



## Application of CFD and ANN in Predicting the Flow Nature of Flue Gas in the Catalytic Converter

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The main objective of this research is to improve the performance of the catalytic converter by achieving uniform flow distribution of petrol engine exhaust gas using a distributor plate in the upstream section. The flow analysis in the catalytic converter is conducted using computational fluid dynamics (CFD) Solid works 2017 simulation software. Totally, flow simulation is carried out for twelve different cases. It has been observed that a 140 mm diffuser and distributor plate positioned 117 mm from the entrance delivers the optimal flow trajectory. This catalytic converter highly exhibits a non-linear correlation between the input and output variables. Results of such simulation study are then considered as an input for artificial neural network (ANN) model, an artificial intelligence (AI) technique. Results predicted by the ANN model are compared with CFD output. Compared outputs are in good agreement with each other. To sum up, we conclude that by introducing the distributor plate in the flow regime of the conventional catalytic converter, we can accelerate the rate of uniform flow distribution.

**Keywords:** Diffuser plate, Flow trajectory, Laminar flow, Turbulence, Uniform flow distribution

### Introduction

The toxic gases coming out of Internal Combustion engines are ruminated as one of the significant air pollutions. Incomplete combustion leads to more toxic emissions.<sup>1</sup> As per the derived standards, exhaust gases should be treated well to ensure human safety. The scientists developed a catalytic converter to reduce the toxic gases coming out of Spark Ignition (SI) Engine. The efficiency of the catalytic converter depends upon several parameters such as temperature, nature of fuel supplied to the engine, exhaust gas residual time, exhaust gas flow distribution, etc. Presently, the usage of flow analysis on catalytic converters plays a crucial role in the automobile, manufacturing, nuclear, and marine industries. The effectiveness of catalytic converter relies on various parameters endured in engine exhaust gases such as temperature, velocity, pressure, turbulence, flow distribution, residual time of exhaust gas and nature of fuel entering the SI engine. The catalytic converter's efficiency depends on proper flow distribution, operating temperature, fuel composition, and chemical reaction at all engine running conditions.<sup>2</sup>

The velocity fluctuations are high at the beginning of the converter even though the flow is laminar

inside the converter since the flow is turbulent before entering the converter. The velocity depends on the turbulence viscosity ratio. It might even persist throughout the channel, which may influence the heat transfer and mass diffusion.<sup>3</sup> Wall with 100 cells per square inch has the lowest pressure drop. The cone angle with 15 degrees at the inlet section has led to a 4 Pascal pressure drop. Fixed parameters such as gap width and higher substrate length and variable parameters of larger substrate length ratio improve the flow distribution and conversion efficiency. Increased light off time and reduced flow uniformity index reduced the conversion efficiency. The conversion efficiency is decreased with reduced residual time resulting from high velocity and reduced cell size. The flow distribution is highly increased in a honeycomb arc structure, although it increases pressure drop slightly. The pressure drop can be reduced by increasing the ratio of an opening area of an arc to the section area of the inlet.<sup>4</sup>

CFD modelling of the catalytic converter is done using experimental data. A simulation is done with specific perforated plates in the inlet of the converter. It is not effective to remove the non-uniformity velocity through the catalytic converter, but it leads to a slight increase in pressure drop. But there was an increase of 12.9% inflow uniformity index.<sup>5</sup> Modeling is done for two monolith cell densities, one with 400

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cells per square inch and another with 900 cells per square inch. There is a temperature rise of about 2% in 900 cells per square inch when compared with 400 cells per square inch. Pressure drop was also high on 900 cells per square inch (up to 33%) due to increased flow resistance. 400 cells per square inch are preferred, but the velocity will be high and residual time is also less.<sup>6</sup>

A converter has three sections, inlet diffuser, Monolith, and outlet nozzle. The high-velocity inlet mainly causes the flow mal-distribution through the diffuser. The flow is mal distributed in the peripheral region, and it distributes uniform at the centre due to a pressure drop at each cell. The flow distribution can be as high as 20% at the centre. It also affects the conversion efficiency of the monolith.<sup>7</sup> Three different types of distributor plates (perforated, bubble cap and porous) were used in fluidized bed hydrodynamics and change in pressure was determined across the distributor plates. Among the three types, pressure drop was very minimal in both perforated plate and bubble cap.<sup>8</sup> Improvement of gas radial momentum in fluidized bed gasifier was achieved by swirl distributor plate over conventional distributor plate. Swirl distributor plate enhanced the gas-fuel mixing in both vertical and radial directions.<sup>9</sup> Effect of distributor plate in fluidized bed dryer was analyzed using ASPEN PLUS steady-state simulator. Effective uniform distribution of gas was achieved when the distributor plate was used.<sup>10</sup>

The above literature survey reveals that the following conditions are dominantly retarding the existing catalytic converter's performance. (i) Velocity of the exhaust gas influences the heat transfer and mass diffusion, (ii) lesser cpsi minimizes the pressure drop, (iii) higher velocity of exhaust gas causes mal-distribution and reduces the conversion efficiency due to less residual time, and (iv) non-uniform flow distribution at the diffuser region reduces the efficiency of the catalytic converter.

