involving NO. The reaction between hydrocarbon and O_2 gas yields H_2O and CO_2.

Methodology

The primary aim is to enhance the fluid flow within the nano-based catalytic converter, hence augmenting its overall operational efficiency. In light of this approach, our intention is to suggest a novel configuration for the monolithic structure that is normally found within a catalytic converter.

- The present model exhibits a conventional monolithic shape.
- The present study introduces a novel model, termed the aero filter, which features a distinct monolith shape.
- The proposed model incorporates a novel monolith shape and an updated aero filter.

Analysis

The models are meticulously crafted and constructed within the NXCAD software platform. The assembled component is imported into the ANSYS software. The entire model is meshed using the built-in meshing option, taking into account fluid considerations and designating areas for the inlet and outflow. The computational fluid dynamics study is conducted using the FLUENT solver integrated within ANSYS, employing appropriate boundary conditions and inlet flow parameters as shown in table 1. The velocity distribution, dynamic pressure distribution, and turbulence intensity were measured for all of the models. To analysis the model the mesh details are used in the ANSYS software as shown in table 2.

Table 1: Flow conditions.

Outer case material	Aluminum 6061
Monolith material	Calcium carbide
Inlet condition	50 m/s
Outler condition	No back pressure
Outside operating temperature	300 K
Fluid consideration	Carbon dioxide
CAD software	NXCAD
Mesh and analysis	ANSYS
SOLVER	FLUENT

Table 2: Mesh details.

Mesh detail	Domain	Nodes	Elements
Current model	Cats	13434	40289
	Filter	6030	4048
	Fluid	6888	5368
	All domains	26352	49705
Aero filter model	Cats	13434	40289
	Filter	3924	12718
	Fluid	6888	5368
	All domains	24246	59375
Updated aero filter model	Cats	13434	40289
	Filter	5115	16036
	Fluid	6888	5368
	All domains	25437	61693

Results and Discussion

The velocity, dynamic pressure, and turbulence contour representations depicted in figure 1, figure 2, and figure 3 were obtained using computational fluid dynamics analysis utilizing the FLUENT solver within the ANSYS software. Figure 4 to figure 8 depict the contour outcomes of the corresponding planned models. The velocity distribution of the newly proposed shape exhibits uniformity in contrast to the standard model. The conventional model exhibits a higher-pressure distribution in the dynamic pressure contour following the entrance neck section, while experiencing a significant reduction in pressure towards the exit section. Nevertheless, the pressure contour of the new shape exhibits a seamless transition as a result of its design, facilitating a consistent distribution

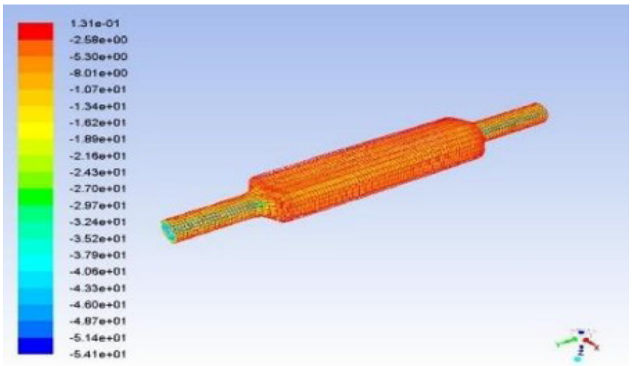

Figure 1: Velocity contour.

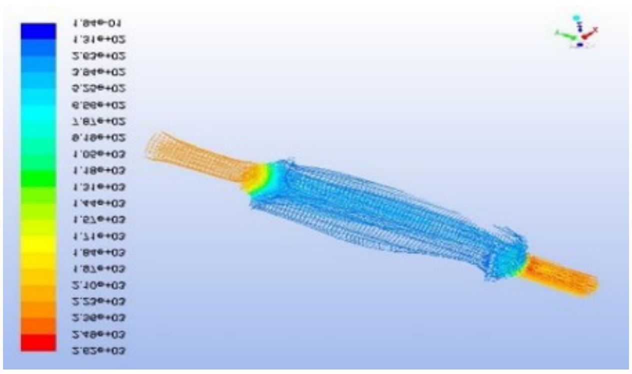

Figure 2: Dynamic pressure.

