INVESTIGATION OF PRESSURE EFFECT ON METHANE CONVERSIONS IN CATALYTIC COMBUSTION SYSTEM

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ABSTRACT

Catalytic Converter is a device to clean up the exhaust gases by breaking down the harmful gas compounds. When the engine burns fuel, it produces gases that pollute the air such as hydrocarbons, carbon monoxide and nitrogen oxides. This project is carried out to investigate the influences of reactor pressure on the methane conversion and to find the effect of reverse flow on methane conversion. The single channel has been considered as a part of a monolith structure and from the modeling point of view only one channel needs to be investigated, assuming that symmetry holds for the inlet conditions. The single channel reactor is a cylindrical tube with diameter 2 mm and length 20 mm. Computational fluids dynamic (CFD) analysis simulate the reaction of burned methane with oxygen and show the graphical result of path line the reaction flow from the inlet to the exhaust. From the graph the simulation has show that the optimum pressure for the methane conversion rate is at 1 atm pressure. The Reverse flow that develops near the outlet of channel when the reactor pressure reach at 5 atm slightly increase the conversion rate of burned methane.

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ABSTRAK

Pemangkin amat diperlukan untuk membersihkan gas-gas yg keluar dari eksoz dengan memecahkan sebatian gas-gas yang berbahaya ini. Pembakaran bahan bakar dalam enjin, akan menghasilkan gas-gas yang akan mencemarkan udara sebagai contohnya hidrokarbon, karbon monoksida dan nitrogen oksida. Projek ini dijalankan untuk mengkaji pengaruh tekanan reaktor dan kesan aliran berbalik terhadap tindak balas pembakaran gas metana. Satu saliran dari keseluruhan struktur monolit saja yang dipertimbangkan dalam kajian ini, dengan menganggap bahawa keadaan simetri berlaku dekat lubang kemasukan. Saluran ini mempunyai diameter 2 mm dan panjang 20mm. Aplikasi perkomputeran bendalir dinamik analisis akan menghasilkan simulasi tindakbalas pembakaran gas metana dengan oksigen dan akan menunjukan gambar keputusan aliran pergerakan tindakbalas dari lubang kemasukan hingga ke lubang keluaran. Berdasarkan keputusan simulasi dari graf, menunjukan optimum tekanan untuk kadar penukaran gas metana adalah 1 atm. Aliran berbalik yang berlaku dekat lubang keluaran apabila tekanan reaktor mencapai kepada 5 atm akan meningkatkan kadar penukaran pembakaran gas metana.

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CHAPTER 1

INTRODUCTION

1.1 BACKGROUND

The use of three way catalysts converter become important because the emission came from internal combustion engine. The majority of gasoline-fueled engine now day equipment with catalytic converter. The main purpose of catalytic converter is to convert carbon monoxide (CO), nitrogen oxide (NO_x) and unburned hydrocarbons to carbon dioxide, water and nitrogen so that the emission from gasoline engine can be reduce or less harmful to environment [1].

Catalytic converters are built from structures called monoliths. The monolith forms the basic framework of the converter, and acts as an inert substrate for the catalytic coating. A layer of washcoat is first deposited on the substrate, and the catalysts (often precious metals such as platinum, palladium, and rhodium) are then deposited on the washcoat. In order to reach the required conversion efficiencies for a practical converter, the surface area for reactions must be very large, and this large area is provided by the monolith geometry and the highly porous wash coat. To optimize the design of a catalytic converter, it is important to investigate not only the flow field, but the chemical reactions and heat transfer in the system as well. The distributions of temperature and species throughout the device play an important role in its performance.

1.2 PROBLEM STATEMENT

1.2.1 Important of Catalyst converter

When the engine burns fuel, it produces gases that pollute the air such as hydrocarbons, carbon monoxide and nitrogen oxides. The function of the exhaust system is to clean up the emissions that are harmful to the environment. Catalytic Converter is needed to clean up the exhaust gases by breaking down the harmful gas compounds. Chemicals in the catalytic converter act as catalysts, changing the highly hazardous gas compounds to less harmful ones. Because air pollution is a major environmental problem that affects us all, catalytic converters are a necessity.

