Experimental and Numerical Investigations of Fluid Flow through Catalytic Converters

By

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ABSTRACT

Experimental and Numerical Investigations of Fluid Flow through Catalytic Converters

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The need for better automotive technologies to improve fuel economy, while meeting stringent vehicle emission standards, grows with the demand for environmental protection and rising fuel prices. A new technology, designed and patented by Vida Fresh Air Inc., offers emission reduction while improving fuel economy. In this study, experimental and numerical investigations are performed to understand the flow through the catalytic converter, commercially known as Cleanalytic™, using a scaled-down test rig. Experiments are conducted using hot air flow to evaluate the thermalhydraulic characteristics of the new technology. The measurements are performed for Reynolds number of 43,000 and free stream temperature of 177 °C. These conditions were selected to achieve thermal and hydraulic similarity of actual test conditions for engines. The numerical investigations are performed using ANSYS Fluent and the model predicted the experimental measurements within ±6 %. The use of Cleanalytic™ improved the performance of the catalytic converter.
Dedication

This thesis is proudly dedicated to my beloved parents Shahinaz A. Moneeb and Ahmed S. Ibrahim and my siblings Kareem, Eslam and Heba. Thank you for your support, love, sacrifices and prayers.
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Nomenclature

\( A \) Surface area
\( B_R \) Bias error
\( C_p \) Specific Heat
\( D \) Inlet pipe Diameter
\( d \) Instrument diameter
\( e_f \) Effective
\( \vec{F} \) Momentum sink or source
\( f \) Fluid
\( G \) Generation term
\( HW \) Hot-wire
\( h \) Convective heat transfer coefficient
\( \rho_h \) Stagnation enthalpy
\( h_s \) Static enthalpy
\( IR \) Monolith inertial resistance
\( k \) Thermal conductivity or turbulence kinetic energy
\( K \) Monolith axial permeability
\( L \) Length
\( Nu \) Nusselt number
\( \Delta P \) Pressure difference
$p_s$ Static pressure

$p_t$ Total pressure

$Pr$ Prandtl number

$P_R$ Precision error

$R$ Monolith container radius

$R'$ Inlet pipe radius

$R''$ Monolith substrate radius

$Re$ Reynolds number

$RMSD$ Root mean square difference

$RMSE$ Root mean square error in percentage

$r$ Radial direction

$S$ Source term or modulus of the mean rate of strain

$s$ Solid or substrate

$T$ Temperature

$T_0$ Stagnation temperature

$TC$ Thermocouple

$U_R$ Total uncertainty

$u$ Flow velocity

$u'$ Fluctuating component of the velocity

$V$ Electric voltage

$VR$ Monolith viscous resistance
\( \bar{v} \) Average flow velocity

\( w \) Wall

\( x \) \( x \) coordinate

\( Y \) Dissipation term

\( y \) \( y \) coordinate

\( z \) Axial direction

**Greek letters**

\( \Gamma \) Effective diffusivity

\( \beta \) Turbulence model constant

\( \beta^* \) Turbulence model constant

\( \gamma \) Flow uniformity index

\( \varepsilon \) Emissivity

\( \mu \) Viscosity

\( \mu_t \) Turbulent or eddy viscosity

\( \rho \) Density

\( \sigma \) Stefan Boltzmann’s constant or turbulent Prandtl number

\( \tau \) Stress tensor

\( \phi \) Monolith porosity

\( \omega \) Specific dissipation rate
Chapter 1 Introduction

Nowadays, automobiles are one of life essentials. This need encouraged the industry to increase the production of automobiles. Most automobiles produced are operated with fuel for which combustion is necessary. This combustion process is associated with releasing harmful emissions including carbon monoxide (CO), unburnt hydrocarbons (HC) and nitrogen oxides (NOx) which have negative effects on humans and the environment. This has led to the development of emission control units to treat exhaust gases and convert them to less harmful products. These units are called catalytic converters (Kummer, 1980 and Taylor, 1984).

Catalytic converters consist of honeycomb-like structures often referred to as “the monolith substrate” as shown in Figure 1.1, the catalyst which primary consists of one or more noble metals that facilitate the oxidation and reduction chemical reactions and a padding mat surrounding the substrate that helps in maintaining higher temperatures necessary for the continued operation of the converter.
The monolith substrate is typically constructed of a ceramic material namely cordierite and is shaped into a honeycomb structure to maximize the surface area to promote the chemical reaction (Heck et al. 2001, Heck and Farrauto 2001 and Shuai and Wang 2004). This honeycomb structure is loaded with the washcoat. The washcoat consists of aluminum oxide, silicon dioxide, titanium dioxide or a mixture of alumina and silica (Kummer 1980 and Ramanathan et al. 2004). The washcoat increases the surface roughness of the substrate to increase the overall surface area and act as a catalyst carrier due to its high porosity (Richardson et al. 2003). The catalysts used are noble metals mostly palladium, rhodium and platinum. These noble metals are oxidation and reduction catalysts (Chen et al. 2004, Gandhi et al. 2003 and Kummer 1980). The oxidation reactions require enough oxygen to complete the reaction. Ceria-zirconia acts as an oxygen storage medium supply and is embedded in the washcoat as wall (Masui et al. 2000, Matsumoto, 2004 and Yao and Yao, 1984). As shown in Figure 1.2, the ceramic substrate is holding the washcoat that carries the catalyst within its porous structure. The catalytic converter assembly is placed after the exhaust manifold and downstream of the internal combustion engine of the automobile to receive the harmful exhaust gases and convert them to more environmentally friendly ones. There are two main types of catalytic converters for gasoline engine applications. The first type is “two-way catalytic” converters in which two chemical reactions take place; oxidation of CO to CO$_2$ and oxidation of unburnt HCs to CO$_2$ and water vapor. Two-way catalytic converters were widely used for diesel and gasoline engines and are no longer used since
1981 as they don’t treat NOx emissions. The second type is “three-way catalytic” converters (TWCC). TWCC incorporate three chemical reactions; two oxidation reactions (similar to “two-way catalytic converters”) and a reduction reaction in which NOx are converted to O₂ and N₂ (DieselNet 2004; Kummer 1980; Pontikakis et al. 2004). A typical catalytic converter assembly is shown in Figure 1.3.

*Figure 1.2: A schematic of a loaded ceramic substrate (DieselNet, 2011)*

*Figure 1.3: A typical catalytic converter (www.crowndautomotive.com)*
The chemical reaction equations for the three-way catalytic converter are exothermic reactions and are shown below:

- Reduction of nitrogen oxides to nitrogen and oxygen:
  \[ 2NO_x \rightarrow xO_2 + N_2 \] (1.1)

- Oxidation of carbon monoxide to carbon dioxide:
  \[ 2CO + O_2 \rightarrow 2CO_2 \] (1.2)

- Oxidation of unburnt hydrocarbons to carbon dioxide and water vapour:
  \[ C_xH_{2x+2} + \left[ \frac{3x + 1}{2} \right] O_2 \rightarrow xCO_2 + (x + 1)H_2O \] (1.3)

The chemical reactions start at the light-off temperature. The light-off temperature is typically from 300 °C to 400 °C (Jeong and Kim, 2000). This high temperature can be achieved by the combustion of fuel that delivers very high temperature exhaust gas to the ceramic brick. However, during idling, the temperature of the brick drops which leads to production of harmful emissions because the temperature of the brick is lower than the activation temperature of the reaction known as “light-off temperature” (Guojiang and Song, 2005 and Ramanathan et al. 2004). Another challenge is the cold-start period. During this period, the catalytic converter is cold and cold-start emissions are heavily produced. The engine has to consume more fuel to increase the heat supply to the catalytic converter and allow for faster light-off to minimize the harmful emissions produced. This mechanism consumes more fuel and reduces the efficiency of the engine. For these reasons, regulations came in place to encourage the automotive industry to lower the amount of harmful emissions to maintain a healthy environment and sustain the energy resources.

With the massive demand for transportation in Canada, the automotive market is growing larger and production of greenhouse gasses has drastically increased. Transportation is the second largest source of GHG emissions in Canada after the oil and gas industry covering almost one quarter of the entire GHG
emission production spectrum as shown in Figure 1.4. The figure represents the production of carbon dioxide only because it is the most dominant GHG produced (EPA, 2010).

![Figure 1.4: GHG production in Canada from 1990 to 2014 (EPA, 2010)](image)

Out of this quarter, almost 80% of the production is linked to automobiles and heavy trucks as shown in Figure 1.5. The total GHG production in 2014 was approximately 130 megatonnes which is a substantial amount of emissions produced by a single source (EPA, 2010). This issue forced the Canadian along with many other governments to enforce more strict emission standards on the automotive industry (Farrauto and Heck 1999, Heck et al. 2001, Koltsakis 1997 and Shelef and McCabe 2000). To satisfy these regulations, new designs of emission control units (catalytic converters) must be achieved.

### 1.1. Catalytic Converter Performance

Cold start emissions and idling are the main sources of harmful emissions in automotive industry. Starting the vehicle after a cold period doesn’t allow immediate initiation of chemical reaction due to the delayed light-off. The sooner the light-off starts, the less emissions are released due to thermal performance improvement. Thermal performance is associated with the monolith ability to heat up to the light-off
temperature as fast as possible and retain the heat as long as possible. The hydraulic performance is associated with the pressure drop across the ceramic substrate and the flow distribution. The lower the pressure drop, the lower the load on the engine hence less fuel consumption. (Agrawal et al. 2012, Bella et al. 1991, Cho et al. 1998, Tsingolou and Koltsakis 2004 and Windmann et al. 2003). All these aspects are discussed further in chapter 2.

Cleanalytic™ is a new catalytic converter technology designed and patented by Vida Fresh Air Corp., shown in Figure 1.6. It enhances the flow distribution within the monolith and hence improves the thermo-fluid performance by dividing the substrate into two smaller chambers which allow for faster light-off. These chambers are thermally insulated with an insulation layer (Figure 1.6) that allows for a controlled heat diffusion from the inner to the outer chamber as shown in Figure 1.7. This behaviour allows the core of the monolith to heat up faster during the cold start period and improves the conversion efficiency.

![Figure 1.5: Automobile and GHG emissions in Canada from 1990 to 2014 (EPA, 2010)](image-url)
Figure 1.6: Cleanalytic™ catalytic converter (www.vidafreshair.com)

Figure 1.7: Direction of heat diffusion in catalytic converters
Improving the thermo-fluid performance of the catalytic converters is necessary to meet the more stringent emission regulations. Improving the performance of catalytic converters requires intensive experimental investigations to study the flow behaviour inside the catalytic converter. Understanding the fluid flow behaviour inside the catalytic converter will allow to highlight what is needed to be improved. This requires very accurate fluid flow and pollutant concentration measurement instruments and a safe environment for researchers to perform these tests. Those restrictions decrease the feasibility of such studies and a more feasible approach is needed.

With the help of computational fluid dynamics (CFD) tools, challenging problems can be simplified and solved effectively and accurately. Therefore, it is intended to use numerical simulations along with experimental validation to investigate and improve the thermal performance of catalytic converters by being able to optimize the converter design. This will substantially reduce the cost of implementing the new converter design. Consequently, this study investigates the performance of both typical and Cleanalytic\textsuperscript{TM} catalytic converters experimentally and numerically. The experimental measurements obtained include temperature, velocity and static pressure distribution across the converter which are also used to validate the numerical model. These specific measurements affect the performance of the catalytic converter in three ways; the monolith temperature is an indication on the light-off temperature which is a key parameter in quantifying the thermal performance of catalytic converters. The velocity distribution describes the space of the monolith that is being utilized by the exhaust. The larger the utilized space, the larger the amount catalyst that is utilized and hence the chemical reaction is enhanced. The pressure drop measurements quantifies the amount of back pressure on the engine. The higher the pressure, the higher the fuel consumption required to deliver the same amount of power. Furthermore, the performance of the new Cleanalytic\textsuperscript{TM} design has also been evaluated.

1.2. Thesis Objectives:

The aim of this study is to:

- Experimentally investigate the thermalhydraulic performance of a typical catalytic converter design by looking at temperature, velocity and static pressure distribution across the converter.
• Study the effect of using the Cleanalytic™ on the thermalhydraulic performance of the converter.
• Develop and validate computational fluid dynamics (CFD) techniques that more accurately predicts the fluid flow and thermal performance of the catalytic converter.
• Use the developed numerical methodology to predict and evaluate the performance of the Cleanalytic™ catalytic converter using the temperature, velocity and pressure distributions.

1.3. Thesis outline:

This thesis is organized in seven chapters as follows:

Chapter 1: Provides an introduction to catalytic converters.

Chapter 2: Discusses the background history of the technology and surveys the relevant literature.

Chapter 3: Includes a description of the experimental setup used in this study as well as the methodology.

Chapter 4: Describes the computational fluid dynamics model developed for this study.

Chapter 5: Presents the results obtained from experiments and simulations and provides a comprehensive discussion on the findings.

Chapter 6: Summarizes the findings accompanied and suggests future recommendations.

Chapter 7: Provides references used for this study.
Chapter 2 Literature Review

2.1. The Pellet Catalytic Converters

Engine exhaust gas treatment has been a major concern for decades. In the thirties, automobile manufacturers realized the need to treat the products of the combustion process that occurred within the internal combustion engines (Farrauto and Heck, 1999). The initial solution for this challenge was the utilization of pellet catalytic converters. These pellets were the major component of the catalytic converters in the 1970s. The pellets were spherical particles with diameter ranging from 2.5 mm to 5 mm and made of gamma-alumina. The pellets were enclosed in a steel shell to form the catalytic converter and loaded with noble metals and stabilizers for the exhaust treatment as shown in Figure 2.1. This catalytic converter technology had many disadvantages. Due to the shape of the pellets, a large pressure drop occurred across the converter which directly affected the performance of the engine. Moreover, the risk of losing the catalyst was higher due to particle wear (DieselNet, 1998). These disadvantages encouraged scientists and engineers to develop monolithic catalytic converter which are being used today.
2.2. The Monolith Substrate

Monolith substrates are the main component of the exhaust after treatment system found in the automobiles today. They provide a superior performance in comparison to the pellets support. They are characterized with small channels that vary in hydraulic diameter and wall thickness. Monolith substrates are specified with the cell density and the wall thickness. Due to their large surface area, they have an enhanced heat transfer which improves the chemical reaction and hence the conversion efficiency which indicates an improved thermal performance. The thermal performance can be coherentized by the time needed for the catalytic converter to reach the light-off temperature. The “light-off” temperature is quantified as the temperature at which the conversion of pollutants is more than 50% which is typically more than 350 °C (Jeong and Kim, 2000) for a typical catalytic converter.