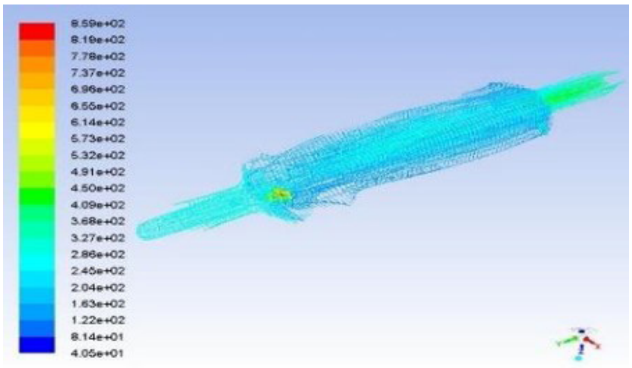

Figure 3: Turbulent intensity.

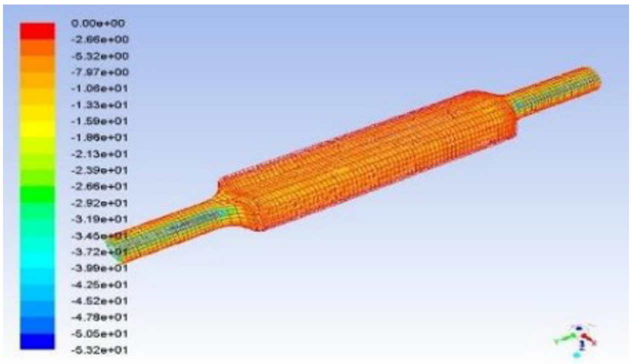

Figure 4: Velocity contour.

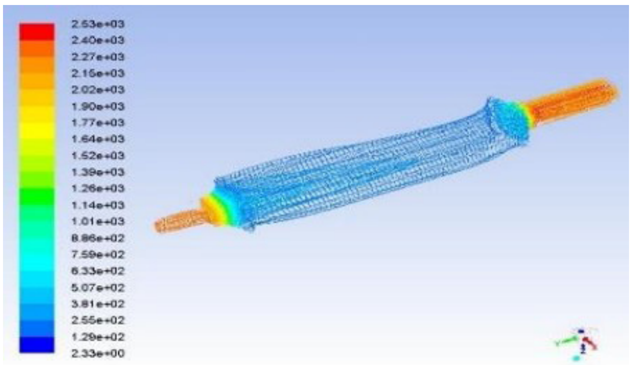

Figure 5: Dynamic pressure.

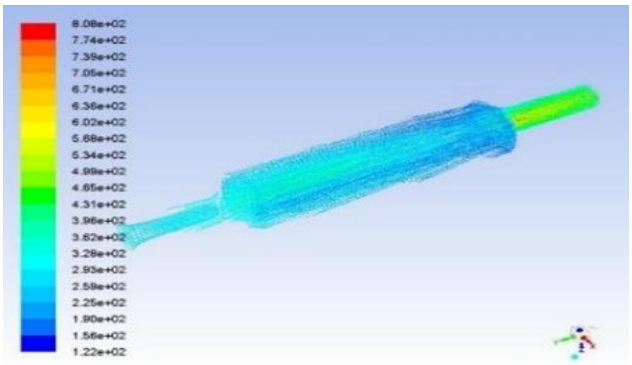

Figure 6: Turbulent intensity.

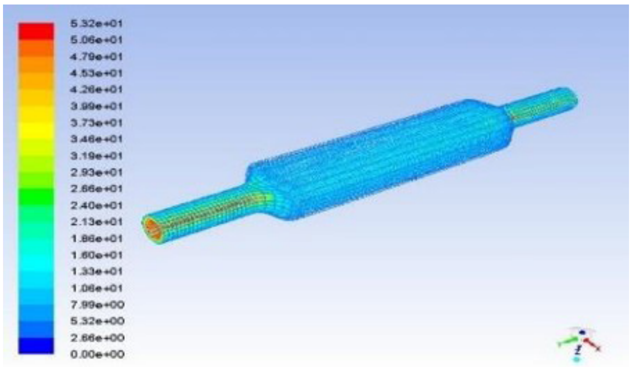

Figure 7: Velocity contour.