1.3 OBJECTIVE

i. To investigate The influences of reactor pressure on the methane conversion
ii. To find The effect of reverse flow on methane conversion

1.4 SCOPE

i. Develop a two-dimensional numerical model for simulation of a monolith honeycomb catalytic reactor.

ii. From the data, the geometry model and mesh were created using the program Gambit 2.16.

iii. Perform the simulation with program Fluent for the model.

1.5 ORGANIZATION OF REPORT

This project report was organized with a few chapters which describe details about the progress and time frame of the project. The report was detailed in all five chapters and the project management (time frame) is attached in the appendix.

Chapter	Description
Introduction	Introduction to catalytic combustion material and a discussion of the motivation behind and objectives of this research
Literature Review	Information, article, research and journal that related to the title. Also get the data and privies study about catalyst converter
Methodology	Next, there is a description of methods undertaken in this research
Result and Discussion	There is a discussion of the results obtained from the solved computer simulations
Conclusion	The implications of the research results and future work for improve the current research

Tables 1: Organization of the Report

CHAPTER 2

LITERATURE REVIEW

2.1 Introduction

The aim of this chapter is to give some overview information about the catalytic converter which in the subject emission reduction from combustion engine. In this chapter, the explanations and details of function and principle work of catalytic converter, the previous research and findings, the theories are included. It also will describe the basic model design, analysis process for catalytic converter.

2.2 Background

Air pollution generated from mobile sources is a problem of general interest. In the last 60 years the world vehicle fleet has increased from about 40million vehicles to over 700 million; this figure is projected to increase to 920 million by the year 2010 [2]. Engine exhausts consist of a complex mixture, the composition depending on a variety of factors such as: type of engine (two- or four-stroke, spark- or compression (diesel)-ignited), driving conditions, e.g. urban or extra-urban, vehicle speed, acceleration/deceleration, etc. Table 1 reports typical compositions of exhaust gases for some common engine types.

Exhaust component and condition[a]	Diesel Engine	Four –stroke spark ignited-engine	Four stroke lean-burn spark ignited-engine	Two-stroke spark ignited-engine
NO_x	350–1000 ppm	100–4000 ppm	≈1200 ppm	100-200 ppm
HC	50–330 ppm C	500-500 ppm c	≈1300 ppm C	20,000-30,000 ppm C
CO	300–1200 ppm	0.1-6%	≈ 1300 ppm	1-3%
O_2	10–15%	0.2-2%	4-12 %	0.2-2%
H_2O	1.4–7%	10-12%	12%	10-12%
CO_2	7%	10-13.5%	11%	10-13%
SO_x	10–100 ppm[b]	15-60ppm	20 ppm	≈20 ppm
PM	65 mg/m^3			
Temperature (test cycle)	r.t.–650 ^0C (r.t.–420 ^0C)	r.t.-1100 ^0C[c]	r.t.-850 ^0C[c]	r.t.-1000 ^0C[c]
GHSV (h^{-1})	30,000–100,000	30,000-100,000	30,000-100,000	
λ (A/F)[d]	≈1.8 (26)	≈1 (14.7)	≈1.16 (17)	≈1 (14.7)[e]

[a] N2 is remainder.

[b] For comparison: diesel fuels with 500 ppm of sulphur produce about 20 ppm of SO2 [6].

[c] Close-coupled catalyst.

[d] λ defined as ratio of actual A/F to stoichiometric A/F, $\lambda = 1$ at stoichiometry (A/F = 14.7).

[e] Part of the fuel is employed for scavenging of the exhaust, which does not allow to define a precise definition of the A/F.

