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Pressure Drop Prediction of Square-cell Honeycomb Monolith Structure

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Abstract— **Stringent emission regulations around the world necessitate high efficiency catalytic converter to be used in vehicles exhaust system. It is essential to determine optimum geometry of honeycomb monolith structure which required high surface area to treat the gases while maintaining low pressure drop to the engine. In this paper, adapted sub-grid scale modeling is used to predict the pressure loss of square cell shape of honeycomb monolith structure in catalytic converter application. This sub-grid scale modeling represents the actual variations of pressure drop between the inlet and outlet for various combinations of wall thickness and cell density. Comparison is made to the experimental and numerical work established in the literature. This approach is found to give better and more comprehensive results over the single channel technique.**

Keywords-honeycomb monolith, pressure loss, sub-grid scale modeling

I. INTRODUCTION

Air pollution and global warming is a major issue nowadays. For this reason, emission limits are introduced around the world and continually being made stricter every year. The enforcement of this regulation has led to the compulsory utilization of catalytic converter as an emission treatment to the exhaust gas of vehicles.

The installation of catalytic converter in the exhaust system has not been without a problem. The catalyst surface area needs to be sufficient to treat the gases to meet the emission limits. However, this will increase the pressure drop and becomes the major issue to overcome since it indicates the engine loss in terms of power and fuel economy. Typically, the engine will lose about 300 W per 1000 Pa of pressure loss [1]. As a result, a trade-off between the pressure loss and total surface area has become the main concern in determining the appropriate geometry of catalytic converter.

Pressure drop in catalytic converter are associated with two major components: substrate and flow distribution devices (including manifold, inlet and outlet pipe, inlet and outlet diffuser) [2]. The largest contribution of the exhaust backpressure is coming from the substrate. Its earlier shape was in pellet form (using spherical particulate γ-Al_2O_3 particles) before being replaced with the honeycomb monolith. The latter was more advantageous in term of lower pressure drop by having high open frontal area (about 70%) and parallel channels [3]. Honeycomb monolith is also available in different cell density and shapes offering potential flexibility. However, the geometries have to be optimized to meet the demanding application in the automotive industry.

Many researchers have proposed models to predict the pressure loss of the channels substrate with various cell shapes. The most common is the classic Hagen-Poiseuille for a fully developed laminar flow through a circular duct [4]. There were also model for a square duct [4] and Luoma's expression [5]. Based on the comparison between the measured data and the prediction of these models, several conclusions had been made. Thorough investigation reveals that none of these models able to capture the exact behaviour of the pressure losses. Equation for square duct is accurate in getting the value of static pressure at the exit of monolith. Nevertheless, its flow profile is different from the accepted laminar profile and it is thought from the highly surface roughness of the channel [6].

An empirical model also had been developed by Ekstrom and Andersson [7] to predict the pressure drop suitable for one dimensional (1D) and three dimensional (3D) simulations. In here, only one channel was modeled. The Hagen-Poiseuille equation was used to describe the pressure drop of the laminar flow in a channel. However, literature values can be found for most of the simple shapes. For some other complicated shape, CFD simulation of a single channel can give the constant value. It can also be determined experimentally by measuring substrates of different length according to the pressure drop difference between the substrates.

Inlet and outlet effects will also contribute to the overall pressure drop. Entrance effects are due to the boundary layer growth, flow maldistribution and sudden contraction when flow enters the monolith. There was a deceleration effect at the channel outlet and it influenced the pressure loss in that region. Therefore, a fully developed laminar flow profile would develop after certain distance in the channel.

In the substrate, the typical honeycomb channels have a hydraulic diameter to length ratio in 1:100. In performing

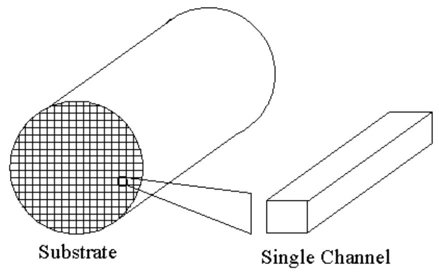


Figure 1. Single channel modeling [8].

the calculations; if each channel is represented by a 10 x 10 x 100 cells, modeling all the channels produce millions of cells which will take tremendous computational efforts and high cost to solve it. As a result, modeling of honeycomb monolith is rather complicated due to the massive numbers of channels.