In terms of introducing the distributor plate in the upstream section of the catalytic converter, the present study is novel, and it addresses the above-mentioned research gap. The distributor plate increases the flow distribution uniformly throughout the catalytic converter, which enhances the contact surface area between exhaust gas and catalyst. Residual time of the exhaust gas was increased by

reducing the exhaust velocity, which increases the catalytic reaction rate. Finally, the artificial neural network model was developed to predict the performance of the catalytic converter.

## Materials and Methods

### Catalytic Converter Model

The regular conventional catalytic converter consists of the diffuser at the inlet section, the ceramic or metallic substrate at the centre and the nozzle at the end. The catalytic converter shown in Fig.1(a) and (b) is designed and modelled using Solid Works 2017 software. To achieve uniform flow distribution, especially near the wall surface, a distributor plate with three different dimensions is designed, as shown in Fig. 1(b). Detailed technical specifications of the catalytic converter without distributor plate (conventional) and with distributor plate (modified) of various cases are given in Table 1 and Table 2.

### Catalytic Converter Flow Analysis

Solid Works – Computational Fluid Dynamics (CFD) flow analysis 2017 software is used to conduct flow analysis through the catalytic converter. Table 3 consists of software and system requirements for CFD analysis. Input conditions are taken from petrol engine with 1489 cubic capacity, power of 40.5 kW/54 HP and torque of 108 Nm. Table 4 and Table 5 consist of input and output conditions of working fluid for CFD analysis. The IS2062 isotropic material has been selected for the outer shell. The ceramic substrate with a porosity of 0.335 is chosen. During flow analysis, it has been observed that the flow properties became saturated at 322039 nodes.

### Assumptions

The characteristics of the fluid flow problem are assumed as follows:

- (1) 3D and steady flow.
- (2) Newtonian fluids.
- (3) Compressible flow.
- (4) Zero slip at wall surfaces.
- (5) A periodic boundary condition is used.