Moreover, the monolith channels provide a more uniform flow distribution across the substrate which improves the chemical reaction and the durability. Therefore, improving the thermal-hydraulic performance of the monolith substrate enhances the light off characteristics of the catalytic converter and improves the efficiency of the converter (Holmgren et al, 1997 and Tsinoglou et al. 2004). When the thermal performance of the catalytic converter is enhanced, the temperature inside the monolith is increased and the light off temperature is obtained faster.
CFD simulations have been the most commonly used tool to evaluate the performance of the catalytic converter for the last three decades because they offer a great advantage in terms of time and cost efficiency. Researchers used CFD to predict the fluid behaviour, thermal characteristics and conversion efficiency of the monolith substrates. They suggested many techniques to mathematically model the flow field inside the brick starting from 1D unidirectional models to full and comprehensive 3D models (Chen et al. 2008, Kumar and Mazumder 2010, Ozhan et al. 2014 and Hayes et al. 2012).

### 2.3. Thermalhydraulic Performance of Catalytic Converters

Early work done on this topic involved steady state and transient analysis and these two types of flow conditions were investigated under different conditions. Many researchers investigated and simulated steady state flow under reacting flow conditions (Groppi and Tronconi 1997, Tsinoglou et al. 2004, Hayes et al. 2012 and Taylor 1999) and other researchers investigated the non-reacting steady state flow inside the catalytic converter (Holmgren et al. 1997, Lai et al. 1991 and 1992). The transient flow condition was also studied by some researchers to investigate the performance of the catalytic converter during the cold-start period (Braun et al. 2002, Chakravarthy et al. 2003, Hayes et al. 2012, Ramanathan et al. 2003 and Tsinoglou et al. 2004). Moreover, some researchers studied only the hydraulic behaviour of the flow within the monolithic substrate under steady state cold flow conditions (Holmgren et al. 1997, Benjamin et al. 2001 and Hayes et al. 2012).

Koltsakis 1997 and Shelef and McCabe 2000 reviewed the catalytic converter systems in automobile emission control. The study also covered the main principles and the performance of the catalytic converter. Moreover, they discussed the durability of the catalytic converter as well as the effect of the catalytic converter performance on the thermal management of the engine. In addition, a comprehensive review on the concurrent mathematical models developed to monitor and optimize the catalytic converter as well as studying the catalytic interactions and the physical characteristics. Chen et al. 2008 presented an overview of the state of the art of the mathematical models used to model the monolith and the catalytic reactions. They discussed various aspect of the modeling process including steady state and transient modeling, gas uniformity and flow distribution, chemical kinetics and conversion characteristics and heat and mass transfer within the monolith. Moreover, they provided a guideline to help researchers choose the proper
model in their studies including 1-D, 2-D and 3-D models. Furthermore, they also demonstrated different scales used in modeling the flow inside the monolith channels including washcoat models, single channel models and multi-channel full reactor models.

2.3.1. Hydraulic Performance of Catalytic Converters

Many researchers investigated the effect of the hydraulic performance of the catalytic converter on the overall performance of the converter. Improving the hydraulic performance means improving flow distribution of the flow within the monolith substrate and minimizing the generated back pressure. More uniform flow distribution tends to enhance the conversion efficiency and the durability of the catalytic converter (Bella et al. 1991, Jeong and Kim 1998, 2000, Karvounis and Assanis 1993 and Martin et al. 1998). When the flow is not uniformly distributed, the catalyst within the ceramic substrate becomes partially utilized and that leads to a reduction in the conversion efficiency and the life time of the monolith. Moreover, lower back pressure improves the engine performance resulting in more fuel-efficient vehicles. This leads to less GHG emissions (Ekstrom and Andersson 2002, Amirmordin et al. 2011 and Hayes et al. 2012).

2.3.1.1. The effect of flow distribution on hydraulic performance

Flow distribution inside the monolith substrate is affected by three main factors. Namely, the exhaust manifold design, monolith properties and the inlet flow conditions. The following design parameters (Figure 2.2) were investigated by many researchers throughout the literature as they directly affect the flow distribution and hence performance of the catalytic converter:

1. Inlet pipe length
2. Inlet diffuser geometry
3. Bending angle of the inlet pipe
4. Brick geometry and properties
Figure 2.2: Exhaust manifold design parameters.


Cho et al. 1998 studied the flow distribution for steady and transient flow conditions. They investigated the flow distribution at the exit of the first monolith of a two-brick system under the assumption that the flow through each channel does not interfere with the flow in adjacent channels. Steady tests yield more flow maldistribution than the transient tests and the configuration of the exhaust manifold has a significant influence on the flow distribution within the monolith.

Lai et al. 1991 and 1992 studied the effect of the exhaust manifold geometry on the flow distribution as bent pipes tend to distort the flow and increase the flow maldistribution. They utilized 3D simulations with incorporation of the brick resistance to the simulation to obtain accurate predictions. They concluded that the flow becomes more uniformly distributed when the inlet pipe is shorter in length and the bending angle is smaller. Moreover, they investigated the effect of brick properties on the flow distribution concluding that the higher the brick resistance the more uniform the flow distribution is observed.
Similar conclusions have been reached by Amirnordin et al. 2011, Karvounis and Assanis 1993, Ramanathan et al. 2003, Weltens et al. 1993, Chen et al. 2004 and Lun et al. 2010. They also added that with multi-brick catalytic converters, the second brick tends to show more uniform flow distribution than the first one due to the gap between the two bricks which allows the flow to redistribute more uniformly. They specifically suggested using smaller channel hydraulic diameter and shorter ceramic substrates to overcome the pressure drop developed by higher brick resistance.

Jeong and Kim 1998 and Martin et al. 1998 investigated the effect of inlet pipe diameter on the flow distribution numerically under steady state and transient conditions and concluded that with smaller pipe diameters, the flow becomes distorted and less uniformly distributed. The investigation was extended to study the effect of the inlet Y junction on the flow distribution and they found that the flow is non-uniformly distributed around the Y junction due to streamline separation which lead to flow non-uniformity inside the monolith. Moreover, the flow distribution in a dual flow catalytic converter is enhanced for longer mixing pipes and larger junction volume especially under unsteady conditions as they allow flow adjustment. In addition, they investigated the effect of the flow uniformity on the light-off behaviour of the catalytic converter by including chemical and thermal models. They found that the cross-section area ratio of the inlet pipe to the monolith has a significant influence on the exhaust distribution in the monolith for high flow unsteady conditions since the conversion efficiency is degraded when the cross-section area ratio is decreased due to high temperature and velocity gradients which lead to high flow concentrations in the core of the monolith.

Bella et al. 1991 utilized 3D simulations to model the flow inside the exhaust manifold and concluded that with the existence of the inlet diffuser, the flow became significantly more uniformly distributed. Complimentary conclusion reached by Chen and Schirmer 2003; Hayes et al. 2012 who implemented 0D steady state catalyst model, 1D transient plug model and 2D model to further investigate the design of the inlet diffuser. They stated that with increasing the inlet diffuser angle, the flow tends to be non-uniformly distributed and that effect is more severe when increasing the volume flow rate. Figure 2.3 is a sample of the work of Hayes et al. 2012 in investigating the effect of the diffuser angle on the flow uniformity index which is an indication on the variation of the local velocity from the average velocity at the upstream face of the monolith.
Figure 2.3: Effect of diffuser angle on the flow uniformity index (Hayes et al. 2012)

As shown in Figure 2.3, a flow index of 0.25 represents ideally uniform flow and GHSV is the gas hourly spaced velocity. It can be clearly seen from the figure that the flow index is greatly affected by the diffuser angle at high angles and the gas flow rate. Similar unsteady and multi-dimensional study was done by Shuai and Wang, 2004 and concluded that the flow was more uniform for a 40˚ inlet diffuser more than a 60˚ one.

Weltens et al., 1993 investigated the flow distribution within close-coupled catalytic converters using CFD. They used 3D modeling and optimized different design parameters. They investigated design parameters are the geometry of the inlet pipe and cone, the geometry as well as the placement of the monolith, the shape of the exit cone. They added that the condition at the inlet of the first monolith of a multi-block system is dominant in which the second monolith tends to have a uniform flow based on the inlet condition with optimal gap width between both monoliths to be less than 10 mm. Moreover, they suggested the first monolith to be longer to increase the flow resistance and allow the flow to uniformly distribute at the upstream face of the monolith.

Karvounis & Assanis, 1993 developed a finite element code to solve the flow field through the inlet diffuser, the ceramic brick and the nozzle sections of the catalytic converter for different flow rates and channels hydraulic diameters and investigated the effect of non-uniform inlet flow distribution on the conversion efficiency of the catalytic converter. They predicted the reactant concentration across the honeycomb’s
outlet based on the velocity distribution at the inlet. However, the lower the hydraulic diameter of the channels, the higher the conversion efficiency and the pressure drop which can be decreased by shortening the catalytic converter monolith.

Holmgren et al. 1997 investigated the effect of shaping the inlet face of the monolith on the flow distribution utilizing the flat, parabolic and conical shapes. They implemented a 3D, isothermal, incompressible and axisymmetric model to predict the flow field in the exhaust pipes and a 1D laminar flow model was used to model the monolith and the study concluded that using parabolic and conical monolith inlet face increases the efficiency and the utilization of the catalyst hence the conversion efficiency and reduces the pressure drop due to the shorter channels at the periphery. Figure 2.4 shows the effect of shaping the inlet cone on the velocity profile 3 cm downstream the monolith.

Figure 2.4: The effect of the substrate front face shape on the velocity distribution (Holmgren et al. 1997)
At mass flow rate of $3.2 \times 10^{-2}$ kg/s, it can be seen in Figure 2.4 that using shaped inlet face of monolith enhances the flow distribution due to less flow resistance at the outer channels which helps increasing the flow through these channels. The effect of elevated temperature on the flow distribution is also shown in Figure 2.5 which represents Reynolds number of 60,000, 44,000 and 28,000 for 750°C, 650°C and 550°C cases, respectively. The effect of the shape of the inlet face is more pronounced with elevated temperatures as the temperature gradients are higher which directly affect the flow velocity. The parabolic inlet face offered a slightly more uniform flow distribution than the conical shape especially at higher temperatures.

Chen and Schirmer 2003 employed a semi-empirical 0-D steady state catalyst model and a 1-D transient plug flow model to optimize the design of the catalytic converter for internal combustion engines. They utilized CFD simulations and modeled the monolith substrate as a porous medium with empirically calculated viscous and inertial resistances. They solved the flow field over a perforated plate as an inlet condition to the monolith substrate. They concluded that the assumption of the perforated plate was reasonable as a surface of pressure discontinuity. Moreover, they observed higher flow uniformity with installation of a perforated plate at the front face of the monolith substrate.

Guojian & Song, 2005 utilized a 2D symmetrical transient model to study the effect of the flow and temperature distribution on the performance of the catalytic converter and introduced a honeycomb...
spherical arc shown in Figure 2.6 at the exit of the inlet pipe to redistribute the flow across the inlet face of the monolith and investigated the flow distribution. The arc improved the flow distribution with a small increase in pressure drop which can be reduced by manipulating the opening area of the arc and cross section area of the pipe.

![Diagram of Honeycomb Spherical Arc](image)

*Figure 2.6: Honeycomb spherical arc (Guojiang and Song, 2005)*


Bressler et al. 1996 investigated the unsteady flow within close coupled converter (CCC). They performed experimental and computational investigations to analyse the efficiency when uniformly distributing the flow within the entire volume of the converter. The study introduced the exhaust pulsation in their analysis to replicate the real conditions and utilized different engine load conditions in their study. They concluded that when running the engine at lower loads, the monolith bricks are utilized more efficiently and the flow uniformity is higher. Arias-Garcia et al. 2001 investigated the flow distribution in the CCC for steady and pulsating conditions experimentally and numerically. They subjected the catalytic converter to a four-port rig that can supply air flow separately. They observed flow maldistribution when each port was running alone. Moreover, they noticed that with increasing Reynolds number, the flow maldistribution increases for steady air flow. On the other hand, pulsating the flow tends to decrease the flow maldistribution at the back
of the monolith brick. Their CFD simulations underestimated the velocities by 50% because they were not sensitive to the entrance effects.

Badami et al. 2003 investigated the unsteady flow effect on the catalytic converter by developing a CFD model and validating it against experimental data using hotwire anemometry for steady state conditions. They concluded that under steady state conditions, Reynolds number can affect dramatically the flow uniformity index and developed a new formulation of flow uniformity index under transient conditions and a new correlation between the transient uniformity index and the steady state index with a good agreement with experimental data.

Chen et al. 2004 utilized a 3D CFD flow modeling and a heterogenous reaction model of the catalytic converter. They calculated the pressure and the velocity field with incorporating the flow resistance within the monolith substrate. They concluded that the flow field is influenced by the monolith substrate resistance for a specific geometry and Reynolds number. Moreover, the flow uniformity at the front face increased with increasing cell density of the monolith and decreased when increasing the flow Reynolds number.

Jeong and Kim 1997 and 1998, Lai et.al 1992, Weltens et al. 1993 and Karvounis and Assanis 1993 utilized their developed CFD models discussed earlier to investigate the effect of the inlet Reynolds number on the flow distribution and they reported similar conclusions that the flow uniformity decreases when increasing Reynolds number and the inlet velocity. However, when testing the the effect of pulsating flow on the flow distribution they found that flow pulsations tend to enhance the flow uniformity.

Liu et al. 2007 and Liu et al. 2001 performed an experimental and a numerical study on the reverse flow catalytic converter for a natural gas/diesel dual engine. The simulation involved a 1-dimensional single channel model to monolith substrate. They concluded that the conversion efficiency of CO and HC was improved for the reverse flow catalytic converter for low inlet temperature and light engine load only when the catalytic converter initial temperature is high enough given that the converter initial temperatures was varied from 694 K to 919 K.
2.3.1.2. The effect of the pressure drop on the hydraulic performance

The effect of the pressure drop on the hydraulic performance of the catalytic converter has been investigated by many researchers (Bressler et al. 1996, Benjamin et al. 2001, Ekstrom and Andersson 2002, Agrawal et al. 2012 and Hayes et al. 2012). They investigated the effect of the inlet flow conditions, substrate properties and the catalytic converter geometry on the pressure drop utilizing various modelling strategies. Below is a summary of their findings.

In Bressler et al. 1996 study discussed earlier, the pressure drop was significantly decreased when pulsating the exhaust flow at engine full loads which resulted from a more uniform flow distribution. Moreover, Benjamin et al. 2001 simulated the flow distribution within the catalytic converter. They considered the entrance effects on the flow to accurately calculate the pressure drops. They concluded that treating the flow within a single channel as one-dimensional laminar flow under predicts the effect of flow maldistribution. Moreover, incorporation of pressure-drop improved the peak velocity predictions at the middle of the monolith of the catalytic converter.

Ekstrom and Andersson 2002 experimentally investigated the pressure drop across the monolith brick of the catalytic converter. They investigated different types of bricks with different cell density, coating and wall thickness. They did not include combustion in their experimental work and used cold and hot air flow instead. They developed an empirical model that could predict the pressure drop with good agreement with experimental data and previous models and can be used for 1-D and 3-D CFD simulations. They found that the main sources of pressure drop are viscous and inertial effects.

