COMPUTATIONAL FLUID DYNAMICS (CFD) ANALYSIS FOR A CATALYTIC CONVERTER DESIGN

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ABSTRACT

Design of catalytic converters involves four major components including casing, washcoat, catalyst and substrate. However, the design process is complicated as it involves various parameters. One of the problems faced by designers is obtaining the performance of catalytic converters where the substrate is made up of a large number of cells. Therefore, an effort to solve the problem using Computational Fluid Dynamics (CFD) with an alternative modeling technique is deployed. This study involved a preliminary design which employed an adapted sub-grid scale modeling as an alternative method for the analysis of substrate performance. The Pahl and Beitz's model was applied in the design process. The adapted sub-grid scale modeling was used to predict the pressure loss, select the cell shape and produce the performance chart which could show the relationship between the parameters involved. The proposed adapted sub-grid scale modelling method was found to give results within 5 % error which was better compared to the single channel method. Results also indicated the advantage of hexagonal-shaped over square-shaped cells in terms of pressure loss where the former showed a 43 % lower value than the latter. The Mechanical-Chemical Performance Mapping (MCPM) was finally obtained. The mapping could be used to assist in the substrate design of catalytic converters.

ABSTRAK

Rekabentuk penukar bermangkin melibatkan empat komponen utama termasuk bekas, lapisan, pemangkin dan substrat. Namun begitu, proses rekabentuk adalah kompleks kerana ia melibatkan pelbagai parameter. Salah satu masalah yang dihadapi oleh perekabentuk adalah untuk memperolehi prestasi penukar bermangkin di mana substrat terdiri daripada banyak sel. Oleh itu, usaha telah dilakukan untuk menyelesaikan masalah dengan menggunakan Pengiraan Dinamik Bendalir (CFD) sebagai kaedah permodelan alternatif telah digunakan. Kajian ini melibatkan rekabentuk awalan di mana ia mengadaptasikan kaedah sub-grid yang telah diperbaiki sebagai kaedah alternatif dalam analisis prestasi substrat. Model Pahl and Beitz's telah digunakan dalam proses merekabentuk. Kaedah sub-grid telah digunakan untuk meramalkan kejatuhan tekanan, memilih bentuk sel dan memperolehi carta prestasi yang menunjukkan hubungan antara parameter terlibat. Kaedah sub-grid yang dicadangkan telah menunjukkan bentuk heksagon memberikan perbezaan keputusan sebanyak 5 % dan ia lebih baik berbanding kaedah satu sel. Keputusan juga menunjukkan kelebihan sel berbentuk heksagon berbanding bentuk segiempat dari segi kejatuhan tekanan di mana bentuk heksagon menunjukkan 43 % lebih rendah kejatuhan tekanan berbanding bentuk segiempat. Carta Prestasi Mekanikal dan Kimia akhirnya diperolehi. Ia boleh digunakan untuk membantu dalam merekabentuk substrat sesebuah penukar bermangkin.

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LIST OF ABBREVIATION

AEA	-	The United Kingdom Atomic Energy Authority
Al_2O_3	-	Aluminium Oxide (Alumina)
ASC	-	Advanced Scientific Computing
CFD	-	Computational Fluid Dynamics
CFX-Pre	-	Solver in ANSYS CFX Software
cpsi	-	Cell Per Square Inch
cpsc	-	Cell Per Square Centimeter
EURO	-	European Standards of Emission Regulations
FeCrAl	-	Ferum Chromium Aluminium
GSA	-	Geometric Surface Area
MAA	-	Malaysian Automotive Association
OFA	-	Open Frontal Area
OSC	-	Oxygen Storage Capacity
PEC	-	Performance Evaluation Criteria
PDE	-	Partial Differential Equation
RMS	-	Root Mean Square
RS	-	Root Square
TWCC	-	Three-Way Catalytic Converter
U.S	-	United States of America
1D	-	One Dimensional
2D	-	Two Dimensional
3D	-	Three Dimensional

LIST OF SYMBOLS

A	-	Surface Area (mm^2)
atm	-	Atmosphere
A/V	-	Specific Surface Area (mm^2/mm^3)
C	-	Carbon
cc	-	Volume of Combustion Chamber (cm^3)
CeO_2	-	Cerium Oxide (Ceria)
CO	-	Carbon Monoxide
CO_2	-	Carbon Dioxide
^oC	-	Degree Celsius
D_h	-	Hydraulic Diameter (mm)
ε	-	Height of Surface Roughness (µm)
f	-	Darcy Friction Factor
f'	-	Fanning Friction Factor
HC	-	Hydrocarbon
h_{tot}	-	Specific Total Enthalphy (m^2/K^2)
H_2	-	Hydrogen
H_2O	-	Water
L_e	-	Developing Length
MgO_2	-	Magnesium Oxide
mil	-	1/1000 inch
NO_x	-	Nitrogen Oxide
n	-	Number of Data
O_2	-	Oxygen
p	-	Static Pressure (Pa)
Pd	-	Palladium
Pt	-	Platinum