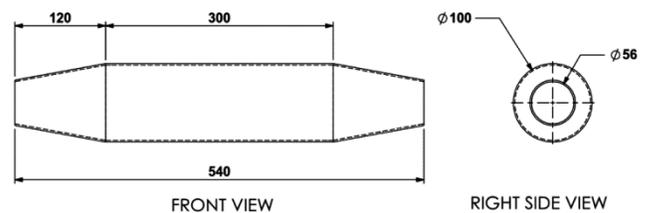


Fig. 1(a) — Front and right-side view of the catalytic converter

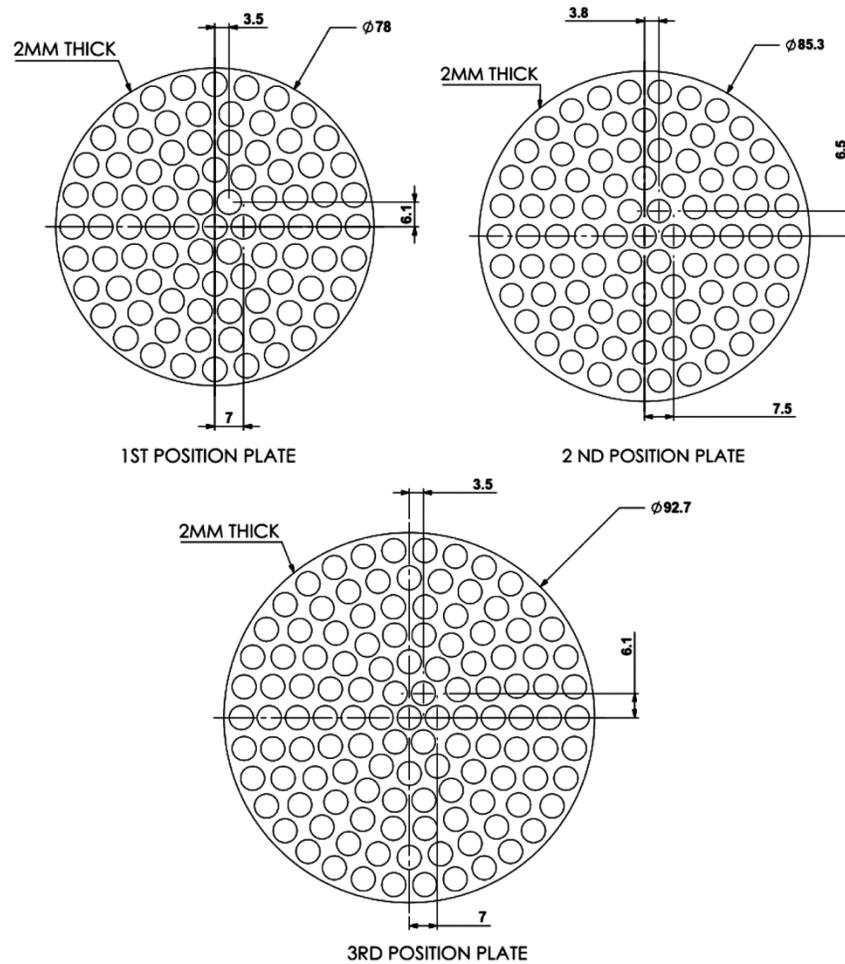


Fig.1 (b) — Distributor plates used in the catalytic converter

Table 1 — Detailed technical specifications of conventional and modified catalytic converter

Case No.	Conventional / Modified	Diffuser / Upstream Length (mm)	Cone angle	Diameter of the distributor plate (mm)	Distributor plate position from the leading edge (mm)
1	Conventional	—	—	—	—
2	—	120	10.4°	78	60
3	Modified	—	—	85.3	80
4	—	—	—	92.7	100
5	Conventional	—	—	—	—
6	—	130	9.6°	78	65
7	Modified	—	—	85.3	87
8	—	—	—	92.7	109
9	Conventional	—	—	—	—
10	—	140	8.9°	78	70
11	Modified	—	—	85.3	94
12	—	—	—	92.7	117

### Governing Equations

Many designs can be obtained by changing the diffuser length and its angle and substrate geometry, such as cell density, length, and void fraction. The required basic governing equations of conservation of

momentum, mass and energy are given in Eqs 1–3. The flow of fluid in the diffuser is always turbulent due to higher Reynolds number, and RANS (Reynolds averaged Navier Stokes) equations are generally used to generate any flow model.

Table 2 — Detailed geometrical specifications of conventional and modified catalytic converter

COMPONENT / SECTION	PARAMETER	TYPE	DIMENSION
DIFFUSER	Diffuser inlet and outlet diameter	Fixed	56 mm and 100 mm
	Diffuser lengths	Variable	120 mm, 130 mm and 140 mm
	Diffuser cone angle	Variable	10.4°, 9.6° and 8.9°
	Diameter	Variable	78 mm, 85.3 mm and 92.7 mm
DISTRIBUTOR PLATE	Longitudinal pitch	Variable	3.5 mm, 3.8 mm and 3.5 mm
	Transverse pitch	Variable	6.1 mm, 6.5 mm and 6.1 mm
	Thickness	Fixed	2 mm
SUBSTRATE	Length	Fixed	300 mm
NOZZLE	Length	Fixed	120 mm
OVERALL	Length	Variable	540 mm, 550 mm and 560 mm

Table 3 — Software requirements and boundary conditions

S.No.	Description	Conditions
1	Software Product	Flow Simulation 2018 SP2.0. Build: 4123
2	CPU Type	Intel(R) Core(TM) i7-2670QM CPU @ 2.20GHz
3	CPU Speed	2201 MHz
4	RAM	16327 MB / 8388607 MB
5	Operating System	Windows 7 Service Pack 1 (Version 6.1.7601)
6	Thermodynamic parameters	Static Pressure: 101325.00 Pa, Temperature: 30°C
7	Total Nodes	322039
8	Flow Type	Laminar and turbulent
9	Fluid Type	Air
10	Type	Inlet Mass Flow
11	Coordinate system	Face Coordinate System

Table 4 — Input conditions of working fluid for CFD Analysis

S.No.	Description	Conditions
1	Type	Static Pressure
2	Coordinate system	Face Coordinate System
3	Thermodynamic parameters	Static pressure: 101.325 kPa Temperature type: Temperature of initial components Temperature: 30.00°C
4	Boundary Layer Type	Turbulent

Table 5 — Flow analysis of minimum and maximum output values

S.No.	Name	Minimum	Maximum
1	Density (Fluid) kg/m <sup>3</sup>	1.15	1.18
2	Pressure [kN/m <sup>2</sup> ]	100.54	102.38
3	Temperature [°C]	29	32
5	Velocity [m/s]	0	43.293
6	Mach Number	0	0.12
7	Vorticity [rotation/sec]	8.96	232565.49
9	Shear Stress [N/m <sup>2</sup> ]	0	34.11
13	Turbulence Intensity [%]	4.53e-04	1000.00
14	Acoustic Power [W/m <sup>3</sup> ]	2.143e-63	0.020
15	Acoustic Power Level [dB]	0	102.99