Since honeycomb material is a unitary structure with uniform-sized and parallel channels, it is available in various channel shapes and dimensions including hexagon, square, sinusoidal, triangular and circle. Macroscopic modeling of catalytic activities is seen to be limited to a single channel of the substrate monolith. It is valid by considering the velocity profile is uniform at the inlet face of the monolith sample (it is assumed that flow maldistribution does not occur when the exhaust gas enters a substrate from the diffuser). Individual channels are separated from each other in term of mass transfer, hence provides information to the pressure loss, heat and mass transfer and chemical behavior of the catalyst. Single channel method of analysis are seen to be employed by many previous researchers [6][7][8][9][10]. Fig. 1 displays a concept of single channel modeling of a circular substrate with a square cell shape.

The increasing needs of design and optimization of the full scale catalytic converters requires further modeling techniques to be improved. Sub-grid scale modeling (Fig. 2) had been used to predict the temperature and concentration

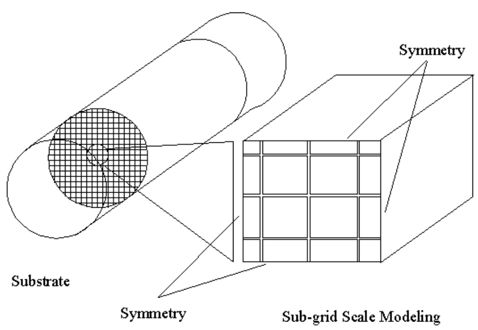


Figure 2. Sub-grid scale modeling [11].

of a catalytic combustion in a full scale catalytic converter [11]. The simulation had provided certain pressure drop values from the beginning of monolith until its end. This technique is primarily focused on heterogeneous chemical reaction in which the prediction of temperature and concentrations within the entire catalytic converter is obtained based on a complex combination of the properties of the gas and solid parts. Such effects cannot be predicted by single channel method and provides better accuracy compared to single channel [12].

This paper proposes the adapted sub-grid scale modeling to predict the pressure drop of square cell shape honeycomb monolith structure in exhaust aftertreatment application. This method offers closer approximation in pressure loss prediction compared to established technique with additional advantages of fewer elements which reduces the computing cost.

Beginning from the next section, this paper is organized as follows: Section II describes the geometry, computational domain, meshing and boundary conditions of the model. Section III discusses the results of the Computational Fluid Dynamics (CFD) calculation including grid independence study and comparison with the experiment and other models and finally, the paper is concluded in Section IV.

II. METHODOLOGY

A. Computational Domain

The geometry of honeycomb monolith structure employed in this study was square shape with 600 cpsi/4.5 mil (cpsi is cells per square inch and 4.5 mil (0.114 mm) is

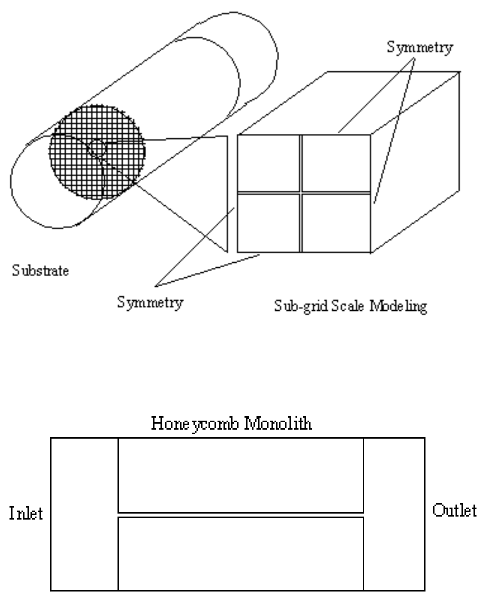
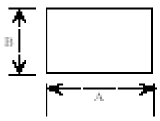
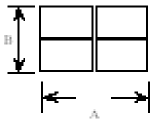


Figure 3. Adapted sub-grid scale modeling applied on square-cell honeycomb.

TABLE 1. GEOMETRY OF SINGLE CHANNEL [8] AND SUB-GRID SCALE MODELING

Parameters	Single channel 	Sub-grid scale modeling 
Cell shape	Square	Square
A (mm)	0.950	1.064
B (mm)	0.950	1.064
Cell length (mm)	118	118
Cell density (cpsi)	600	600
Wall thickness (mm)	0.114	0.114

the wall thickness). The domain was built using the approach adapted from sub-grid scale modeling [12] as in Fig. 3. Instead of considering single channel only [8], this method utilizes four channels which were taken into account simultaneously its inlet and outlet length. Its geometrical difference in domain set up was compared to single channel method and tabulated in Table 1.

Fig. 4 shows the actual domain with solid T- shaped represent the wall thickness of honeycomb structure. Unstructured Tri-Mesh (0.2 mm spacing) with 121,718 elements was depicted in Fig. 5.