Amirnordin et al., 2011 adopted a sub-scale model to predict the pressure drop of different sizes of the square and hexagonal cell shapes of the catalytic converter. They used the model to investigate the effect of the channel design on the performance of the catalytic converter. They tested various combination of wall thickness and cell density in their study and the developed model showed better results than the single channel model utilized commonly in the literature. They concluded that the hexagonal cells are dynamically more efficient as they offer lower pressure drop compared to the square cells. By contrast, the square
channels are chemically more efficient as they have higher surface areas. The authors suggested that the hexagonal cells are a better choice as they dominate the dynamic performance in comparison to the insignificant surface area reduction compared to square cells. Figure 2.7 represents a comparison between the hexagonal and square cells in terms of pressure drop and specific surface area. The cell density for both designs is 900 cells per square inches with a wall thickness of $2.5 \times 10^{-3}$ inch ($6.4 \times 10^{-2}$ mm). The monolith length is 152.4 mm and the average flow velocity is 20 m/s.

A 2D steady and transient model was developed by Hayes et al., 2012 found that the flow distribution for reacting and non-reacting condition is a function of the catalytic converter properties like cell density, diffuser angle and aspect ratio of the monolith. In addition, the mass flow rate highly influenced the distribution. Moreover, faster light-off behaviour was obtained with higher monolith cell densities. Dual monolith configurations with high cell density cores and low cell density at the periphery showed the worst flow uniformity. The effect of the cell density and the flow velocity on the pressure drop is shown in the Figure 2.8. It can be seen from the figure that increasing the flow velocity increases pressure drop for the tested cell densities with a diffuser angle of 40°. Moreover, increasing the cell density increases the pressure drop and it has a more significant effect on the pressure drop when applying the washcoat.

![Figure 2.7: Comparison between the hexagonal and the square cells of monolith substrates (Amirnordin et al., 2011)](image)
Figure 2.8: The effect of the inlet flow velocity on the pressure drop for different monolith types (Hayes et al., 2012)

Agrawal et al., 2012 developed a planar two-dimensional model to study the interactions between flow, reactions and thermal effects of the catalytic converter. They utilized a full-scale model consisting of 85 channels and a reduced-scale model consisting of 21 channels. They investigate the effect of the friction coefficient for the channels on the flow distribution. They investigated the effect of the flow distribution on the conversion of carbon monoxide. They concluded that the flow tends to be non-uniformly distributed with the flow expansion within the inlet diffuser. Moreover, the higher the pressure drop across the channels the more uniform flow distribution is obtained. The implementation of the reduced-scale model yielded matching results to the full-scale model. Furthermore, the conversion efficiency of the catalytic converter decreased as the flow mal-destination was increased and the reactions taking place within the monolith did not have any effect on the flow distribution.

2.3.2. Thermal behaviour of ceramic substrate

The thermal behaviour of the catalytic converter has been investigated by many researchers (Chakravarthy et al. 2003, Groppi and Tronconi 1997, Shamim et al. 2002, Hayes et al. 2012, Jeong and Kim 2000 and Chung et al. 1999). The conversion efficiency and the thermal response of the monolith under different load conditions are crucial to understand the thermal characteristics of the catalytic converter. Understanding
the interactions between the chemical and physical processes within the monolith channels is a key factor in modelling the monolith reactors (Chen et al. 2008). Ferguson and Finlayson 1974, Heck et al. 1976 and Young and Finlayson 1974 developed the earliest mathematical models to study the physical and chemical process within the catalytic converter. Their model incorporated heat and mass transfer effects inside the monolith and the laminar flow inside the monolith channels. In this section, the summary of the key studies established in the literature will be presented.

Kočí et al. 2004 developed two models to simulate the flow and the chemical kinetics within the three-way catalyst monolith converter. The models describe the dynamic behaviour of flow in the short monolith and the kinetics of oxidation and reduction reactions and included the effect of diffusion in the washcoat on the light-off and the conversion of the outlet. Also, Pontikakis et al. 2004 developed a mathematical model to predict the thermal performance of the catalytic converter. Their model predicted the solid phase temperature through 1-D transient conditions and a quasi-steady 1-D model to predict the gas temperature. They utilized a simplified redox reactions scheme in their model along with an oxygen storage sub model.

Groppi & Tronconi, 1997 investigated the heat and mass transfer for a monolith with equilateral triangular channels. They implemented 3-D modeling to approach the analysis in which they assumed a fully developed laminar flow and equal thermal and mass diffusivity. Their analysis concluded lower heat and mass transfer for the triangular channels due to the acute corners of the triangles compared to square and circular channels which resulted in reaching operating temperatures and lower gas heating rates for the coefficients of heat and mass transfer.

Shamim et al. 2002 developed a numerical simulation to predict the performance of the three-way catalytic converter. The model incorporates heat conservation and chemical reaction sub model with oxygen storage mechanism and it showed that the conversion efficiency was improved when operating under rich oxygen content.

Bella et al. 1991 investigated the effect of flow uniformity on the conversion efficiency in their 3D model discussed earlier. When the flow was non-uniform, it became concentrated in the central region of the honeycomb which resulted in non-uniformity of the chemical reaction in the catalytic converter that caused noble metal depletion and lower conversion efficiencies.
Martin et al., 1998 studied the relation between flow maldistribution and ageing, light-off and conversion for steady state conditions. They conducted emission test for engine cycles and concluded that light-off temperature increases as the catalytic converter ages and at high exhaust gas velocities with insignificant effect on the conversion efficiency once light-off temperature is reached. The central region of the catalytic converter aged faster due to flow maldistribution that led to higher velocities in that region. Moreover, lower catalyst efficiencies for all pollutants were obtained by small inlet pipe diameters that caused flow non-uniformity during the early stage of the ECE emission test cycle and at the final stages of the EUDC especially for NOx. These lower conversion efficiencies can be decreased further with ageing.

Chung et al. 1999 predicted the temperature, thermal response and light-off behaviour of the catalytic converter using CFD. They incorporated heat transfer and chemical formulations into the numerical simulations. They obtained temperature distribution for the catalytic converter components and concluded the conversion properties of the catalytic converter can be adjusted by changing the precious metal concentrations.

Jeong and Kim 2000 numerically simulated the cold start of a vehicle when the catalytic converter is placed closer to the engine exhaust manifold. They considered a 3D, transient compressible reacting flow in the warm-up to investigate the effect of the warm-up period on the thermal behaviour of the main catalyst and the emissions. They also examined the effect of the flow distribution as well as the catalyst loading on the temperature distribution and the emission performance. They concluded that flow maldistribution and large pressure drops occurred more significantly in the warm-up period of the catalyst systems. Moreover, during the warm-up stage, the velocity and temperature distributions have similar patterns due to the dominance of heat transfer by convection of the incoming exhaust gas. The catalyst did not contribute in the conversion of the exhaust gas during the warm-up process due to lower temperatures at the middle regions. Furthermore, when the space velocity was very large, concentrating the precious metal in the entrance will have no effect on the conversion efficiency which suggested taking the flow distribution into consideration when loading the precious metal within the warm-up catalytic converter to ensure higher conversion efficiencies.
They also performed another numerical study in the same year (Jeong and Kim 2000) to investigate the light-off and thermo-fluid performance of the catalytic converter. The developed model incorporated the flow maldistribution to obtain more reliable representation of the actual conditions. They developed a 2-dimensional model that predicts the catalyst performance that is coupled with turbulent reacting flow and concluded that with increased cell density and geometric surface area and reduced cell thickness, the light-off performance and the conversion efficiency can be improved.

Flow non-uniformity during cold start transient period of catalytic converter was investigated by Chakravarthy et al., 2003 utilizing multi-dimensional channel model. It was recorded that the ignition behaviour can be dramatically affected by flow recirculation at the inlet of the substrate which lead to high flow maldistribution especially at lower exhaust temperatures. The study concluded that flow non-uniformity effects were more significant with increasing flow temperature. In addition, the pressure drop distribution remained constant and was dependant on the recirculation pattern at the front face of the monolith.

Braun et al., 2002 utilized a 3D transient flow model with a 2D multi step heterogeneous chemical reaction model to predict the emissions of the system. They ran the simulations with variable inlet conditions which lead to various temperature distributions and pollutants profiles. Similarly, Windmann et al., 2003 studied the effect of the flow distribution at the upstream face of the monolith on the thermal behaviour of the catalytic converter. They concluded that the flow maldistribution has a negative effect on the conversion efficiency of the catalytic converter in the first few minutes of the test cycle. They noticed that the overall conversion efficiency was lower even if the first part of the monolith was lit off earlier and faster only for the limited flow conditions tested.

An analytical 1D two-phase model was obtained by Ramanathan et al. 2003 and 2004 to describe the light-off characteristics of washcoated straight channel catalytic monolith using CFD tools under transient flow condition. The model predicted the transient time and the total emissions released during the cold-start stage for a non-uniform catalyst loading. They found that a proper redistribution of the metal catalyst enhances the front-end ignition hence further reduction of the cumulative cold start emissions. They also investigated
the effect of various design parameters and catalyst loading condition on the cumulative emission and the transient time.

The effect of the flow uniformity on the conversion efficiency of pollutants was investigated using 2-D symmetrical transient model discussed earlier and developed by Guojiang & Song, 2005. It was found that increasing the flow uniformity increases the conversion efficiency for the pollutants CO, unburnt HCs and NOx as shown in Figure 2.9.

Figure 2.9: Conversion efficiency for varies uniformity indices and pollutant species (Guojiang and Song 2005)
where $\gamma$ represents the flow uniformity index and $S_v$ is the space velocity and is equal to 69,444 $\text{hr}^{-1}$. The space velocity is the exhaust flow rate entering the catalytic converter divided by the volume of the catalytic converter. Further investigations on the conversion efficiency was carried out by Santos & Costa, 2008 at which the influence of the geometric and physical properties of the monolith substrate on the conversion efficiency of a three-way catalytic converter was investigated. They utilized the ceramic and metallic substrates in their study under steady state and variable engine operation conditions and concluded that the ceramic substrate resulted in higher conversion for lower space velocities due to lower thermal conductivity that enhanced local ignition. On the other hand, the metallic substrate had a higher conversion rate at higher space velocities due to lower transverse Peclet number and higher geometric surface area.

Lun et al. 2010 utilized CFD simulation to study the light-off performance of the catalytic converter. The model incorporated 3D flow calculations coupled with 1D heat and mass transfer equation in the monolith region and was validated against experimental data with a good agreement. A significant impact on the light-off performance of the catalytic converter was found as the monolith wall thickness varies as shown in Figure 2.10.

![Figure 2.10: Monolith solid temperature as a function of wall thickness (Lun et al. 2010)](image-url)
Figure 2.10 represents the effect of the wall thickness on the temperature of the solid where w is the wall thickness. It can be seen in the figure that increasing the wall thickness decreases the solid temperature due to the increase in the thermal mass hence worse light-off performance. The effect of the monolith wall thickness on the conversion efficiency for carbon monoxide is seen in Figure 2.11. Increasing the wall thickness is inversely proportional to the conversion efficiency. The figure represents the best monolith thickness of 0.1 mm which yields light-off (50% conversion efficiency) significantly earlier than the rest of the tested wall thicknesses.

From the literature, it is very challenging to quantify the optimum operating conditions and the design parameters of catalytic converters. This can be affected by many factors such as fuel prices, manufacturing costs, and emissions standards. In general, a catalytic converter design that yields faster temperature response, lower pressure drop and highly utilized monolith space would be an optimum solution.
2.4. Scope of Current Study

As discussed above, many researchers in the literature utilized CFD extensively in their studies and some of them validated their models against experimental data. Most researchers used pressure drop and velocity measurements to validate their simulations and a little validation was done for the thermal part. The validation done on the thermal part was either temperature measurements inside the monolith at very limited locations due to the complexity of the geometry or pollutants concentration measurements. To the best of the author’s knowledge, no studies addressed the flow temperature measurements downstream the monolith substrate in the literature. This study utilizes local temperature, velocity and turbulence intensity profile measurements downstream the monolith to validate the CFD. Moreover, pressure drop measurements across the monolith is also used for the validation. Incorporation of temperature measurements to validate CFD models provides confidence when addressing the thermal performance numerically due to the significant influence of the temperature on the flow behaviour. This study focuses on studying the thermal-hydraulic performance for the conventional catalytic converter and the new technology (Cleanalytic™) under steady state and non-reacting flow for different monolith cell densities utilizing ANSYS Fluent software.
Chapter 3 Experimental Setup and Methodology

To investigate the thermalhydraulic performance of catalytic converters, an experimental setup was built to measure local temperature and velocity profiles downstream of the monolith substrate as well as static pressure along the longitudinal axis of the catalytic converter. Measurements were taken for monolith cell densities of 400 CPSI with wall thickness of $6.5 \times 10^{-3}$ inch ($1.7 \times 10^{-1}$ mm) and 900 CPSI with wall thickness of $2.5 \times 10^{-3}$ inch ($6.4 \times 10^{-2}$ mm). Both conventional as well as Cleanalytic™ catalytic converters were studied under identical operating conditions at a steady mass flow rate of $5.18 \times 10^{-2}$ kg/s and a free stream temperature of 177 °C.
3.1. Scaling of the Actual Catalytic Converter

The operation conditions of the tested catalytic converter were selected to achieve dynamic and thermal similarity to the operation conditions of the actual catalytic converter. The dynamic similarity is achieved by finding the proper pipe diameters and inlet mass flow rate that yield the same Reynolds number as the actual operation Reynolds number. The thermal similarity is achieved by finding the inlet temperature that yields the same Nusselt number inside the monolith as the actual one.