The governing continuity equation is:

$$\rho \left[ \frac{\partial u}{\partial t} + u \cdot \nabla u \right] = 0 \quad \dots (1)$$

The momentum equation is:

$$\rho \left[ \frac{\partial u}{\partial t} + u \cdot \nabla u \right] = -\nabla p + \mu \nabla^2 u \quad \dots (2)$$

To define the turbulence term, additional closure is required. The Boussinesq assumption gives the most common turbulent viscosity model, and it is expressed as:

$$\rho \left[ \frac{\partial u}{\partial t} + u \cdot \nabla u \right] = -\nabla p + (\mu(\nabla u + (\nabla u)^T) - \frac{2}{3}\mu(\nabla \cdot u)I) + F \quad \dots (3)$$

Where,

$$\rho \left[ \frac{\partial u}{\partial t} + u \cdot \nabla u \right] = \text{inertial forces,}$$

$$-\nabla p = \text{pressure forces,}$$

$$\mu \nabla^2 u = \text{viscous force,}$$

$$(\mu(\nabla u + (\nabla u)^T) - \frac{2}{3}\mu(\nabla \cdot u)I) = \text{viscous forces,}$$

$$F = \text{external forces applied to the air}$$

$$\frac{\partial u}{\partial t} = \text{Local or temporal acceleration} = 0$$

$$u \cdot \nabla u = \text{Convective acceleration}$$

#### Artificial Neural Network (ANN)

ANN is an excellent artificial intelligent tool to deal with non-linear function approximation. It can be used to solve a wide range of engineering and science problems. A well-trained neural network model works much faster than simulation and mathematical models because of its simple architecture and accuracy. The predictive capacity depends on the training and validation with experimental data and by selecting the appropriate topology. Table 6 lists the merits and demerits of such an ANN model. In general, neural networks learn to solve a simple or complex problem rather than being programmed. Learning of neural networks is achieved through proper training. ANN uses the support of various training algorithms.<sup>11</sup>

Architecture of ANN consists of an input layer, processing or hidden layer and an output layer, as shown in Fig. 2; the process flow chart of the entire process is shown in Fig. 3.

In this research, an ANN model for predicting the output conditions of the catalytic converter is developed based on feed-forward back-propagation (FFBP). Data were obtained from the catalytic converter CFD simulated results. The diffuser length, diffuser cone angle and distributor plate position are taken as input parameters, and pressure and velocity are taken as output parameters.

In this analysis, the catalytic converter's flow performance was carried out by varying diffuser lengths from 120 mm to 140 mm. A nonlinear relationship between input and output parameters were determined with a total of 162 observed data

Table 6 — Merits and demerits of artificial neural network

MERITS	DEMERITS
1. Simple architecture	1. Uncertainty from experimental/simulation data sets leads to reduction in accuracy
2. Flexible model for any set of data	2. Not suitable for experiments/simulation with minimum data sets
3. Suitable for large set of variables	3. Architecture will become complex when multiple hidden layers are considered
4. Shorter processing time (66–69ms)	
5. Accurate prediction	
6. Manipulating non-linear functions are possible	
7. Capable of inferring relationship between unseen data sets	

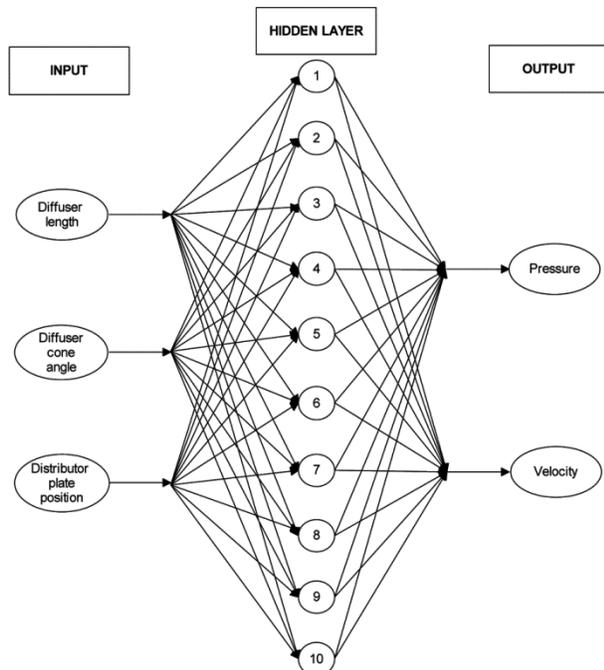


Fig. 2 — Schematic Layout of ANN model for 3 inputs and 2 outputs

sets. The 60% data (98 data sets from 162) were trained from the computational fluid dynamics (CFD) results. Later 20% of data (33 data sets from 162) were taken for validating the developed ANN tool. The remaining 20% (31 data sets from 162) were tested to improve the developed network.