B. Boundary Condition

Inlet was defined as its flow regime in subsonic, assumed of uniform velocity in 5 m/s and air inlet temperature at 20 ^{o}C (293 K). Air inlet temperature was selected based on the experimental and numerical condition conducted by Miyairi *et al.* [8]. As the simulation proceeds, the velocity was changed to 10, 15 and 20 m/s. Pressure outlet was set at atmospheric pressure. The wall was defined as no slip condition and the temperature was fixed at 100 ^{o}C (373 K).

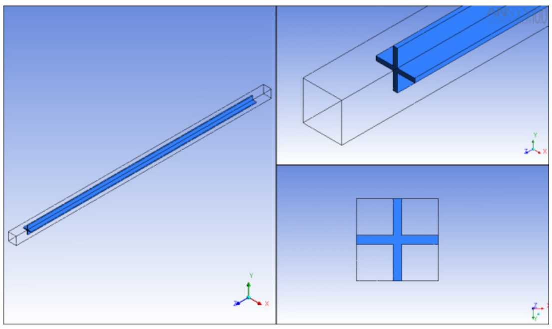


Figure 4. Actual domain of square-cell using sub-grid scale modeling.

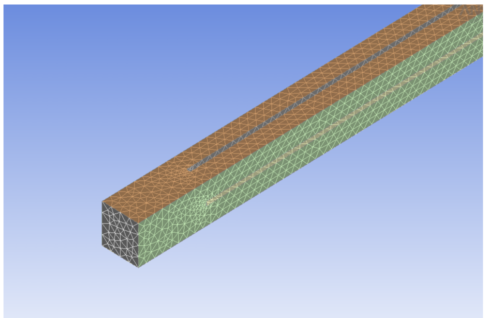


Figure 5. Meshing of square cell-shape using sub-grid scale modeling.

The fluid properties of air used in this model was given in Table 2. A three dimensional (3D) steady state incompressible solution of the Navier-Stokes was performed using ANSYS CFX. The equations involved are outlined in (1) and (2). During the solver definition, upwind advection scheme was used and the convergence criteria mentioned residual type as Root Mean Square (RMS) with residual target was set on $1x10^{-5}$.

The Continuity Equation [14]

$$\frac{\partial \rho}{\partial t} + \nabla \bullet (\rho U) = 0 \quad (1)$$

The Momentum Equation [14]

$$\frac{\partial \rho U}{\partial t} + \nabla \bullet (\rho U \otimes U) = \nabla \bullet (-p\delta + \mu(\nabla U + (\nabla U)^T)) + S_M \quad (2)$$

C. Validation

Pressure drop calculation was performed on the honeycomb structure with the cell density, wall thickness and length stated in Table 1. At 5 m/s inlet velocity, the

TABLE 2. AIR PROPERTIES AT 20 ^{O}C AND 1 ATMOSPHERE IN BOUNDARY CONDITION

Thermodynamic properties (unit)	Properties
Molar mass (kg/mol)	28.96
Density (kg/m^3)	1.205
Specific heat capacity (J/kg.K)	1005
Dynamic viscosity (kg/m.s)	18.207x10^{-6}
Thermal conductivity (W/m.K)	0.0257

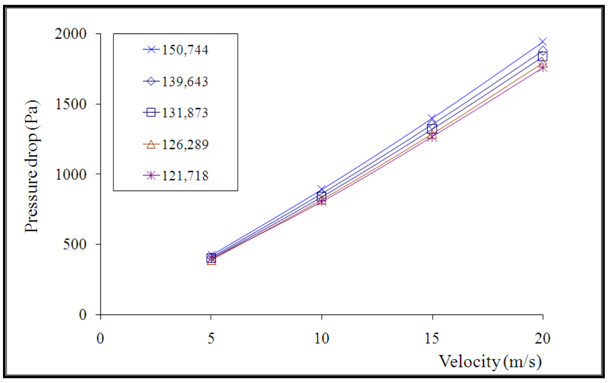


Figure 6. Grid independence study for square-cell shape using sub-grid scale modeling.

calculated results were compared to the experimental data as in [8]. The difference was calculated using Root Square (RS) and RMS shown in (3) and (4). The difference was tabulated in percentage. The same steps was applied for 10, 15 and 20 m/s of inlet velocity.

$$\text{Root Square (RS)} = \sqrt{\left(\frac{X_{sim} - X_{exp}}{X_{exp}}\right)^2} \ \% \qquad (3)$$

where

X_{sim}: Calculated data
X_{exp}: Experimental data

$$\text{Root Mean Square (RMS)} = \frac{1}{n}\sum_{i=1}^{i=n} RS_i \ \% \qquad (4)$$

where

n: number of data

III. RESULTS AND DISCUSSION

Grid sensitivity tests were conducted using the same geometry of the experiment by Miyairi *et al.* [8]. Fig. 6 illustrates the experimental and calculated pressure drop for different velocity and mesh density. Small deviation of pressure drop values compared to the experiment indicates the reliability of the meshing scheme to be employed further.