A typical catalytic converter has an inlet pipe diameter of 3 inches (76.2 mm) and substrate diameter of 4.5 inches (114.3 mm). The typical operation conditions are mass flow rate of 0.1 kg/s and free stream temperature of 630 °C. The average flow velocity inside the inlet pipe 40 m/s and Reynolds number is 43,000 (see similar calculations in Appendix C). To calculate Nusselt number inside the monolith, both Reynolds number and Prandtl number were calculated. Reynolds number is calculated as shown in Appendix C and Prandtl number is calculated as follows:

$$ Pr = \frac{C_p \cdot \mu}{k} = 0.696 $$  \hspace{1cm} (3.1)

where $C_p$, $\mu$ and $k$ are the specific heat, dynamic viscosity and thermal conductivity. The Nusselt number inside the substrate can be calculated from Dittus-Boelter equation as follows:

$$ Nu = 0.023 \cdot \frac{Re_{ch}^{4/5} \cdot Pr^{0.4}}{Pr} = 3.7 $$  \hspace{1cm} (3.2)

where $Re_{CH}$ and $Pr$ are the channel Reynolds number and Prandtl number, respectively. The same procedure is followed to obtain the Reynolds number and Nusselt number for the scaled experiment with chosen inlet pipe diameter of 2 inches (50.8 mm) and substrate diameter of 3 inches (76.2 mm). To achieve dynamic and thermal similarities for the chosen dimensions and the calculated dimension less parameters, the inlet mass flow rate and free stream temperature are found to be $5.18 \times 10^{-2}$ kg/s and 177 °C, respectively.
3.2. Experimental Test Rig

The test rig was designed to supply air with a varying flow rate ranging from 0 to 4500 L/min supplied by a 124-kPa air blower derived by a variable speed motor that is controlled by a manual control panel. The air passes through a vertical catalytic converter (test section). The test rig was divided into three sections; the inlet pipe, the catalytic converter and the exit pipe. Air was heated by a Leister LHS 61L SYSTEM 11 kW electric heater. The heater supplies a wide range of temperatures from 50 °C to 650 °C (see Appendix B). The temperature can be controlled by the heater within ± 5 °C step. The inlet pipe, catalytic converter and outlet pipe were equipped with various instruments to monitor temperature, velocity and pressure drop which will be discussed in section 3.3.

The test setup is a scaled down automotive catalytic converter system. The Reynolds number based on inlet pipe diameter is $43 \times 10^3$ at an inlet flow temperature of 177 °C and inlet mass flow rate of $5.18 \times 10^{-2}$ kg/s. The flow is non-reacting with steady hot air supply. The study is more focused on the physical behaviour of the flow within the catalytic converter using a controlled experiment with the minimum number of uncontrollable factors that coexist with chemical reactions. The schematic diagram and actual pictures of the experimental setup are shown in Figure 3.1 and Figure 3.2, respectively. There are two temperature and one pressure measurement locations along the length of the inlet pipe. Two traversing mechanisms were mounted downstream of the catalytic converter section (test section) to measure temperature and velocity profiles 5 mm downstream the monolith substrate as shown in Figure 3.3 and Figure 3.4. Velocity and temperature measurements were taken using a hot-wire anemometer and a thermocouple, respectively. The outlet section was equipped with a single pressure measurement location.

The inlet section consists of an inlet pipe with an inside diameter of 2 inches (50.8 mm) and length of about 530 mm the pipe was connected to the catalytic converter section through an inlet diffuser that is 25 mm long and has an angle of 45° as shown in Figure 3.5. The catalytic converter section that contains the monolith substrate is 76 mm long with an inside diameter of 76 mm as shown in Figure 3.6. The outlet section shown in Figure 3.7 consists of a 25-mm long extension to the monolith container that has a 76 mm inside diameter and equipped with threaded holes to mount the traversing mechanisms. The section is then connected to an exit converging cone 30 mm long with an angle of 30°. The exit cone is connected to the
exit pipe. The pipe is 180 mm long with an inside diameter of 2 inch (50.8 mm). The material used to build the test rig is stainless steel grade 441 with a wall thickness of 2 mm.

Figure 3.1: Experimental setup schematic
Figure 3.2: Actual experimental setup
Figure 3.3: Test section showing the temperature and velocity traversing mechanisms

Figure 3.4: Temperature and velocity measurements locations (a) actual picture with measurements location 5 mm downstream the monolith. (b) schematic of the container showing traversing directions of instruments.
Figure 3.5: Inlet pipe dimensions

Figure 3.6: Monolith container dimensions
The conventional catalytic converter consists of the monolith substrate and a thermally insulating padding material wrapped around the monolith with thickness varying from 2 - 4 mm. The monolith substrate had a diameter of 73 mm and after being wrapped with the padding material was pressed inside the metallic can to ensure a tight fit as shown in Figure 3.4(a) above.

The Cleanalytic™ catalytic converters modify a typical catalytic converter substrate by adding an insulation layer at a prescribed diameter. Cleanalytic™ technology divides the monolith into two chambers via thermal barrier. This insulation layer redistributes the flow passing through the monolith between the inner and outer regions and enhances flow distribution. This results in improved thermal performance and higher temperatures inside the substrate. The thickness of the circular insulation pattern is typically 2 cells wide and varies from 1.5 mm to 2.5 mm. Patterns tested in this thesis had inside diameters of the insulation varying from +10% to -10% of the inlet pipe diameter (46 mm - 56 mm) as shown in Figure 3.8.
Figure 3.8: Monolith Substrate with the insulation layer (a) and (b) schematics of the ceramic substrate with and without installation layer, (c) dimensions of the insulation layer and (d) actual picture of Cleanalytic™ technology
3.4. Mass Flow Rate and Blower Frequency

The air flow is supplied by a variable speed blower. The blower is controlled by an electric motor with a variable speed frequency drive. A relationship between the blower frequency and the air mass flow is obtained to monitor the experiment and maintain a steady state operation. Figure 3.9 shows the linear relation between the blower frequency and the air mass flow rate. The blower frequency that provide the required mass flow rate is 10.2 Hz.

3.5. Instrumentation

3.5.1. Velocity Measurements and Hot Wire Anemometry

Constant temperature anemometry (CTA) was used for velocity measurements 5 mm downstream the monolith substrate. A Dantec Dynamics Inc. hot wire probe model with 2 % accuracy was used. The hot wire probe was connected to a single channel MiniCTA 54T42 provided by Dantec Dynamics Inc. with frequency bandwidth of 10 kHz at 50 m/s in air. The hot wire probe was 10 µm in diameter and 2.2 mm in length. It had maximum measurement flow velocity limit of 350 m/s and temperature limit of 800 ºC.

The hot-wire probe was calibrated against a pitot tube as shown in Figure 3.10 for a range of flow velocities at prescribed flow temperatures. Flow temperature was held constant at a prescribed value and the flow velocity was varied to obtain the calibration data at that temperature. The process was then repeated for different temperatures.

The pitot tube measures the local dynamic head which is the difference between the total and the static pressure and is read through a digital manometer. The velocity was then calculated from Bernoulli’s equation as shown in Equation (3.3).

\[ u = \sqrt{\frac{2 \times (p_t - p_s)}{\rho}} \] (3.3)
Figure 3.9: Blower frequency vs air mass flow rate based on inlet pipe.

Figure 3.10: Hot-wire is placed as close as possible to the pitot tube for calibration
where $\rho$ is the density of air at the flow temperature, $p_t$ and $p_s$ are total and static pressure respectively. Since the interest of this measurement was to scan the velocity profile downstream the catalytic converter ceramic substrate, two calibration curves were obtained to cover the variation of velocities due to the variation of temperatures. The calibration curve fitting must be of the 4th order as suggested by the manufacturer for best measurements accuracy. The calibration was performed at a steady flow temperature of 165 °C and 145 °C. Figure 3.11 shows the calibration curves and equation used for measuring the velocity throughout the experiments.

For flow temperatures within ± 10 °C from the calibration temperature, a voltage correction formula suggested by the manufacturer was used to compensate for the temperature difference as shown in Equation (3.4).

$$V_{corrected} = V_{HW} \times \left( \frac{T_{wire} - T_r}{T_{wire} - T_c} \right)^{0.3}$$

(3.4)

where $V_{HW}$ is the voltage output of the hot-wire, $T$, $T_{wire}$ and $T_r$ are the local, the wire and the reference temperatures, respectively. The wire temperature was held constant at 520 °C.

![Figure 3.11: Hot-wire calibration curve with 4th degree fit polynomials](image)

Figure 3.11: Hot-wire calibration curve with 4th degree fit polynomials
The hot wire probe is mounted on a traverse mechanism with a dial gauge. The traverse was moved in steps of 3 mm to obtain measurement points that cover the cross section of the brick. Measurements are collected using a DAQ system. The signal was captured with a sampling frequency of 3000 samples/second for 40 seconds.

### 3.5.2. Temperature Measurements and Thermocouples

T-type thermocouples supplied by Omega Inc. with diameter of 3/16 inch (4.8 mm) and length of 6 inches (152 mm) were used to measure flow temperature in the inlet pipe and temperature profile downstream the monolith with ± 0.5 °C accuracy as specified by the manufacturer. The voltage output of the thermocouples was calibrated using the reference temperature of boiling water and ice. A controlled temperature heater was used to obtain additional calibration temperatures. A 4-point calibration curve was obtained for each thermocouple and were identical. The calibration curves for each thermocouple were identical for the three thermocouples as shown in Figure 3.12. The reference temperature for calibration was measured using a thermometer with accuracy of ± 0.1 °C and the voltage was measured with multimeter that has an accuracy of ± 0.0001 volt. Two thermocouples were located at 76 mm and 279 mm from the inlet to measure the flow temperature in the inlet pipe. A third thermocouple was mounted on a traverse mechanism with a dial gauge as shown in Figure 3.3 and was used for temperature profile measurements downstream of the substrate. Temperature measurements were taken across the rear face of the brick in steps of 3 mm.

![Figure 3.12: Thermocouple calibration curve with linear regression fit](image-url)
The effect of convection and radiation from the thermocouple probe was examined to investigate the effect on measurement accuracy. To investigate the effect of convection, the stagnation temperature was calculated. At the stagnation point, the stagnation enthalpy is equal to the summation of the static enthalpy and the dynamic enthalpy as show in Equation (3.5)

\[ h_0 = h_s + \frac{V^2}{2} \]  

(3.5)

where \( h_0 \) is the stagnation enthalpy, \( h_s \) is the static enthalpy and \( V \) is the average velocity of the flow. Assuming constant specific heat \( (C_p) \), \( h_0 = T_0 \times C_p \) and \( h_s = T \times C_p \). Where \( T_0 \) and \( T \) are the stagnation and static temperature, respectively. Dividing Equation (3.5) by \( C_p \), Equation (3.6) is obtained.

\[ T_0 = T + \frac{V^2}{2 \times C_p} \]  

(3.6)

The second term on the right-hand side of Equation (3.6) describes the difference between the stagnation and static temperatures which is the effect of convection. Figure 3.13 represent the stagnation effect on the temperature measurement. As seen in the Figure 3.13, the effect of convection is negligible with an average variation of \( \pm 0.01 \% \) for measured temperatures.

![Figure 3.13: Effect of stagnation on temperature measurement](image)
Due to the lower temperatures at the pipe walls compared to the mid-flow temperature, the effect of radiation was investigated as well. Making an energy balance at the surface of the thermocouple between the convection heat transfer into the thermocouple and the radiation heat transfer out of the thermocouple, Equation (3.7) was obtained.

\[ h * (T - T_{TC}) = \varepsilon_{TC} * \sigma * (T_{TC}^4 - T_w^4) \]  

(3.7)

where \( h \) is the convection heat transfer coefficient, \( \varepsilon_{TC} \) is the emissivity of the thermocouple surface, \( \sigma \) is Stefan Boltzman’s constant and \( T_{TC} \) and \( T_w \) are the thermocouple and wall temperatures, respectively. Dividing both sides by \( h \) will lead to Equation (3.8).

\[ T - T_{TC} = \frac{\varepsilon_{TC} * \sigma * (T_{TC}^4 - T_w^4)}{h} \]  

(3.8)

The right-hand side of Equation (3.6) represents the effect of radiation on the thermocouple reading. The convective heat transfer coefficient was calculated from Nusselt number \( (Nu) \) as shown in Equation (3.9).

\[ Nu = \frac{h * d_{TC}}{k} \]  

(3.9)

Where \( d_{TC} \) and \( k \) are the diameter and the thermal conductivity of the thermocouple. For cross-flow over a cylinder (the thermocouple), Churchill-Berstein (1977) correlation was used to calculate the Nusselt number as shown in Equation (3.10).

\[ Nu = 0.3 + \frac{0.62 * \text{Re}_d^{1/2} * \text{Pr}^{1/3}}{[1 + \left( \frac{0.4}{\text{Pr}^{3/4}} \right)^{1/4}]} \left[ 1 + \left( \frac{\text{Re}_d}{282000} \right)^{5/8} \right]^{4/5} \]  

(3.10)

Where \( \text{Re}_d \) and \( \text{Pr} \) are Reynolds number and Prandlt number, respectively. The effect of radiation on temperature measurements was calculated and shown in Figure 3.14. The effect of radiation shown to be very small with an average variation of ± 0.002 % and is then neglected.
The thermocouples are connected to the DAQ system for data processing. The data is sampled at a frequency of 100 samples/second for 20 seconds.

### 3.5.3. Other Instruments

Pressure drop measurements were obtained using a differential pressure transducer provided by Omega Inc. that has a pressure range of ±17 kPa, accuracy of ±0.25 % full scale accuracy and voltage range of 5 Vdc. It was used to measure pressure drop across the catalytic converter. A calibration sheet for the pressure transducer provided by the manufacturer was used and it is represented in Figure 3.15. The pressure drop across the catalytic converter was measured as the difference in pressure between two locations, 80 mm (9 diameters) and 150 mm upstream downstream the monolith, respectively. The pressure data was collected using DAQ system. The data was sampled at a frequency of 2000 samples/second for 30 seconds.

The flow rate through the test section was measured using a rotameter with ±5 % accuracy and is controlled by a ball valve upstream the rotameter. The pressure across the rotameter is measured by two pressure gages with accuracy of ±3 %. The pressure regulator is used to control the flow pressure upstream of the electric heater to the suitable operation pressure (less than $1 \times 10^5$ Pa).
Temperature and velocity profile measurement instruments are mounted on two traverse mechanisms (shown in Figure 3.3) to scan the measurements across the catalytic converter using 3 mm steps. Dial gauges are mounted on the traverse mechanisms with minimum traversing steps of $2.5 \times 10^{-3}$ mm.

The thermocouples are connected to a temperature data acquisition (DAQ) card (NI 9214) provided by National Instruments with 16 thermocouples channels, 68 sample/second aggregate and output of $\pm 78$ mV. The DAQ isothermal terminal block accuracy is up to $0.45^\circ$C with sensitivity of $0.02^\circ$C sensitivity. MiniCTA 54T42 and the differential pressure transducer are connected to another DAQ model number (NI9215) provided by National Instruments with $\pm 10$ V, simultaneous analog input, 100k Sample/second and 4-channel characteristics. All DAQs are connected to a desktop computer and a LabVIEW software to monitor and record data.

### 3.6. Uncertainty and Error Analysis

The uncertainty analysis is performed for temperature, velocity, pressure and location measurements. The bias and precision errors are accounted for and the values are averaged for the recorded measurements. Equation (3.11) is used to find the total uncertainty for the measurements.
\[ U_R = \sqrt{(B_R^2 + P_R^2)} \]  

(3.11)

where \( U_R, B_R \) and \( P_R \) are the total uncertainty, the bias error and the precision error, respectively. The bias error is the fixed systemic error of the instrument and it is given by the manufacturer as the accuracy of the instrument. However, the precision error is a randomized error due to environmental conditions and is calculated by repeating each measurement 4 times and comparing the results obtained for a single measurement (a sample is shown in Figure 3.16). Table 3.1 summarizes the uncertainty analysis for the experiments. The values shown in the Table 3.1 are presented in the results plots as error bars for the given uncertainty percentages.