**Investigating the ANN Model Accuracy and Error with Experimental Data Sets**

Sridharan *et al.*<sup>11–13</sup> observed the error range between simulation values and predicted values. The error percentage for individual data sets is calculated using Eq. (4).

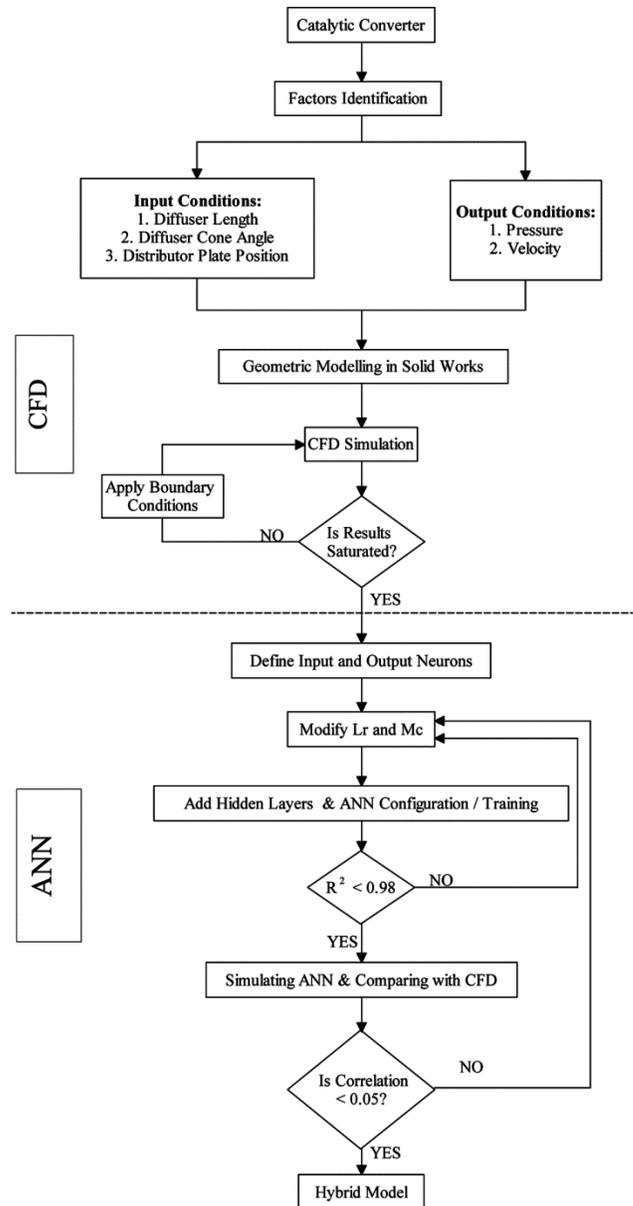


Fig. 3 — Process flow chart for CFD and ANN

$$\text{Error } (e_r) = \frac{|\text{Predicted value} - \text{Measured value}|}{\text{Measured value}} \quad \dots (4)$$

Individual Percentage accuracy ( $A_{in}$ ) is then calculated using Eq. (5)

$$A_{in} = e_r \times 100 \quad \dots (5)$$

The average value of individual accuracy is used to calculate the overall model accuracy ( $A_o$ ) using Eq. (6)

$$A_o = \frac{A_{i1} + \dots + A_{in}}{n} \quad \dots (6)$$

## Results and Discussion

In this study, both the conventional and the modified geometries are designed using the Solid Works 2017 software. In specific, the boundary conditions are applied using the Solid Works – CFD analysis module. The boundary conditions are the same as that of the real-time working conditions. There are 322,039 cells, 1,443,856 faces and 102,089 nodes for the catalytic converter without distributor plate cases. For the catalytic converter with distributor plate cases, there are 405,098 cells, 2,096,123 faces and 405,098 nodes. The computational time duration for the finer mesh is about 6630 seconds. For the coarser mesh, it is about 2257 seconds with a Core 2 Duo core processor. This study utilized the k- $\epsilon$  turbulence model for the simulation of all the twelve cases. In this study, a total of 12 CFD cases are compared for the improvement in the flow distribution. Among these, three cases belong to the conventional catalytic converter without a distributor plate. The remaining nine cases deal with the conventional catalytic converter with distributor plate.

Case —1, 5 and 9: (Without distributor plate)

Conventional catalytic converter with variable diffuser length.