Table 2.1 Example of exhaust condition for two- and four-stroke, diesel and lean four stroke engine [3-6]

2.3 Catalytic Converter

2.3.1 Technology

The catalytic converter is use in wide range of engineering application, including in automotive exhaust after-treatment, hydrogen production for fuel cell systems, and low temperature lean combustion within gas turbines. Catalytic conversion is utilized in automobiles to remove pollutants from engine exhaust to comply with set governmental emission standards. The two types of converters that have been used are bead-pellet catalytic reactors and catalytic monoliths. Bead/pellet catalytic reactors are constructed by filling a containing vessel with small porous ceramic pellets that have been covered in catalytic slurry is shown in Figure 2.1.

The current three-way catalysts (newer technology) consist of either a ceramic (cordierite) or a metallic (stainless steel) honeycomb structure called a monolith, usually with 1mm × 1 mm large square cross sections or channels divided by thin 0.1 mm porous walls. The number of channels varies between around 400 and 600 cells per square inch (cpsi). The honeycomb structure is coated with a highly porous alumina-based washcoat. The washcoat, in turn, is impregnated with the noble metals (Pd, Pt and Rh) constituting the active sites, amenable for the removal of the hazardous exhaust gases. The exhaust flows through the monolith tubes, reacting with the catalyst along the inner surface areas of the tubes and exiting as acceptable emissions. The closed-loop-controlled three-way-catalytic converter is most commonly used catalytic monolith in automotive applications [7], given its name for the three primary pollutants it removes. Carbon monoxide (CO), hydrocarbons (HCs), and nitrous oxides (NOx) are removed from the exhaust flow via a catalytic combustion reaction.

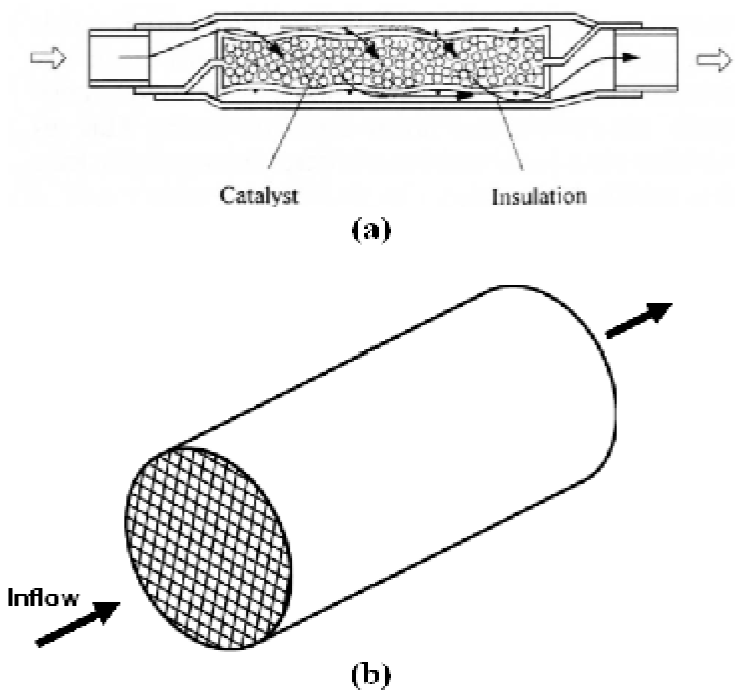

Figure 2.1 Examples of (a) bead/pellet catalytic reactor and (b) catalytic monolith