**Table 3.1: Uncertainty analysis of measurements**

<table>
<thead>
<tr>
<th>Measurement</th>
<th>Bias Error</th>
<th>Precision Error</th>
<th>Total Uncertainty</th>
</tr>
</thead>
<tbody>
<tr>
<td>Velocity</td>
<td>2 %</td>
<td>5 %</td>
<td>5.4 %</td>
</tr>
<tr>
<td>Temperature</td>
<td>0.28 %</td>
<td>0.29 %</td>
<td>0.38 %</td>
</tr>
<tr>
<td>Pressure</td>
<td>0.25 %</td>
<td>4 %</td>
<td>4.1 %</td>
</tr>
<tr>
<td>Location</td>
<td>0.1 %</td>
<td>0</td>
<td>0.1 %</td>
</tr>
</tbody>
</table>

**Figure 3.16: A sample of the measurement repeatability.**
Chapter 4 CFD Modelling

Computational fluid dynamics is a very common tool to aid in solving complex engineering problems. Proper modelling and mathematical representation are critical to approach the correct solutions along with accurate calibration and validation. This chapter presents the methodology followed to model and simulate the hot fluid flow through the catalytic converter monolith substrate including mathematical modelling, solution domain, mesh independence study and parameters implementation.

The solution domain is divided into three regions as shown in Figure 4.1. Regions I & III include inlet and outlet sections where turbulent flow occurs. The third region is the monolith substrate region that is modelled as a porous media region. This region is dominated by laminar flow due to the small hydraulic diameter of the channels. The k-ω turbulence model is used to model the turbulence in the flow and it will be discussed in detail in section 4.2.
Modelling the flow through the porous region requires evaluating the porous model parameters. The parameters required to properly model the porous zone are the channel viscous and inertial resistances and the region porosity. The region porosity is calculated from the geometry of the channels and the monolith specifications. However, finding the viscous and inertial resistances requires modeling a single channel of the monolith and is discussed in detail in the following section.

4.1. Single Channel Model:

Modelling the substrate zone is more challenging than the rest of the flow domain due to the increased computational cost associated with modelling this geometry. There are two main approaches to model the substrate zone: constructing a discrete channel model, where all channels are modelled. This would require meshing every channel to exactly simulate the air flow within the channels including entrance, viscous and inertial effects. Although this approach is more accurate, it is the most computationally expensive option due to the need of a very fine mesh. The second approach to this problem is to use the porous media model to model the flow inside the substrate. This requires the use of a 3D single channel model which characterizes the flow inside a single channel and provide the value of the parameters required for the porous media model. This model is computationally less expensive and relatively accurate for these types of simulations (Chen et al., 2008 and Hayes et al., 2012). The channel dimensions are obtained from the actual monolith dimensions and are shown in the Table 4.1. All the dimensions are standard for substrate production and obtained from the manufacturer.
A series of calculations at various mass flow rates and inlet temperatures that correspond to the experimental operating conditions are performed. The pressure drop across the channel is calculated and recorded for each case. The pressure drop is then plotted against the mass flow rate in the channel. Using Ergun Equation (4.1) which states that the total pressure drop across the channel is the summation of the viscous and inertial losses as shown below, the viscous and inertial resistances can be obtained using a best fit second order regression.

\[
\frac{\Delta P}{\Delta L} = VR \ast \mu \ast u + IR \ast \rho \ast \frac{u^2}{2} \tag{4.1}
\]

where \( \frac{\Delta P}{\Delta L} \), \( VR \), \( IR \), \( v \), \( \mu \) and \( \rho \) are the pressure drop per unit length, viscous resistance, inertial resistance, fluid average velocity, average dynamic viscosity and average density, respectively. The resistances obtained from these calculations are then specified for the porous media model calculations as the porous properties and are adjusted to obtain the pressure drop for the same variations of mass flow rate and inlet temperature. The calculations are based on the conditions represented in the Table 4.2. The temperature and mass flow rate range selected are obtained from the total mass flow rate and the experimental temperature measurements shown in chapter 5. Also, the solution domain is divided into 4 sections. Inlet and outlet sections to include the entrance and exit effects, flow channel and channel walls as shown in Figure 4.2.

The viscous and inertial resistances depend on the mass flow rate and temperature. The governing equations for the flow field are the continuity, momentum and energy equations. The steady state continuity Equation (4.2) can be written as:
\[
\frac{\partial}{\partial x_i} \left( \rho_f u_i \right) = 0
\] (4.2)

Table 4.2: Inlet flow conditions for the single channel model calculations.

<table>
<thead>
<tr>
<th>Inlet Temperature (°C)</th>
<th>Density (kg/m³)</th>
<th>Dynamic Viscosity ((10^6 \text{ Pa.s}))</th>
<th>Inlet Mass flow rate (kg/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>130</td>
<td>0.86672</td>
<td>23.218</td>
<td></td>
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<tr>
<td></td>
<td></td>
<td></td>
<td>1 \times 10^6</td>
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<td></td>
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<td>3.5 \times 10^6</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>7 \times 10^6</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>1.5 \times 10^5</td>
</tr>
<tr>
<td>150</td>
<td>0.8226</td>
<td>24.07</td>
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</tr>
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<td></td>
<td></td>
<td></td>
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<td></td>
<td>3.5 \times 10^6</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>7 \times 10^6</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>1.5 \times 10^5</td>
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<tr>
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<td>24.878</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>1 \times 10^6</td>
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<td></td>
<td>7 \times 10^6</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>1.5 \times 10^5</td>
</tr>
</tbody>
</table>

Figure 4.2: Single channel solution domain.
where \( \mathbf{u} \) is the velocity vector and \( \rho_f \) is the fluid density. The steady state momentum Equation (4.3) can be written as:

\[
\nabla \cdot (\rho \mathbf{u} \mathbf{u}) = -\nabla p + \nabla \cdot \mathbf{\tau} + \mathbf{F}
\]

(4.3)

where \( p, \mathbf{\tau} \) and \( \mathbf{F} \) are the pressure, the stress tensor and any momentum source or sink such as viscous and inertial resistances terms, respectively. The steady state energy Equation (4.4) for the fluid can be written as:

\[
\frac{\partial}{\partial z} \left( k_{\text{eff}}^f \frac{\partial T_f}{\partial z} \right) - \rho_f C_p \frac{\partial u_s}{\partial z} \frac{\partial T_f}{\partial z} = h A_u (T_f - T_s)
\]

(4.4)

where \( k_{\text{eff}}^f, T_f, C_p, u_s, h, A_u \) and \( T_s \) are the fluid thermal conductivity, fluid temperature, fluid specific heat, superficial velocity, convective heat transfer coefficient, surface area and substrate temperature. All fluid properties are functions of temperature. The radiation is neglected due to the lack of large temperature gradients in the axial and radial direction.

Figure 4.3 shows the boundary conditions assigned for the single channel model. The solution domain is assigned a mass flow rate inlet boundary conditions and the channel inside walls are assigned no slip boundary condition. The external walls are assigned symmetry boundary condition because the simulated channel present a single channel in an array of channel that are assumed to have uniform inlet conditions. The outlet is a pressure outlet boundary condition set at atmospheric pressure.

\[\text{Figure 4.3: Boundary conditions of the single channel model.}\]
All the calculations are done for both substrates, the 400 CPSI and the 900 CPSI. Tables 4.3 and 4.4 and Figures 4.4 and 4.5 present the results of the pressure drop calculations for the 400 CPSI and 900 CPSI substrates. The resistance values given by (Hayes et al., 2012) are used as initial estimates to find the porous media properties and then corrected to obtain the pressure drop within variation of ±5% from the results obtained from the single channel calculations. Table 4.5 represents the viscous and inertial resistance values that are used throughout this study.

Table 4.3: Pressure drop calculation results for the 400 CPSI substrate.

<table>
<thead>
<tr>
<th>Inlet Temperature (°C)</th>
<th>Inlet Mass flow rate (kg/s)</th>
<th>∆P/∆L (kPa/m)</th>
<th>Average Channel Velocity (m/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>130</td>
<td>1 x 10^{-6}</td>
<td>0.728</td>
<td>1.14</td>
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<tr>
<td></td>
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<td>1.5 x 10^{-5}</td>
<td>14.750</td>
<td>18.72</td>
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</table>
Figure 4.4: Pressure drop calculation results for 400 CPSI substrate.

Table 4.4: Pressure drop calculation results for the 900 CPSI substrate.

<table>
<thead>
<tr>
<th>Inlet Temperature (°C)</th>
<th>Inlet Mass flow rate (kg/s)</th>
<th>$\Delta P/\Delta L$ (kPa/m)</th>
<th>Average Channel Velocity (m/s)</th>
</tr>
</thead>
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<td>12.96</td>
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<td>$1.5 \times 10^{-5}$</td>
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<td></td>
<td>$1.5 \times 10^{-5}$</td>
<td>36.880</td>
<td>30.27</td>
</tr>
</tbody>
</table>
Figure 4.5: Pressure drop calculation results for 900 CPSI substrate.

Table 4.5: Viscous and inertial resistances values for 400 CPSI and 900 CPSI substrates

<table>
<thead>
<tr>
<th>Cell density (CPSI)</th>
<th>Viscous resistance (1/m²)</th>
<th>Inertial resistance (1/m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>400</td>
<td>7.95 x 10⁷</td>
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</tr>
<tr>
<td>900</td>
<td>12.2 x 10⁷</td>
<td>23.5</td>
</tr>
</tbody>
</table>

The viscous and inertial resistances are assigned for the axial direction. However, they are three order of magnitude larger in the radial direction to force the flow through the porous zone in a straight way similar to the flow passing though discrete parallel channels as suggested by (Hayes et al., 2012).

4.2. Modelling of Flow Through Catalytic Converter:

The flow through the catalytic converter can be separated into three sections. Sections I and III are modelled as turbulent flow and represent flow inside the pipes outside the porous zone. Section II is the flow through the monolith substrate which is dominated by a laminar flow regime (see calculations in Appendix C). Modelling for both sections is discussed.
4.2.1. Geometry

The solution domain is divided into three sections, the inlet pipe and cone, the catalytic converter and the exit pipe and outlet cone. The inlet pipe is connected to the monolith section through a 45° diffuser and the exit pipe is connected to the catalytic converter through a 30° converging cone. These values are identical to the actual geometry which are used commonly for catalytic converter diffuser design. The catalytic converter section contains the monolith substrate that is surrounded by a padding. Figure 4.6 represents the domain for the axisymmetric 2D model. The axisymmetric 2D model is used for the rest of this study and a comparison between the 2D and 3D models is presented in section 4.3.

![Figure 4.6: Baseline substrate solution domain with all simulated components.](image1)

![Figure 4.7: Cleanalytic™ substrate solution domain.](image2)
The measuring plane in Figure 4.6 above refers to the plane where the experimental data were collected and CFD results were for validated as discussed in chapter 5. The solution domain for the Cleanalytic™ is shown in Figure 4.7 with the X-20 Filler insulation layer. Table 4.6 and Figure 4.8 summarize the dimensions for the solution domain that are identical to the dimensions of the developed experimental setup:

![Figure 4.8: Dimensions of solution domain](image)

Table 4.6: Dimensions of the components of simulated catalytic converter assembly.

<table>
<thead>
<tr>
<th>Geometry</th>
<th>Dimension (mm)</th>
<th>Geometry</th>
<th>Dimension (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>a</td>
<td>530</td>
<td>h</td>
<td>35.5</td>
</tr>
<tr>
<td>b</td>
<td>2.5</td>
<td>i</td>
<td>37</td>
</tr>
<tr>
<td>c</td>
<td>89</td>
<td>j</td>
<td>25.5</td>
</tr>
<tr>
<td>d</td>
<td>114</td>
<td>k</td>
<td>25.5</td>
</tr>
<tr>
<td>e</td>
<td>1.5 - 2.5</td>
<td>l</td>
<td>30.5</td>
</tr>
<tr>
<td>f</td>
<td>23 - 28</td>
<td>m</td>
<td>180</td>
</tr>
<tr>
<td>g</td>
<td>2 - 4</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>
4.2.2. Material and Fluid Properties

The materials used in the model are presented in Table 4.7 provided by Vida Fresh Air Corp. and air properties are presented in the Figures 4.9, 4.10, 4.11 and 4.12. All the properties are taken from (www.engineeringtoolbox.com). All materials listed in Table 4.7 are solids and for that the properties are independent of temperature.

Table 4.7: Material properties

<table>
<thead>
<tr>
<th>Part</th>
<th>Material</th>
<th>Density (kg/m$^3$)</th>
<th>Specific Heat (J/kg-K)</th>
<th>Thermal Conductivity (W/m-K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pipes</td>
<td>Stainless Steel 441</td>
<td>770</td>
<td>460</td>
<td>25</td>
</tr>
<tr>
<td>Padding</td>
<td>Fiberfrax</td>
<td>2700</td>
<td>1040</td>
<td>0.1</td>
</tr>
<tr>
<td>Insulation</td>
<td>X-20 Filler</td>
<td>480</td>
<td>1000</td>
<td>0.12</td>
</tr>
<tr>
<td>Monolith</td>
<td>Cordierite</td>
<td>2600</td>
<td>1465.4</td>
<td>2.5</td>
</tr>
</tbody>
</table>

Figure 4.9: Air density as a function of temperature

\[ y = 2\times10^{-6} - 1\times10^{-4}x^2 + 3\times10^{-11}x^4 - 3\times10^{-8}x^3 + 1\times10^{-5}x^2 - 0.005x + 1.3126 \]
Figure 4.10: Air specific heat as a function of temperature

Figure 4.11: Air thermal conductivity as a function of temperature
4.2.3. Zones I & III Flow Modeling

The turbulent flow regime is dominant in these zones. The k-ω turbulence model is utilized to model turbulence in these zones when solving the Reynolds Averaged Navier-Stokes (RANS) equations where k and ω are the turbulent kinetic energy and the specific dissipation rate, respectively. This model was selected as it is more suitable for free shear flows and wall-bounded boundary layer problems (Karthik, 2011 and Zhang et al. 2007). The governing equations for the flow within these zones are presented below.