Case — 2–4, 6–8 and 10–12: (With distributor plate)

Modified catalytic converter with variable diffuser length, diameter, and positions.

The Table 1 presents the detailed variations in the length, diameter and positions related to the distributor plate.

### CFD Analysis

Initially, the analysis is conducted without the distributor plate (Case—1, 5 & 9). Then the analysis is conducted with the distributor plate (Case—2, 3, 4, 6, 7, 8, 10, 11 & 12) by varying diameter (78mm, 85.3mm and 92.7mm) and position of the distributor plate (60mm to 117mm) for three different diffuser lengths (120 mm, 130mm and 140 mm). The

comparison is made to observe the effects of introducing the distributor plate at the upstream section of the catalytic converter. Substrate and nozzle dimensions are kept constants for all the cases. Pitch, Monolith and Nozzle dimensions are shown in Table. 1.

### Comparison of Flow Trajectory for with and without Distributor Plate System

#### Flow Distribution without Distributor Plate:

The Fig. 4 shows the flow trajectory simulation results for case-9. Flow trajectory result indicates that the flow concentration of supplied inlet air at the central region is maximum, while the flow concentration nearer to the wall surface is comparatively minimum. Thus, the velocity of air at the centre portion of the substrate is high. Such an increase in the velocity of air at the centre portion reduces the residual time. The reduction in residual time reduces the catalytic converter efficiency because of less reaction time.

#### Flow Distribution with Distributor Plate:

The Fig. 5 shows the flow trajectory simulation results for case—2. This flow trajectory justifies the improved uniform flow distribution and concentration all through the catalytic converter. Such presence of a distributor plate slightly increases the stagnation pressure of air. At the same time, the velocity at the centre portion is reduced by 34%. The slight increase in pressure drop is due to the distributor plate. The pressure drop level is reduced by changing the diffuser length and cone angle. Among all the cases, case—12 is considered the best in terms of better flow distribution, reduction in velocity at the centre portion, and minimum pressure drop.

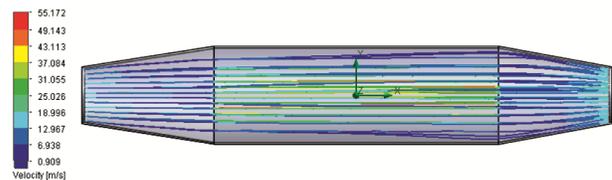


Fig. 4 — Flow Trajectory for Diffuser Length 140 mm (without distributor plate)

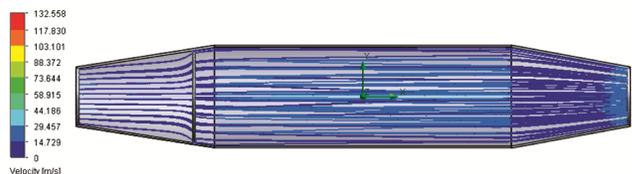


Fig. 5 — Flow Trajectory for Diffuser Length 140 mm (with distributor plate at 117 mm from leading edge)

Table 7 — Average change in pressure for catalytic converters with distributor plate

S.No.	Case Number	Diffuser Length (mm)	Distributor Plate distance from the diffuser entry (mm)	Average change in pressure ( $\Delta P$ ) (Rounded off to 2 digits) (kN/m <sup>2</sup> )
1	case-2	120	60	172.08
2	case-3	120	80	153.39
3	case-4	120	100	14.45
4	case-6	130	65	142.25
5	case-7	130	87	125.27
6	case-8	130	109	26.19
7	case-10	140	70	161.85
8	case-11	140	94	123.89
9	case-12	140	117	1.63

#### Comparison of Pressure, Velocity and Turbulence with and without Distributor Plate

The Table 7 shows the average change in pressure between the inlet and outlet of the diffuser. A significant reduction in pressure drop was found for the case—4 and case—8. The Fig. 6 and Fig. 7 show the pressure values of the catalytic converter for case—9 and case—12. The Fig. 7 (case—12) shows the minimum pressure drop among all the cases. The presence of distributor plate nearer to substrate entrance gives minimum pressure drop, and its average change in pressure is within the acceptable range. The Fig. 8 shows the velocity at the centre portion of the substrate reaches the maximum due to the nozzle's drag force, which reduces the residual time. The Fig. 9 shows the reduction in velocity at the centre portion due to the presence of a distributor plate. The reduction in velocity increases the residual time, which improves the catalytic converter efficiency. The Fig. 10 and Fig. 11 show the turbulence effect. The presence of a distributor plate gives minimal improvement in turbulence.