The calculation achieves the grid independence result between 121,718 and 150,744 with mean deviation ranges between 1.14 to 5.15 %. RMS difference for each set of data at each particular velocity exhibits the consistency of computed pressure loss compared to the values from the experiment. Preferred mesh density is selected by obtaining the best fit of predicted pressure drop to the experimental data. Therefore, the lowest mean difference chosen is 5.14 % representing the mesh density 121,718. This meshing scheme is selected to be used further in the simulation.

The present work is validated by comparing the simulation results from the preferred meshing to the experimental data and numerical work conducted by Miyairi *et al.* [8]. Table 3 shows the mean RMS difference of the present simulated results is 5.14 %.

TABLE 3. VALIDATION FOR SQUARE CELL SHAPE

	Miyairi *et al.* (2003)			**Present work**	
	Experiment	***Simulation***		***Computed***	
Air velocity (m/s)	***Pressure drop (Pa)***	***Pressure drop (Pa)***	***RS difference (%)***	***Pressure drop (Pa)***	***RS difference (%)***
5	417	476	14.16	400	4.00
10	857	987	15.10	806	5.97
15	1339	1527	14.00	1266	5.47
20	1857	2132	14.78	1762	5.12
		RMS difference (%)	14.51	RMS difference (%)	5.14

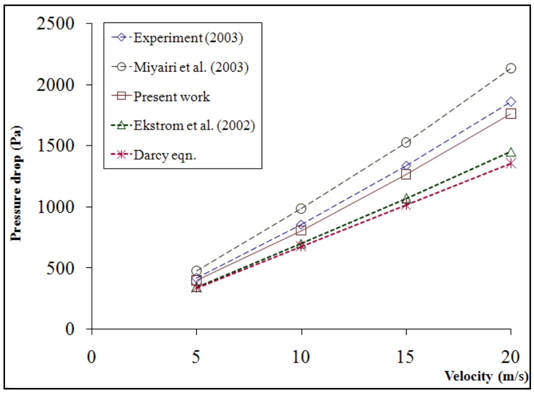


Figure 7. Comparison of pressure drop for square-cell using different technique.

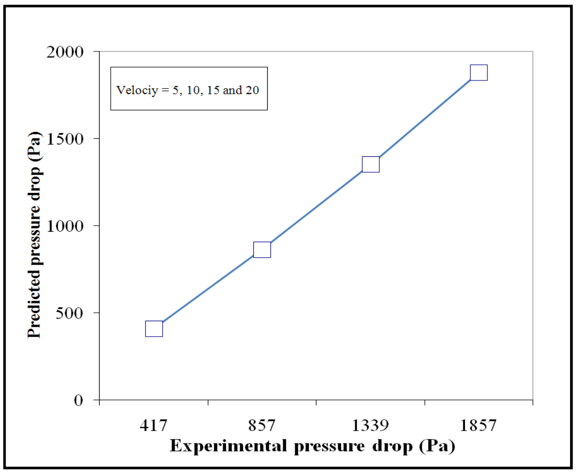


Figure 8. Parity chart of correlation between simulation and experimental pressure drop.

Compared to the previous numerical work [8], it exhibits higher deviation with mean RMS difference is 14.51 %. Fig. 7 shows the comparison of all models including Ekstrom and Andersson [7] and the established Darcy equation [4]. It was found that deviation of these two models compared to the experiment is higher which are 19.41 and 22.73 % respectively.

The present method of prediction exhibits higher accuracy up to 5 % deviation from the actual experiment. A parity chart is also plotted in Fig. 8 showing that the present numerical work is in good agreement with the experimental data.

Evidently, the present numerical approach has its advantage in predicting the pressure drop across the square cell-shape channel. It shows that the sub-grid scale modeling is a better approach in giving good results compared to single channel approach and other available models as indicated in Fig. 7. Its advantage is highlighted in terms of computational cost (lower number of cells and computing time) and accuracy (lower difference in pressure drop compared to the experiment). It only employs up to 150,000 elements for square-cell compared to 300,000 to 500,000 elements using single channel method.

IV. Conclusion

The sub-grid scale model approach gives better agreement in pressure drop compared to the numerical work using single channel approach. This present method also possesses lower computational cost based on the less computing time and number of elements in the simulation.

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