The continuity equation (4.5) for the steady state condition is:

$$\frac{\partial}{\partial x_i}(\rho u_i) = 0$$  \hspace{1cm} (4.5)

The steady state Reynolds Averaged Navier-Stokes equation (4.6) can be written as:

$$\frac{\partial}{\partial x_j}(\rho u_i u_j) = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \left[ \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \frac{\partial u_l}{\partial x_l} \right) \right] - \frac{\partial}{\partial x_j}(\rho u_i' u_j')$$  \hspace{1cm} (4.6)
where \( u' \) is the fluctuating component of the velocity. After implementing the Boussinesq assumption which states that the turbulent stress tensor can be expressed in terms of the mean rate of strain, the turbulent stresses term \(- (\rho u'_i u'_j)\) can be written as shown in Equation (4.7):

\[
- (\rho u'_i u'_j) = \mu_t \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} (\rho k + \mu_t \frac{\partial u_k}{\partial x_k})
\]

where \( \mu_t \) is the eddy or turbulent viscosity. The k- \( \omega \) turbulence transport equations (4.8) and (4.9) are utilized to calculate the turbulent viscosity.

\[
\frac{\partial}{\partial x_i} (\rho ku_i) = \frac{\partial}{\partial x_j} \left( \Gamma_k \frac{\partial k}{\partial x_j} \right) + G_k - Y_k + S_k
\]

\[
\frac{\partial}{\partial x_i} (\rho \omega u_i) = \frac{\partial}{\partial x_j} \left( \Gamma_\omega \frac{\partial \omega}{\partial x_j} \right) + G_\omega - Y_\omega + S_\omega
\]

where \( \Gamma, G, Y \) and \( S \) are the effective diffusivity, generation terms, dissipation terms and source terms, respectively. The subscripts \( k \) and \( \omega \) represent turbulent kinetic energy and specific dissipation rate, respectively. The effective diffusivity equations can be written as shown in Equations (4.10) and (4.11):

\[
\Gamma_k = \mu + \frac{\mu_t}{\sigma_k}
\]

\[
\Gamma_\omega = \mu + \frac{\mu_t}{\sigma_\omega}
\]

where \( \sigma_k \) and \( \sigma_\omega \) are the turbulent Prandtl numbers for \( k \) and \( \omega \), respectively. The turbulent viscosity \( \mu_t \) can be represented as follows in Equation (4.12):

\[
\mu_t = \frac{\rho k}{\omega}
\]

The generation of turbulent kinetic energy can be written as shown in Equation (4.13):

\[
G_k = \mu_t S^2
\]
where $S$ is the modulus of the mean rate-of-strain tensor and can be represented as

$$S = \sqrt{2S_{ij}S_{ij}}$$

where the mean strain rate $S_{ij}$ is presented in Equation (4.14):

$$S_{ij} = \frac{1}{2} \left( \frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j} \right)$$  \hspace{1cm} (4.14)

The generation of the specific dissipation rate can be expressed in Equation (4.15) as:

$$G_\omega = \frac{\omega}{k} G_k$$  \hspace{1cm} (4.15)

The dissipation of $k$ and $\omega$ can be written in Equations (4.16) and (4.17) as:

$$Y_k = \rho \beta^* k \omega$$  \hspace{1cm} (4.16)

$$Y_\omega = \rho \beta \omega^2$$  \hspace{1cm} (4.17)

The default values of the model constant utilized in Fluent are used. These values are:

$$\sigma_k = 2, \quad \sigma_\omega = 2, \quad \beta^* = 0.09, \quad \beta = 0.072$$

The energy balance for the fluid flow through the pipes can be written in Equation (4.18) as:

$$\frac{\partial}{\partial z} \left( k_{\text{eff}} \frac{\partial T_f}{\partial z} \right) - \rho_f C_{p_f} u_s \frac{\partial T_f}{\partial z} = h A_v (T_f - T_s)$$  \hspace{1cm} (4.18)

### 4.2.4. Zone II Flow Modeling

In this zone, the flow is laminar with Reynolds number range of 200 to 700 (see Appendix C) based on the channel hydraulic diameter. The Volume Averaged Navier-Stokes (VANS) equation is used for the momentum balance with a momentum sink term that represents the flow resistance. The steady state continuity equation can be written in Equation (4.19) as:
\[
\frac{\partial}{\partial x_i} \left( \rho_f u_i \right) = 0
\]  
(4.19)

The velocity used in this equation is the superficial velocity which is the product of the physical velocity and the medium porosity. The volume averaged Navier-Stokes equation can be written as:

\[
\nabla \cdot (\rho_f \mathbf{u} \mathbf{u}) = \nabla p + \nabla \cdot \mathbf{r} + \mathbf{F}
\]  
(4.20)

The source term \( \mathbf{F} \) is defined by (Hayes & Kolaczkowski, 1997) and can be written in Equation (4.21) as:

\[
\mathbf{F} = -\left( \frac{\mu}{K} u_i + \frac{1R_f \rho f}{2} |u| u_i \right)
\]  
(4.21)

From the above equation, the first term on the right-hand side is the viscous losses and the second term is the inertial losses where \( K \) represents the medium permeability. For monolith substrates, the axial permeability is significantly higher than the radial permeability due to the unidirectional nature of the flow within these types of structures. The permeability is the reciprocal of the viscous resistance obtained from section 4.1.

The energy balance of the solid phase is represented in terms of axial and radial conduction, and convection. In Fluent, the thermal equilibrium model is assigned for the porous region which assumes that fluid and solid temperatures are equal which is a reasonable assumption because of the steady state non-reacting conditions. The steady state energy balance for the porous zone can be written in Equation (4.22) as:

\[
\frac{\partial}{\partial r} \left( r k_{r,eff} \frac{\partial T_s}{\partial r} \right) + \frac{\partial}{\partial z} \left( k_{a,eff} \frac{\partial T_s}{\partial z} \right) = hA_u (T_f - T_s)
\]  
(4.22)

where \( k_{r,eff} \) and \( k_{a,eff} \) are the substrate radial and axial thermal conductivities, respectively. The axial and radial thermal conductivities are calculated based on the symmetric model developed by (Visconti et al. 2013) and presented in Equations (4.23) and (4.24) as:

\[
k_{a,eff} = k_s \times (1 - \emptyset)
\]  
(4.23)
\[ k_{r,eff}^2 = k_s \frac{1 - \varnothing}{1 + \varnothing} \]  

(4.24)

where \( k_s \) and \( \varnothing \) are the solid thermal conductivity and the porosity, respectively.

4.2.5. Boundary Condition

At the inlet, a mass flow inlet boundary is set as a mass flow rate of \( 5.18 \times 10^{-2} \) kg/s and free stream temperature of 177 °C. The hydraulic diameter and the turbulence intensity are set at 48.8 mm and 5 %, respectively. At the outlet, a pressure outlet boundary condition is set as an atmospheric pressure with back flow temperature set at 23 °C. The walls of the pipes and are assigned walls boundary conditions with specified thickness of 2 mm and convection heat transfer coefficient. The radiation and shell conduction effects incorporated in the convection heat transfer coefficient of 120 W/m²-K. The interfaces between the padding and the monolith and the insulation layer and the monolith are assigned a slip boundary condition as the wall effects are taken into consideration when calculating the viscous and inertial resistances. An axis boundary condition is assigned for the centerline to model the axisymmetric geometry.

4.2.6. User Defined Functions

Two user defined functions (UDF) were used in Fluent. The first one was used to damp the turbulent kinetic energy and the turbulent dissipation rate inside the monolith. Damping these two parameters to the appropriate values damps the turbulent kinetic energy and the turbulent dissipation inside the monolith which prevents the flow to be influenced downstream of the monolith by the generation of these parameters inside the monolith. This UDF was provided by Vida Fresh Air Crop. where the turbulent parameters were fixed to be nearly zero. The second UDF was used to inject turbulence downstream of the monolith. This region is located at the interface between the laminar flow and the turbulent in the downstream direction of the flow. The turbulence intensity values injected in this region were obtained from the experimental data and varied from 25 % to 33 % depending on the type of monolith tested. Further details on this used defined function are discussed in chapter 5.
4.3. **Meshing**

The mesh is constructed utilizing Ansys software package built-in mesher. The mesh used is a hexahedral mesh with number of elements of 162,000. To capture the boundary layer for the turbulent flow, an inflation layer is used with the height of the elements at the walls varies from $1 \times 10^{-2}$ mm to $5 \times 10^{-2}$ mm to ensure that the Y+ values for the solution is at the order of 1 over the entire domain. Figure 4.13 shows the mesh utilized in this study. The solution is obtained for the 3D mesh and compared to the 2D mesh. It was found that the solution of the 2D mesh varies between $\pm 5\%$ from the 3D mesh with significant decrease in the computational cost (from 7 hours to 6 minutes). The 2D mesh was used for the rest of this study. The mesh independence study for the 2D and 3D meshes is discussed below.

4.3.1. **Mesh Independence Study**

This study is utilized to ensure that solution is independent of the mesh used. Two separate mesh independence studies are performed for 3D and 2D meshes. The 3D mesh independence is performed for 150,000, 550,000, 800,000, 900,000 2500,000 and 3,000,000 elements meshes. The results obtained from the 3D meshes are compared to a 210,000 elements 2D mesh to show the effect of utilizing the 2D and 3D meshes on the solution as shown in the Figure 4.14.

![Figure 4.13: The utilized mesh for the inlet sand outlet pipes and cones](image-url)
Figure 4.14: Mesh impedance study for 3D mesh and the effect of using 2D mesh on the solution (a) temperature profiles & (b) velocity profiles.
The temperature and velocity profiles 5 mm downstream of the monolith for an inlet mass flow rate of $7.2 \times 10^{-2} \text{ kg/s}$ and temperature of 177 °C are used to evaluate the effect of mesh size. This location was chosen for this study because the numerical results are validated using experimental measurements at the same location which indicates that this location is more important than any other location in the entire domain for the mesh independence study.

The results are compared using root mean square error (RMSE) percentage method and the effect of using the 2D mesh on the solution is within ± 5 % as shown in Table 4.8. The variation is calculated based on the results obtained from the 2,500,000 elements 3D mesh. As shown in Table 4.8 above, mesh independence is obtained for meshes have more than 800,000 elements with maximum RMSE of ± 1.2 % effect on the results. Moreover, the 2D 210,000 elements mesh shows variation of ± 5 % of the results compared to all the 3D meshes which can be considered acceptable taking into consideration the reduction of the computational cost from 7 hours to 6 minutes. The 2D analysis is selected for the rest of this study.

Another mesh independence study is performed for the 2D meshes. The used 2D meshes are 36,000, 73,000, 162,000 and 210,000 elements and the results obtained 0.5 cm downstream the monolith for inlet mass flow rate and temperature of $7.2 \times 10^{-2} \text{ kg/s}$ and 177 °C, respectively. The results are shown in the Figure 4.15.

On the other hand, the results are compared using root mean square error (RMSE) percentage method. The variation is calculated based on the results obtained from the 210,000 elements 2D mesh. The results are summarized in Table 4.9:

<table>
<thead>
<tr>
<th>Mesh number of elements</th>
<th>Temperature RMSE %</th>
<th>Velocity RMSE %</th>
</tr>
</thead>
<tbody>
<tr>
<td>3D 150,000</td>
<td>± 3</td>
<td>± 3</td>
</tr>
<tr>
<td>3D 550,000</td>
<td>± 2.7</td>
<td>± 2</td>
</tr>
<tr>
<td>3D 800,000</td>
<td>± 1.8</td>
<td>± 1.6</td>
</tr>
<tr>
<td>3D 900,000</td>
<td>± 1.5</td>
<td>± 1.4</td>
</tr>
<tr>
<td>3D 3,000,000</td>
<td>± 1</td>
<td>± 1.2</td>
</tr>
<tr>
<td>2D 210,000</td>
<td>± 5</td>
<td>± 4</td>
</tr>
</tbody>
</table>
Figure 4.15: Mesh independence study for the 2D mesh. (a) Temperature profiles and (b) Velocity profiles.
As shown in Table 4.9 above, mesh independence is achieved for meshes that are have more than 162,000 elements with maximum variation of ± 0.9 % with s computational cost varying from 5 to 7 minutes. Therefore, the 162,000 elements 2D mesh is utilized for the rest of this study.

### 4.4. Discretization and Equations Solving

The general scalar transport equations are converted into algebraic equations using a control-volume-based technique. This technique utilizes integrating the transport equations over each single control volume to obtain discrete conservation equations on a control volume basis.

The pressure based solver is used to implement the discretization of the transport equations. This solver was chosen because the flow is mildly compressible. The algorithm this solver employs is called the projection method in which the velocity field is obtained from the momentum equation and the pressure field is extracted from pressure correction equations after isolation from the continuity and momentum equations. The process is then repeated until the solution converges. The solution algorithm followed for this solver is the coupled algorithm in which the momentum equation and the pressure-based continuity equation are coupled and solved simultaneously. Then, solving for any other scalar quantity is decoupled and each quantity is calculated separately. Figure 4.16 shows the coupling algorithm in Fluent. The advantages of implementing this algorithm are stability and robust convergence (ANSYS Fluent Theory Guide, 2013).
The solutions of the set of equations is going to be assigned to each cell center in the discretized grid and requires interpolation between the center and the faces of the mesh elements. Upwinding is the technique implemented in Fluent in which the cell face values are calculated from the cell in the upstream direction relative the flow velocity direction.

The interpolation scheme utilized for the continuity, momentum, energy, turbulent kinetic energy and specific dissipation rate is second order upwinding. Second order upwinding calculates the quantities at the faces using a multidimensional linear reconstruction approach by incorporating Taylor series expansion about the cell centroid to achieve high order accuracy. This approach requires determination of the gradients for each cell. Least squares cell-based gradients evaluation is utilized and assumed that the solution of two
adjacent cells varies linearly. This indicates that each cell has a matrix of gradients that form a system of linear equations which can be solved by decomposing the coefficients by using Gram-Schmidt process (Anderson & Bonhaus, 1994). This gradient evaluation method is accurate and computationally inexpensive when the mesh elements are aligned and not skewed.

A second order pressure interpolation scheme is used in which the face pressure is reconstructed using central differencing scheme. This scheme was chosen because it provides higher accuracy than the other options that Fluent offers (ANSYS Fluent Theory Guide, 2013).
Chapter 5 Results and Discussion

Results from the experimental work and CFD simulations are discussed in this chapter. The developed CFD model was validated with results obtained from the experimental work for baseline and Cleanalytic™ catalytic converters. The validation was done using temperature, velocity, turbulence intensity and pressure drop measurements. The experimental and CFD results have been used to study the thermalhydraulic performance of both baseline and Cleanalytic™ catalytic converters. The experimental and numerical study were performed under steady state non-reacting hot air flow through the catalytic converters with a free stream temperature of 177 °C and mass flow rate of $5.18 \times 10^{-2}$ kg/s (Re = 43,000 based on inlet diameter).