#### ANN Model for Predicting the Exhaust Gas Parameters

The multilayered perceptron-based algorithm is deployed in this study for predicting the results of 12 different cases of catalytic converters. The input parameters for multilayered perceptron are (diffuser length, diffuser cone angle and distributor plate position). Also, the model output is varied based on the nature of output needed to pressure and velocity. The multilayered perceptron is implemented and designed using MATLAB R2016a software. At first, 60% of data sets (98 from 162) are used for training the model, 20% data sets for its cross-validation (33 from 162), and 20% datasets (31 from 162) for its performance testing. Multilayered perceptron consists

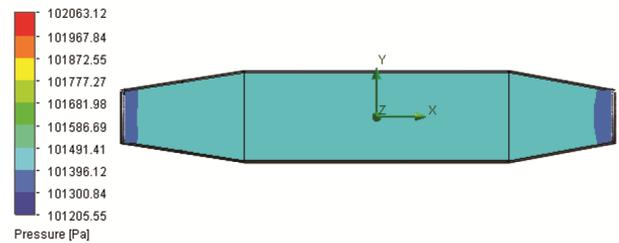


Fig. 6 — Pressure Values - Diffuser Length 140 mm (without distributor plate)

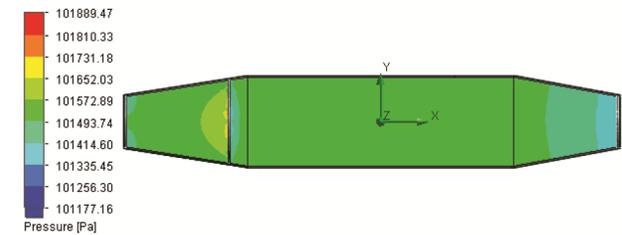


Fig. 7 — Pressure Values - Diffuser Length 140 mm (with distributor plate at 100 mm from leading edge)

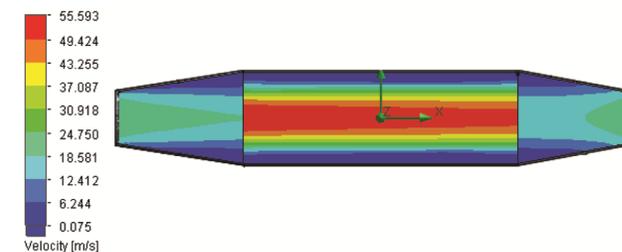


Fig. 8 — Velocity Values - Diffuser Length 140 mm (without distributor plate)

of three inputs and one hidden layer. Also, momentum-based learning methods are carried out with step value equal to 1 and a learning rate of 0.6. The upper limit for epoch is set to 1000. However, the system's reaction under the standard testing conditions at the starting of the training stage is made without any experience. Therefore, artificial neural network

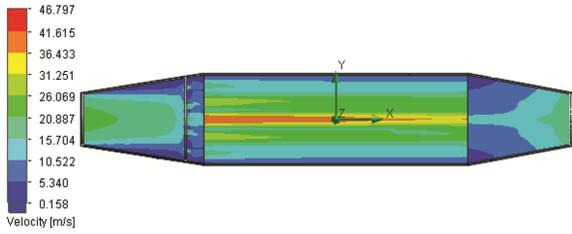


Fig. 9 — Velocity Values - Diffuser Length 140 mm (with distributor plate at 109 mm from leading edge)

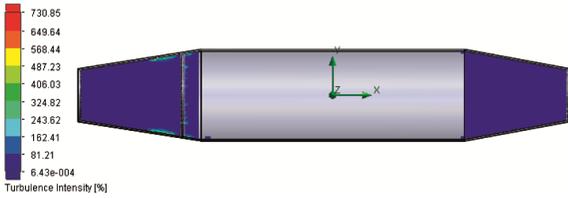


Fig. 10 — Turbulence Intensity - Diffuser Length 140 mm (without distributor plate)

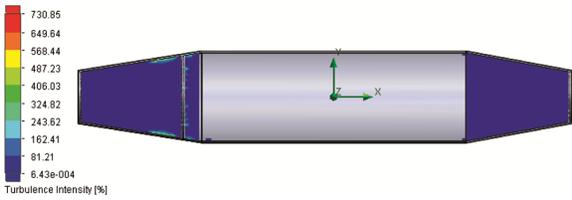


Fig. 11 — Turbulence Intensity - Diffuser Length 140 mm (with distributor plate at 117 mm from leading edge)