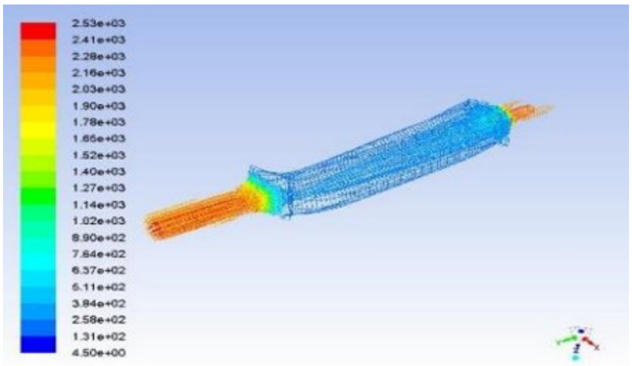

Figure 8: Dynamic pressure.

of pressure. In contrast to the standard model, the proposed model exhibits a uniform distribution of turbulence intensity.

Conclusion

When comparing the fluid flow analysis between the existing conventional design and the suggested design, it is observed that the velocity, dynamic pressure, and turbulence intensity contour yield more favorable outcomes for the proposed design. The fluid entering the nano-based catalytic converter exhibits a homogeneous distribution with less turbulence. The present model exhibits a higher degree of uniform distribution and reduced back pressure as compared to its predecessor, owing to its elevated dissipation rate. The updated recommended form demonstrates more promising outcomes in comparison to the current model.

Acknowledgements

None.

Conflict of Interest

None.

References

1. Presti M, Pace L, Hodgson J, Bella G, De Maio A. 2002. A computational and experimental analysis for optimization of cell shape in high performance catalytic converters. *SAE Tech Paper* 1-11. https://doi.org/10.4271/2002-01-0355
2. Mohiuddin AKM, Nurhafez M. 2007. Experimental analysis and comparison of performance characteristics of catalytic converters including simulation. *Int J Mech Mater Eng* 2(1): 1-7.
3. Michel P, Charlet A, Colin G, Chamaillard Y, Bloch G, et al. 2017. Optimizing fuel consumption and pollutant emissions of gasoline-HEV with catalytic converter. *Control Eng Pract* 61: 198-205. https://doi.org/10.1016/j.conengprac.2015.12.010
4. Chalapathi SK, Murthy CB, Kumar BSP. 2014. Development of automobile catalytic converter during last four decades. *Int J Res Appl Sci Eng Tech* 2: 321-333.
5. Zuo Q, Li Q, Yang X, Chen W, Zhu G, et al. 2023. Investigation of electrically heating catalytic converter flow and temperature field performance improvement based on field synergy. *Energy* 274: 127360. https://doi.org/10.1016/j.energy.2023.127360
6. Pontikakis GN, Konstantas GS, Stamatelos AM. 2004. Three-way catalytic converter modeling as a modern engineering design tool. *J Eng Gas Turbines Power* 126(4): 906-923. https://doi.org/10.1115/1.1787506
7. Shaikh SK, Pathan KA, Chaudhary ZI, Khan SA. 2020. CFD analysis of an automobile catalytic converter to obtain flow uniformity and to minimize pressure drop across the monolith. *CFD Lett* 12(9): 116-128.
8. Gao J, Tian G, Sorniotti A, Karci AE, Di Palo R. 2019. Review of thermal management of catalytic converters to decrease engine emissions during cold start and warm up. *Appl Therm Eng* 147: 177-187. https://doi.org/10.1016/j.applthermaleng.2018.10.037
9. Logesh K, Baskar S, Siddarth BY, Sherwin KA, Naresh P. 2019. Multiwalled carbon nanotube mixed with isopropyl alcohol nano fluid for heat transfer applications. *Mater Today Proc* 18: 4690-4694. https://doi.org/10.1016/j.matpr.2019.07.454
10. Isgoren M, Gengec E, Veli S, Hassandoost R, Khataee A. 2023. The used automobile catalytic converter as an efficient catalyst for removal of malathion through wet air oxidation process. *Int J Hydrogen Energy* 48(17): 6499-6509.
11. Sathyanarayanan S, Suresh S, Uslu S, Shivaranjani RS, Chandramohan VP, et al. 2023. Optimization of gasoline engine emission parameters employing commercial and sucrolite-catalyst coated converter using response surface methodology. *Int J Environ Sci Technol* 20(2): 1725-1738. https://doi.org/10.1007/s13762-022-03968-5