5.1. Flow and Monolith Temperature Measurements

To establish a relation between the temperature measurements inside and downstream of the monolith, the temperature inside the monolith was measured. Figure 5.1 shows the monolith and the flow temperature measurements. In this experiment, the mass flow rate was kept constant at $5.18 \times 10^{-2}$ kg/s and free stream temperature was varied.
Figure 5.1: Monolith and flow temperature (a) schematic of the location of the monolith and fluid temperature measurements (b) experimental measurements

T₁ in the schematic above represents the flow temperature measurement location and T_B represents the temperature measured inside the monolith (brick). The monolith temperature was found to be higher than the fluid temperature by an average of 6%. This difference is due to the increased thermal resistance inside the monolith that allows for higher heat storage and higher temperatures. The thermal resistances inside the monolith are the convection resistance at the ambient side of the walls and the conduction resistances of the monolith, padding and pipe walls. The thermal resistances downstream the monolith are the convection and the pipe walls conduction resistances. It was assumed that this effect remains the same for all other locations inside the monolith. Therefore, the temperature downstream the monolith can be used as an indication on the temperature inside the monolith.

5.2. Effect Turbulence Intensity on Temperature Profiles

The temperature profile downstream of the monolith is affected by several factors. These factors can be the thermal resistance and the flow temperature. Another important factor is the turbulence intensity downstream of the monolith. The higher the turbulence intensity, the higher the mixing hence higher heat transfer from the centerline to the pipe walls. Initially, the use of a user defined function to damp the turbulence kinetic energy and the turbulent dissipation rate was implemented inside the monolith to prevent
these parameters to affect the flow downstream the monolith. However, this didn’t allow the turbulence downstream to be high enough for the mixing which inhibits the heat transfer. Therefore, the temperature profile downstream of the monolith was over-predicted. To overcome this challenge, another UDF was used to inject turbulence downstream of the monolith. The turbulence intensity injected varied from 25% to 33% depending on the monolith type. These values were obtained from the experimental data. The effect of injecting turbulence downstream the monolith on the temperature profile is shown in Figure 5.2. This UDF did not affect velocity and pressure drop predictions, therefore, it was used throughout the rest of this study to improve the temperature predictions.

5.3. Flow Development

The inlet pipe is designed to ensure that the flow reaching the monolith substrate is a fully developed turbulent flow. The flow development profiles include temperature and velocity. The temperature profiles across the inlet pipe are plotted in Figure 5.3 for the 400 CPSI catalytic converter. It can be seen in the figure that the temperature becomes fully developed about 8 diameters length of the inlet pipe. The temperature near the walls are lower due to the convection from the outside surfaces. Near the inlet, the temperature profile is approximately flat due to the imposed inlet boundary condition and it tends to lower at the edges as the flow develops.

![Figure 5.2: The effect of turbulence on temperature profile.](image)
Similarly, the development of the velocity profile followed the same trend as shown in Figure 5.4. A fully developed turbulent flow velocity profile is obtained about 8 diameters length of the inlet pipe. This entrance length was expected as the experimental setup was built to ensure a fully developed turbulent flow. Similar flat trend at the inlet is observed due to the boundary condition. However, the core velocity tends to increase as the velocity develops due to the temperature effects near the walls. The lower the temperature, the higher the density of the air hence the lower the velocity. The same study is done for the Cleanalytic™ and the 900 CPSI monoliths and the results are shown in Appendix A.

5.4. Validation of the Baseline Catalytic Converter

Experimental validation for the baseline catalytic converters includes temperature, velocity and turbulence intensity profile measurements. The validation was done using profile measurements collected 5 mm downstream of the monolith. The data is collected downstream of the monolith because it was very challenging to obtain accurate measurements inside the monolith due to the complexity of its shape. These validations are presented in this section for both types of monolith cell densities (400 and 900 CPSI).

![Figure 5.3: Temperature profiles in the inlet pipe. \( R' \), \( z \) and \( D \) are the inlet pipe radius, the axial location from the inlet and the inlet pipe inside diameter.](image-url)
5.4.1. Temperature Validation

It was observed that the temperature downstream of the 400 CPSI monolith as shown in Figure 5.5 was higher at the core of the monolith. This behaviour is attributed to the heat loss through the pipe walls. The same trend is obtained from the CFD results which are in good agreement with the experimental data with a root mean square error (RMSE) of ± 2.7 %. For the 900 CPSI monolith, the baseline experimental temperature profile monolith shows a similar trend to the baseline 400 CPSI as shown in Figure 5.6. The predicted temperatures follow the same trend and in a good agreement with the experimental data with an RMSE of ± 3.7 %.

5.4.2. Velocity Validation

For the 400 CPSI monolith, the experimental velocity measurements shown in Figure 5.7 show that the flow velocity near the centerline of the monolith is higher than the flow velocity in the periphery region. This occurs because of the flow jet exiting the inlet pipe with the smaller diameter forces the flow to enter the core of the monolith from a cross section area comparable to the cross-section area of the inlet pipe. This effect causes flow non-uniformity and does not allow the monolith to be fully utilized. A similar trend is obtained from the velocity simulation and in good agreement with the experimental data with an RMSE of ± 8.2 %.
Figure 5.5: Temperature profile for the baseline 400 CPSI monolith.

Figure 5.6: Temperature profile for the baseline 900 CPSI monolith.
The velocity profile for the 900 CPSI monolith show in Figure 5.8 is more uniform than the one obtained for the baseline 400 CPSI and this is due to the higher monolith resistance. As the flow jet exits the inlet pipe, it faces a higher resistance caused by the smaller hydraulic diameter of the monolith channels. This acts as a physical barrier that allows the flow to uniformly redistribute at the front face of the monolith. The velocity measurements are approximately constant when approaching the core of the monolith. This flow behaviour allows for a better monolith utilization compared to the case of the 400 CPSI monolith. The same trend was obtained from the simulations and the results are in good agreement with the experimental data with an RMSE of ± 5.2%.

5.4.3. Turbulence Intensity Validation

The turbulence intensity is calculated from the average and the fluctuating component of the velocity using the Equation (5.1) shown below:

\[
Turbulence\ Intensity\ (\%) = \frac{u'}{u} \times 100
\]  

Figure 5.9 shows the turbulence intensity profile for the 400 CPSI monolith. The under-prediction of the turbulence intensity near the padding edge occurs due the shear layer between the stagnant flow at the back
of the padding wall and the flow exiting the monolith. This shear layer causes higher turbulence and was not accounted for in the numerical model because of the transient nature of the vortex shedding taking place and caused by the shear layer. This transient effect only takes place during the experiment though it was at steady state. However, this effect does not affect the other flow properties and was observed for all the tested configurations of Cleanalytic™ and 900 CPSI monoliths. The numerical results are in good agreement with the experimental data with an RMSE of ± 10.2 %.

The turbulence intensity values for the 900 CPSI monolith shown in Figure 5.10 are lower than the values of the 400 CPSI by an average of 3.5 % and this is due to the lower local velocities for the 900 CPSI monolith. The turbulence intensity profile follows the same trend as the velocity profile with a flat plateau. The numerical results are in good agreement with the experimental data with an RMSE of ± 6.9 %.

From the temperature, velocity, turbulence intensity profiles for both 400 CPSI and 900 CPSI baseline catalytic converters, the implemented model successfully predicted the experimental measurements and can be further used to study the thermo-fluid behaviour inside the catalytic converter.

*Figure 5.8: Velocity profile for the baseline 900 CPSI monolith.*
Figure 5.9: Turbulence intensity profile for the baseline 400 CPSI monolith.

Figure 5.10: Turbulence intensity profile for the baseline 900 CPSI monolith.
5.5. Optimization and Validation of Cleanalytic™ Catalytic Converters

This section discusses the selection of the optimum insulation design for the Cleanalytic™ technology. In addition, the validation of the Cleanalytic™ technology using the selected optimum design for both the 400 CPSI 900 CPSI monoliths is discussed.

5.5.1. Cleanalytic™ Insulation Design Optimization

The thickness of the insulation layer is kept constant at 2 mm ± 0.5 mm (around 2 channels wide) to minimize the pressure drop and allow for enough insulation between the monolith chambers. The inside diameter of the insulation layer inside the monolith is the parameter to be optimized. The inside diameter of the insulation layer installed inside the monolith was varied from 46 mm to 56 mm. Local temperature measurements were collected at 5 mm downstream of the monolith to find which insulation design yields the maximum flow temperature and heat retention. The temperature profiles included the temperature profile of the baseline monolith as shown in Figure 5.11.

Using the Cleanalytic™ technology (regardless of the size of the inside diameter of the insulation) increases the flow temperature downstream of the monolith. The insulation diameter was varied based on increments and decrements from the inlet pipe diameter which vary from – 10 % to + 10 % of the inlet pipe diameter. However, when the inside diameter of the insulation is 53 mm (5% larger than the inlet diameter of the pipe), the maximum temperature difference is obtained. This difference indicates that this design is optimum for maximum heat storage inside of the monolith. Table 5.1 shows the temperature difference between the baseline temperature profile and the temperature profiles obtained for the Cleanalytic™ when varying the insulation inside diameter using root mean square difference.
Figure 5.11: Temperature profiles for different Cleanalytic™ insulation layers for the 400 CPSI monolith. Di is insulation inside diameters.

<table>
<thead>
<tr>
<th>Insulation diameter percentage</th>
<th>-10%</th>
<th>+10%</th>
<th>-5%</th>
<th>+5%</th>
<th>0%</th>
</tr>
</thead>
<tbody>
<tr>
<td>Insulation inside diameter (mm)</td>
<td>46</td>
<td>56</td>
<td>48</td>
<td>53</td>
<td>51</td>
</tr>
<tr>
<td>RMSD (°C)</td>
<td>1.8</td>
<td>2.2</td>
<td>1.3</td>
<td>3</td>
<td>2.1</td>
</tr>
</tbody>
</table>

Utilizing the Cleanalytic™ technology with insulation inside diameter of 53 mm yields the highest RMSD from the baseline catalytic converter temperature profile. This effect is caused by the extra thermal resistance of the insulation layer which allows for higher heat retention inside the monolith. Therefore, this diameter is chosen for the validation of the Cleanalytic™ technology and will be used to study its effect on the thermalhydraulic performance of catalytic converters. The same insulation design is chosen for the 900 CPSI monolith.
5.5.2. Temperature Validation

For the Cleanalytic™ technology validation is performed using the same methodology followed when validating the baseline catalytic converters with the same flow conditions and measurements location. As shown in Figure 5.12, the temperature profile for the 400 CPSI Cleanalytic™ monolith for both the experimental and the numerical results followed the same trend obtained for the baseline case. However, temperature was higher for the Cleanalytic™ case by about an RMSD of 3 °C. The numerical results are in very good agreement with the experimental data with an RMSE of ± 2.5 %.

Using the Cleanalytic™ technology for the 900 CPSI monolith has a similar effect on the baseline case with the same trend as the 400 CPSI case as shown in Figure 5.13. The temperature was increased by an RMSD of 2 °C. The numerical results are in good agreement with the experimental data with RMSE of ± 3.2 %.

5.5.3. Velocity Validation

As shown in Figure 5.14, the average flow velocity downstream of the Cleanalytic™ 400 CPSI monolith is higher by an average of 1.5 m/s than the average flow velocity downstream of the 400 CPSI baseline monolith due to channel blockage and smaller monolith cross section area. This blockage divides the monolith into two chambers which forces more of the flow to go through the periphery of the monolith. At r/R = 0.75, the velocity drops because of the channel blockage as this location is directly downstream of the insulation layer where no flow is passing through. The numerical results are in good agreement with the experimental data with RMSE of ± 5.7 %. For the Cleanalytic™ 900 CPSI monolith, the velocity profile is more uniform as it takes a flat trend when approaching the centerline as shown in Figure 5.15. The numerical results are in good agreement with experimental data with an RMSE of ± 4 %.
Figure 5.12: Temperature profiles for the Cleanalytic™ 400 CPSI monolith.

Figure 5.13: Temperature profiles for the Cleanalytic™ 900 CPSI monolith.
Figure 5.14: Velocity profiles for the Cleanalytic™ 400 CPSI monolith.

Figure 5.15: Velocity profiles for the Cleanalytic™ 900 CPSI monolith.
5.5.4. Turbulence Intensity Validation

The turbulence intensity profile follows the same trend as the velocity profile where the average turbulence intensity for the flow downstream of the 400 CPSI Cleanalytic™ monolith shown in Figure 5.16 is higher than the one obtained for the baseline 400 CPSI by average of 2%. The turbulence intensity downstream of the monolith at the periphery are higher due to flow redistribution effects and the numerical results follow the same trend with an RMSE of ± 7.4%. The turbulence intensity downstream the Cleanalytic™ 900 CPSI monolith shown in Figure 5.17 is lower than the baseline case due to lower flow velocity. The numerical results are in good agreement with the experimental data with RMSE of ± 7.2%.

![Figure 5.16: Turbulence intensity profiles for the Cleanalytic™ 400 CPSI monolith.](image)
5.6. 2D Flow Field Results

5.6.1. Baseline 400 CPSI Monolith

The temperature, velocity, turbulence intensity and pressure contours are shown in Figure 5.18. Where Figures a, b, c and d represent the temperature, velocity, turbulence intensity and pressure contours, respectively. The white spaces represent the padding area which is defined as a solid region where the velocity, turbulence intensity and pressure values are undefined. The flow direction is from the left of the page to the right.

The temperature contour shown in Figure 5.18 (a) shows that the temperature distribution across the monolith with higher temperatures in the core of the monolith. The temperature inside the monolith is expected to decrease radially to the direction of the pipe walls due to the heat losses to the ambient temperature. This heat transfer is caused by the radial conduction through the monolith, conduction through the pipe walls and convection at the outside pipe walls.

In Figure 5.18 (b), it can also be seen that flow separation takes place at the inlet diffuser due to the shear layer. This flow separation causes flow circulation at the front face of the monolith which increases pressure.
Another shear layer occurs downstream of the padding and causes flow circulation at the back of the padding due to the stagnant flow interactions with the flow exiting the monolith.

The turbulence intensity contour shown in Figure 5.18 (c) represents the turbulence level inside the monolith which is negligible because the flow inside the monolith channels is laminar. However, high turbulence is taking place at the exit of the monolith channels. The flow inside the monolith is segregated independently in every channel and as the flow exits the monolith, the flow exiting every channel is mixed. This mixing causes high turbulence which decreases when approaching the outlet cone due to the rearrangement of the flow exiting the monolith. It is also noticed that the turbulence near the walls are very small due to lower velocities.

Figure 5.18 (d) represents the pressure contour of the baseline catalytic converter. The pressure drop occurs primarily at the inlet diffuser due to the sudden area expansion which causes flow circulation. Flow circulations causes pressure drop because of the generated turbulence. Downstream of the monolith, the compression of the flow passing through the exit cone from a large pipe cross section to a small one causes pressure drop.

5.6.2. Cleanalytic™ 400 CPSI Monolith

Figure 5.19 shows the flow field contours for the Cleanalytic™ 400 CPSI monolith. The extra white space inside the monolith is the insulation layer which is undefined for velocity, turbulence intensity and pressure contours. For the temperature contour, the insulation is shown as two parallel lines.