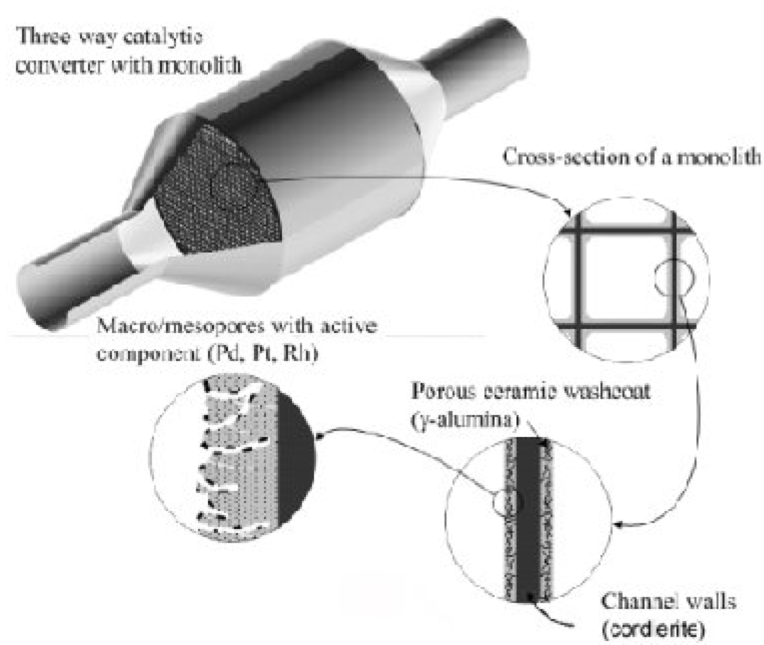

Figure 2.2 Structural design of a monolithic converter in an automotive catalyst

2.4 Monolith

2.4.1 Introduction

Monolithic supports are uni-body structures composed of interconnected repeating cells or channels. They are most commonly composed of ceramic or metal materials but some can also be made of plastic [9]. The most important physical characteristics when used as a catalyst support are the size of the channel through which the gaseous reactants and products traverse. Monolith substrates are usually used in automotive and stationary emission control reactor industry for the selective catalytic reduction of nitrogen oxide. Ceramic monolith for automotive application is made from synthetic cordierites 2MgO・ 2Al2O3・ 5SiO2, that material having a low thermal coefficient expansion [8]. Cordierites are highly anisotropy that leads to orientation during extrusion and overall expansion. Cordierites have a unique combination of several critical characteristics [8];

a) Thermal shock resistance due to a low thermal expansion coefficient
b) Porosity and pore size distribution suitable for ease of washcoat application and good washcoat adherence.
c) Sufficient refractoriness because of the melting point exceeds 1450ºc
d) Sufficient strength for survival in and automotive exhaust environment
e) Compatibility with washcoat and catalysts

2.4.2 Size, Shape and Dimension

Examples of monolithic substrates are shown in Fig. 2.3. The monolith parts itself can be produced in a number of sizes and shapes, typically round or oval cross-sectional areas for automotive applications, or square for stationary emission uses. Cross-sectional part diameters for single pieces up to 35 cm have been produced commercially for heavy duty vehicle uses.

Much larger cross-sectional areas are made by stacking blocks together for stationary emission reactor systems. In addition to the overall part dimension, the geometry of the monolith channels can be produced in many forms including square, round, hexagonal, and triangular.

Cell configurations and properties of monoliths are described in terms of geometric and hydraulic parameters [15, 16]. These properties can be defined in terms of cell spacing *L*, the distance measured from the center of one cell wall of a square channel to the next wall, and wall thickness, *t*. The cell density *N* is defined as the number of cells per unit of cross-sectional area and is expressed in units of cells per square inch (cpsi) or per square centimeter.

$$N = \frac{1}{L^2} \tag{1}$$

The OFA is defined as a function of wall thickness, cell spacing and cell density, as shown in Eq. (2).

$$OFA = N(L - t)^2 \tag{2}$$

The hydraulic diameter defined by Eq. (3) decreases as the cell density increases for a monolith.

$$D_h = L - t \tag{3}$$

The Hydraulic diameter is different for uncoated and washcoated monoliths since washcoating with catalyst or ceramic materials change the wall thickness. In designing monolithic catalysts, there is a balance between geometric surface area and pressure drop. The pressure drop across the monolith depends linearly on flow velocity and length

$$\Delta P = \frac{2f\ell\rho v^2}{G_c D_h} ch \tag{4}$$

Where *f* is the friction factor, dimensionless; *D*h the hydraulic diameter (cm); *G*c the gravitational constant; the monolith length (cm); *v* the velocity in channel (cm/s); and *ρ* the gas density (g/cm3).