Re	-	Reynolds Number
Rh	-	Rhodium
S_E	-	Energy Source (kg/m.K^3)
SiO_2	-	Silicon Oxide (Silica)
S_M	-	Momentum Source (kg/m^2.K^2)
t	-	Time (sec)
T	-	Static Temperature (^{o}C)
u	-	Velocity (m/s)
U	-	Vector Function of U(x,y,z)
V	-	Volume (m^3)
vs	-	Versus
W	-	Watt
X_{exp}	-	Experimental Data
X_{sim}	-	Predicted Data
ρ	-	Density (kg/m^3)
ΔP	-	Pressure Drop (Pa)
λ	-	Thermal Conductivity (W/m.K)
μ	-	Dynamic Viscosity (kg/m.s)
ν	-	Kinematic Viscosity (m^2.s)

$$\nabla = \left[\frac{\partial}{\partial x} + \frac{\partial}{\partial y} + \frac{\partial}{\partial z}\right]$$

$$U = \begin{bmatrix} U_x \\ U_y \\ U_Z \end{bmatrix}$$

$$\nabla \bullet U = \frac{\partial U_x}{\partial x} + \frac{\partial U_y}{\partial y} + \frac{\partial U_z}{\partial z}$$

$$\nabla \bullet (\rho U \otimes U) = \begin{bmatrix} \frac{\partial}{\partial x}(\rho U_x U_x) + \frac{\partial}{\partial y}(\rho U_y U_x) + \frac{\partial}{\partial z}(\rho U_z U_x) \\ \frac{\partial}{\partial x}(\rho U_x U_y) + \frac{\partial}{\partial y}(\rho U_y U_y) + \frac{\partial}{\partial z}(\rho U_z U_y) \\ \frac{\partial}{\partial x}(\rho U_x U_z) + \frac{\partial}{\partial y}(\rho U_y U_z) + \frac{\partial}{\partial z}(\rho U_z U_z) \end{bmatrix}$$

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CHAPTER I

INTRODUCTION

1.1 Research Background

The need for mobility will increase in future, particularly in the fast-developing nations due to the growing world prosperity. In Malaysia, the number of new vehicles registration from 1980-2005 exhibits rapid increase and has contributed to the total of 15 million registered vehicles on the road (MAA Annual Report, 2006). However, this economically necessary development should not come at the expense of the environment. This is particularly important amidst of air pollution and global warming becoming a major issue nowadays. For this reason, the emission limits are being introduced around the world and continually being made stricter every year.

The history began with the introduction of 1970 United States (U.S) Clean Air Act Air which required the steep emissions reduction for the new 1975 and 1976 automobiles. Since 1975, automotive companies have developed technologies that enable the U.S Environmental Protection Agency to successfully adopt the usage of catalytic converter and three-way catalyst (Gerard and Lave, 2000). European countries had also implemented the strict regulations of the European Standard (EURO) beginning from 1992 with the intention to reduce the emissions including carbon monoxide (CO), hydrocarbon (HC) and nitrogen oxide (NO_x) from the combustion engines. Consequently, the enforcement of these regulations had finally led to the compulsory utilization of catalytic converter as an emission treatment for the vehicles exhaust gas around the world.

Looking from the engineering design point of view, it is important to optimize design parameters in order to increase the performance of catalytic converter. Miyairi *et al.* (2003) had investigated the effects of cell shape on mass transfer and pressure loss of substrates design. Structural advantages, mechanical and thermal characteristics of square and hexagonal cells had also been studied by Tanaka *et al.* (2003). Maus (1997) had mentioned that an increase of cell density and Geometric Surface Area (GSA) had reduced the HC emissions efficiency. A reduction in wall thickness also reduces the heat capacity of a substrate; hence improve the cold start problem. Inlet pipe and diffuser geometry and monolithic length also influence the overall performance of catalytic converter.

The installation of catalytic converter in the exhaust system has not been without problem. It has to be highly efficient in treating the emissions without sacrificing the engine performance. The catalyst surface area needs to be sufficient to treat the gases to meet the emission target of the vehicles. However, this will result in the increase of the pressure drop. This is the main issue to overcome since it indicates the engine loss in term of power and fuel economy. Typically the engine will lose about 300 W of power per 1000 Pa of pressure loss (Pannone and Mueller, 2001). As a result, a trade-off between the pressure loss and total surface area has become the major 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) (Lakshmikantha and Meck, 2002). 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 (~70%) and parallel channels (Searless, 2002). The honeycomb monolith is also available in different cell density and shapes offering potential flexibility. However, the geometries have