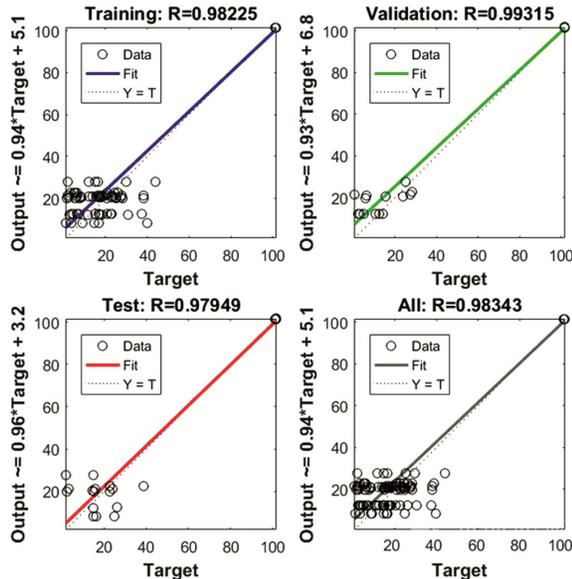


Fig. 12 — Comparison of the simulation results and predicted results derived from the ANN model for training, validation and testing, as well as in all three combined.

initialized training with random weights shows some variations in the network's output in the first epochs, and it will be trained after several epochs and updating the weight values accordingly. The Fig. 12

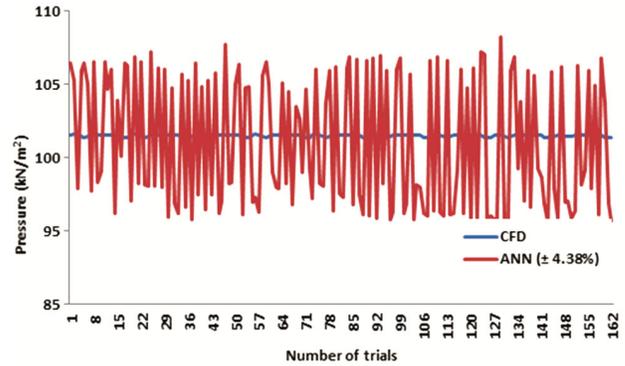


Fig. 13 — Pressure variation between CFD and ANN predicted values

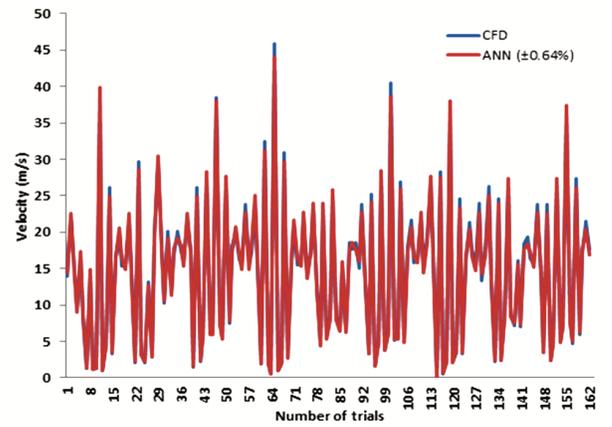


Fig. 14 — Velocity variation between CFD and ANN predicted values

shows the testing, training, validation as well as in all combined.

The Fig. 13 depicts the measured and MLP ANN predicted output results of pressure from the catalytic converters. The Fig. 14 illustrates the measured and MLP ANN predicted output results of velocity from catalytic converters' outlets. The graphs were plotted to represent the deviation between ANN and CFD. It is also evident from the Fig. 13 and Fig. 14 that, proposed ANN model can predict pressure and velocity with an error of  $\pm 4.38\%$  and  $\pm 0.64\%$ . The proposed ANN approach can be used to calibrate/predict the exhaust gas outlet parameters through the catalytic with an accuracy of  $\pm 97.48\%$ .

**Conclusions**

The list of following conclusions is observed from the above study.

1. Based on the output, it has been observed that 140 mm length diffuser and distributor plate position at 117 mm from the entrance gives the best flow trajectory result.

2. About 34% Velocity reduction at the centre portion of the mesh increases the residual time, which will lead to better chemical conversion.
3. Contrarily, the distributor plate's presence at the entrance section of the diffuser and shorter length diffusers does not produce expected results.
4. The results obtained from the CFD are used to develop an ANN model.
5. The proposed ANN model can predict the exhaust gas pressure at the outlet with an accuracy of 95.61%.
6. Similarly, the proposed ANN model can predict the exhaust gas velocity at the outlet with an accuracy of 99.35%.

### Nomenclature

1.  $\rho$  Density of air, kg/m<sup>3</sup>
2.  $u$  Velocity of air, m/sec
3.  $\Delta u$  Change in velocity, m/sec
4.  $P$  Pressure of air, kN/m<sup>2</sup>
5. Pa Pascal
6.  $\Delta p$  Change in pressure, kN/m<sup>2</sup>
7.  $\mu$  Dynamic viscosity of air, Pascal-Sec
8.  $F$  External forces applied to the air, kN
9.  $n$  Number of data sets

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