These fundamental equations allow one to design monolith geometric parameters such as cell density or wall thickness to meet the constraints of external processing requirements such as space velocity, flow rates, pressure drop, etc.

In the case of automotive catalytic converters, the design and durability of advanced ceramics must promote fast light-off, improved conversion efficiency, and reduced backpressure [9]. Current designs are focusing on thinner wall monoliths. Thermal shock resistance and a low coefficient of thermal expansion are important properties of automotive converter substrates, and are a major reason why cordierite is the ceramic material of choice for this application.

The success of cordierite monoliths as catalyst substrates in the treatment of automotive exhaust has given rise to interest in the chemical industry as substrates for catalytic reactors.

For many of these applications, the use of other substrate materials and designs can be utilized since the thermal shock requirements are not as demanding as automotive. In general, many inorganic catalyst support materials used today in conventional chemical and refining application can be extruded into a monolith form. This has ignited interest in monolith reactors as potential replacements for fixed bed and slurry reactors. Monolith reactors offer the advantage of thinner walls, high geometric surface area, low-pressure drop, good mass transfer performance, and ease of product separation.

There may also be advantages in kinetics and mass transfer in gas/liquid phase applications due to better catalyst wetting, higher effectiveness factors, and thin films that are conducive to high mass transfer rates. However, the hydrodynamics and flow distribution of multi-phase flow through a monolith reactor bed is still not fully understood [17 – 21].

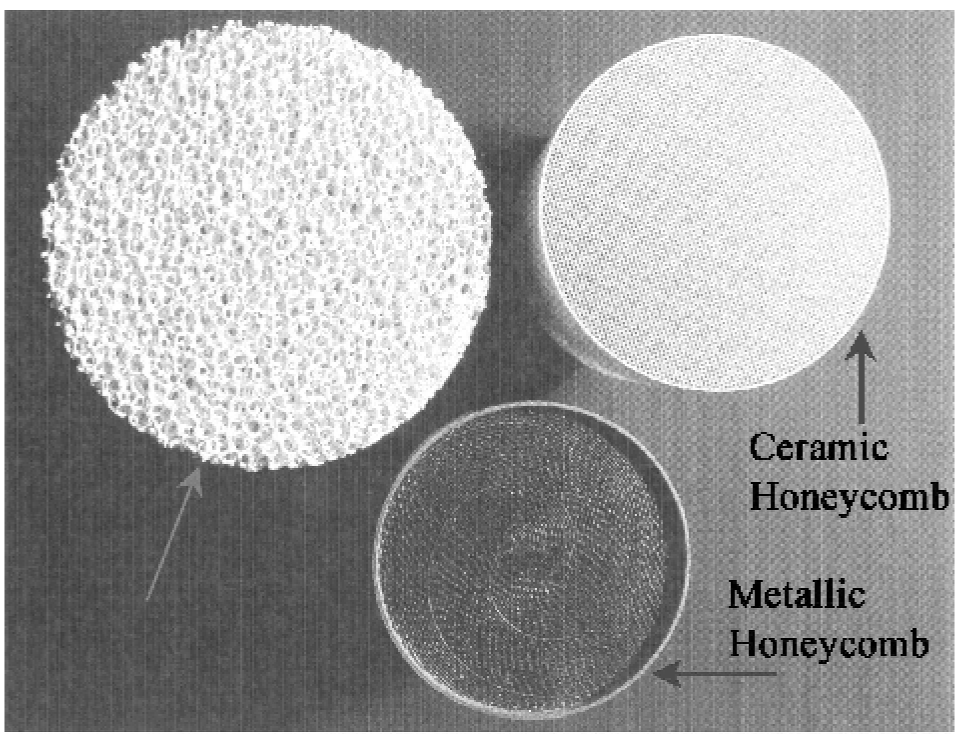

Figure 2.3 Ceramic and metal monolith [9]