The temperature contour shown in Figure 5.19 (a) is similar to the one obtained for the baseline 400 CPSI monolith. However, it is expected that the temperature of the monolith should be higher in the Cleanalytic™ case. This increase in the temperature is due to the installation of the insulation layer inside the monolith which added an extra thermal resistance that opposed the heat transfer to the ambient temperature. This increase is no shown in the contour because of the scale that was intentionally kept consistence when representing the contours. The temperature difference was observed when taking average volume temperature from the CFD in ANSYS. The temperature difference was found to be higher for the Cleanalytic™ case by an average of 13 °C. This difference is further explained in section 5.8.
Figure 5.18: The flow field contours of the baseline 400 CPSI.
From Figure 5.19 (b), the effect of the insulation is clearly seen that blocking a few channels with the insulation tends to force more fluid to the smaller monolith chamber due to the increased flow resistance that allows the fluid to redistribute. The flow tends to traverse radially in the upstream direction across the monolith face and then its velocity increases at the insulation region due to flow accumulation at the back of the blocked channels. This effect can be seen in the red spot at the entrance of the small compartment. In addition to the discussed flow separation and circulation upstream and downstream the padding, another flow recirculation takes place downstream the insulation with very small velocities which indicates stagnant flow interactions with the flow leaving the monolith channels.

In the turbulence intensity contour shown in Figure 5.19 (c), the turbulence intensity increases by average of 2% downstream the smaller and the larger monolith chambers due to the presence of the insulation inside the monolith. When the monolith is divided into two chambers, the flow velocity in each chamber is increased and accordingly the turbulence intensity. The pressure drop contour shown in Figure 5.19 (d) suggests that the pressure drop across the 400 CPSI Cleanalytic™ monolith is higher than the baseline 400 CPSI monolith by about 14% due to the flow resistance added due to the presence of the insulation.

5.6.3. Baseline 900 CPSI Monolith

Figure 5.20 shows the flow field contours for the baseline 900 CPSI monolith substrate. In Figure 5.20 (a), the temperature contour behaves in a similar manner in comparison to the 400 CPSI monolith case where the temperature radially towards the walls of the monolith. This behaviour is expected for a steady state simulation because both monoliths are made from the same material with the same conduction resistance. However, the velocity distribution inside the monolith is more uniform due to the increased 900 CPSI monolith resistance as shown in Figure 5.20 (b). When the monolith resistance is higher, the flow is redistributed at the front face of the monolith and then forced through periphery. This is evident from the turbulence intensity contours shown in Figure 5.20 (c) where the turbulence intensity downstream of the monolith is decreased by about 3.5%. This decrease indicates that the local flow velocity downstream of the monolith is lower but more uniform to maintain the same inlet flow conditions.
Figure 5.19: The flow field contours of the Cleanalytic™ 400 CPSI monolith.
The pressure drop across the 900 CPSI monolith is higher than the pressure drop across the 400 CPSI monolith by about 31 % as shown in Figure 5.20 (d). This increase is observed in the upstream direction due to the increased monolith viscous and inertial resistances.

5.6.4. Cleanalytic™ 900 CPSI Monolith

Figure 5.21 shows the flow field contours for the Cleanalytic™ 900 CPSI monolith. In Figure 5.21 (a), the temperature contour is shown the temperature increased in the outer chamber by an average of 4 °C when compared to the baseline 900 CPSI monolith. This effect is discussed further in section 5.8.

The velocity contour shown in Figure 5.21 (b) shows that the velocity is nearly constant inside the monolith. As discussed in chapter 4, the viscous and inertial resistances are higher for the 900 CPSI monolith. For these high resistance values, the added insulation makes the Cleanalytic™ 900 CPSI monolith has the highest resistances. These high resistances allow the approaching flow to redistribute across the inlet face of the monolith.

The turbulence intensity contour shown in Figure 5.21 (c) indicates similar turbulence intensity trends to the ones obtained for the Cleanalytic™ 400 CPSI monolith with lower values downstream of the monolith due to the lower flow velocity. The turbulence intensity is nearly uniform at the exit of the monolith due to the enhanced flow distribution; however, it drops downstream of the insulation region.

Figure 5.21 (d) shows the pressure drop contour for this configuration which shows that the pressure is highest compared to the rest of the cases due to higher viscous and inertial resistances and smaller cross section area. This increase in pressure is up to 33 % higher than the pressure drop across the Cleanalytic™ 400 CPSI monolith.

From the discussed configurations of the substrate, the most optimized design is the Cleanalytic™ 400 CPSI catalytic converter. It showed a superior enhancement of temperature and flow distribution over the other configuration with a small increase in the pressure drop.
Figure 5.20: The flow field contours of the baseline 900 CPSI monolith.
Figure 5.21: The flow field contours of the Cleanalytic™ 900 CPSI monolith.
5.7. Effect of Padding Thickness on Temperature Profiles

Due to the experimental tolerance in adjusting the dimensions of the padding, the effect of different padding thickness on the numerically predicted temperature profiles is investigated. The flow conditions are identical to the ones used in the validation and the padding thickness varied from 2 mm to 4 mm. Figure 5.22 shows the effect of the padding thickness on the temperature profile 5 mm downstream of the monolith. The effect of padding thickness on the numerical solution is insignificant with RMSD of ± 0.23 % between the 2-mm and the 4-mm padding. The same conclusions were drawn for the 900 CPSI monolith and the Cleanalytic™ monoliths. Therefore, it was assumed that effect of the padding thickness on the temperature profile is negligible.

5.8. Effect of Cleanalytic™ on Thermalhydraulic Performance

This section discusses the effect of using the Cleanalytic™ technology on the thermalhydraulic performance of catalytic converters. The effect of the Cleanalytic™ on different monolith cell densities is also investigated.

![Figure 5.22: Effect of padding thickness on the temperature profile.](image-url)
5.8.1. Thermal Performance of the 400 CPSI Monolith

In this study, the thermal performance of the Cleanalytic™ is investigated by examining the monolith temperature and its heat retention capabilities. This subsection studies the thermal performance of the 400 CPSI and 900 CPSI separately.

The Cleanalytic™ technology improved the thermal performance of the 400 CPSI monolith. The temperature profile in the middle of the monolith is shown in Figure 5.23. The temperature profile of the Cleanalytic™ near the periphery (the smaller monolith compartment) is shifted upwards. This shift means that the temperature in this region is higher in comparison to the baseline 400 CPSI monolith. The temperature in this region is higher by average of 13 °C with RMSD 18 %. This increase in temperature occurs for two reasons. First, when adding the insulating material inside the monolith, the thermal resistance is increased which created a thermal barrier that opposed the heat loss to the surroundings. Second, the insulation allowed more flow with a higher heat input to flow through the

![Figure 5.23: The temperature profile in the middle of the monolith. R'' is the monolith radius.](image)

```plaintext
Figure 5.23: The temperature profile in the middle of the monolith. R'' is the monolith radius.
```
periphery which increased its temperature. This improvement indicates more efficient utilization of the heat within the monolith as well as higher heat retention. This improvement can be taken advantage of when the monolith is loaded with the catalyst, the catalyst will be utilized more efficiently due to the higher temperatures at the periphery of the monolith and the conversion efficiency of the pollutants will be improved. This technology can be used to improve the light-off characteristic during the cold start period as the heat distribution is improved such that the monolith will heat up faster. The same trend is observed at the front and the rear regions of the monolith substrate and are shown in Appendix A.

5.8.2. Thermal Performance of the 900 CPSI Monolith

The Cleanalytic™ technology has a positive effect on the thermal performance of the 900 CPSI monolith catalytic converter. This effect is lower in comparison to the 400 monolith catalytic converters. The temperature profile in the middle of the monolith is shown in Figure 5.24. The temperature of the Cleanalytic™ 900 CPSI monolith followed the same trend as the 400 CPSI in which that it is higher in the smaller monolith chamber. However, it is only higher by average of 4 °C and RMSD of 5 %. This smaller increase in temperature is caused only by the added thermal resistance of the insulation.

![Figure 5.24: The temperature profile in the middle of the monolith. R'' is the monolith radius](image-url)
The effect of the increased heat input is not large in this case because the flow through the baseline 900 CPSI monolith has a better flow distribution which does not give enough potential for further improvement in the thermal performance. Another possible factor that can contribute to this behaviour is the thickness of the insulation layer which was set to be around 2 channels wide. For the 900 CPSI monolith, the channel width is smaller than that for the 400 CPSI monolith. This can cause the overall thermal resistance of the insulation to decrease which may allow for higher heat losses and cause lower monolith temperatures. The same trend is observed for the temperature profiles at the front and rear regions of the monolith due to the steady state nature of this study and shown in Appendix A.

5.8.3. Hydraulic Performance

The effect of installing the Cleanalytic™ on the hydraulic performance of the catalytic converter is studied with regards to the flow distribution inside the monolith and the pressure drop across. Each of these factors is discussed separately.

5.8.3.1. Flow distribution and flow uniformity index

The flow distribution inside the monolith is studied using a dimensionless parameter called “flow uniformity index”. This parameter is an indication of the flow velocity variation across the inlet face of the monolith from the average velocity. Equation (5.2) represents the flow uniformity index:

\[ \gamma = 1 - \frac{\sum_{i=1}^{n} [(v - \bar{v})A]}{2|\bar{v}|nA} \]  

where \( \gamma \), \( v \) and \( \bar{v} \) are the flow uniformity index, local velocity and average velocity. This parameter is calculated based on area-weighted method with ideal uniformity index of 1.

The flow uniformity is very crucial for evaluating the hydraulic performance of the catalytic converter as it represents how efficiently the monolith channels are utilized by the flow. The higher the uniformity index, the more efficient the monolith utilization is hence better catalyst utilization and enhanced conversion efficiency. Other advantages are that improvement of the catalyst wear and faster light-off during the cold
start period. Table 5.2 represents the flow uniformity indices of the 400 CPSI and 900 CPSI baseline monolith and the effect of the Cleanalytic™ on the flow distribution.

<table>
<thead>
<tr>
<th>Monolith substrate</th>
<th>Flow uniformity index</th>
</tr>
</thead>
<tbody>
<tr>
<td>400 CPSI baseline</td>
<td>0.79</td>
</tr>
<tr>
<td>400 CPSI Cleanalytic™</td>
<td>0.83</td>
</tr>
<tr>
<td>900 CPSI baseline</td>
<td>0.87</td>
</tr>
<tr>
<td>900 CPSI Cleanalytic™</td>
<td>0.93</td>
</tr>
</tbody>
</table>

The flow distribution inside the catalytic converter is improved when utilizing the Cleanalytic™ technology for both the 400 CPSI and the 900 CPSI monolith. The flow uniformity index for the 400 CPSI baseline monolith is improved by 6 %. When blocking some monolith channels, the resistance of the monolith is increased and as a result, the flow has the opportunity to redistribute at the front face of the monolith. The same behaviour is observed for the Cleanalytic™ 900 CPSI monolith where the flow uniformity index is improved by 7 %. Although the flow uniformity index is higher in the case of the Cleanalytic™ 900 CPSI monolith, its influence on the temperature distribution is smaller as shown in Figure 5.24 above when compared to the 400 CPSI monolith. This is caused because the flow uniformity index is high enough and did not allow for improvement in the thermal part as discussed earlier. This behaviour suggests that the effect of the Cleanalytic™ on the hydraulic performance of the 400 CPSI monolith is larger and this technology is more suitable for this monolith cell density.

5.8.3.2. Pressure drop across the catalytic converter

The pressure drop across the catalytic converters is a key factor that helps evaluating the hydraulic performance such that the higher the pressure drop is, the higher the engine load and hence higher fuel consumption. The pressure drop experiments are held under steady state condition for 400 CPSI and 900 CPSI Cleanalytic™ and baseline monoliths. The flow temperature is kept constant at 177 ºC and the mass flow rate is varied from $2.6 \times 10^{-2}$ kg/s to $6.2 \times 10^{-2}$ kg/s as shown in Figure 5.25.
Figure 5.25: Pressure drop measurements.

Increasing the mass flow rate increases the pressure drop for all cases. The 900 CPSI measurements hold higher pressure drop than the 400 CPSI due to the increased flow resistance namely, viscous and inertial resistances. In addition, utilizing the Cleanalytic™ technology increases the pressure drop due to the smaller cross section area obtained after blocking some channels insulation layer with a blockage percentage of the cross-section area of 4.12%. The pressure drop is predicted using the numerical model and the results are summarized in Table 5.3.

Table 5.3: Pressure drop measurements and predictions.

<table>
<thead>
<tr>
<th>Method</th>
<th>400 CPSI</th>
<th>900 CPSI</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Baseline</td>
<td>Cleanalytic™</td>
</tr>
<tr>
<td>Experimental (kPa)</td>
<td>3</td>
<td>3.43</td>
</tr>
<tr>
<td>Numerical (kPa)</td>
<td>3.425</td>
<td>3.493</td>
</tr>
<tr>
<td>RMSE %</td>
<td>14.1 %</td>
<td>1.8 %</td>
</tr>
</tbody>
</table>

The pressure drop across the monolith for the Cleanalytic™ 400 CPSI monolith substrate is higher by 0.43 kPa which is about 12.6% of the baseline pressure drop. The pressure drop is about 0.59 kPa (15%) higher
for the Cleanalytic™ 900 CPSI. The predictions of the pressure drop showed the same trend in which that the pressure drop across the Cleanalytic™ monolith is always higher than the baseline regardless of the monolith cell density. However, the pressure drop of the baseline monolith substrate is over predicted for 400 CPSI and 900 CPSI substrates. The over prediction is still within a reasonable agreement with the experimental measurements with RMSE of +14.1 % and +15.6 % for 400 CPSI and 900 CPSI monoliths, respectively. It is important to note that the model accurately predicted the pressure drop across the Cleanalytic™ monolith substrates for both cell densities with RMSE of +1.8 % and +2.7 % for the 400 CPSI and 900 CPSI monoliths, respectively. However, the predicted pressure drop difference between the baseline and the Cleanalytic™ is lower than the experimental difference with 0.068 kPa and 0.096 kPa for the 400 CPSI and 900 CPSI monolith substrates, respectively. The pressure drop across the baseline 400 CPSI monolith is lower by 32 % than the baseline 900 CPSI monolith. This pressure drop study indicates that utilizing the Cleanalytic™ technology for the 400 CPSI monolith substrates is significantly more efficient due to the lower pressure drop generated in comparison to the 900 CPSI monolith with high improvements in the thermal performance as discussed earlier. Furthermore, the numerical model showed reasonable agreement with the experimental data. The axial pressure drop at the centerline of the whole simulation domain (including the monolith) is shown in Figure 5.26 for the 400 CPSI baseline and Cleanalytic™ monolith.

![Figure 5.26: The axial pressure across the simulation domain for the 400 CPSI monolith. z is the axial location and L is the length of the solution domain.](image-url)
The pressure builds up inside the inlet diffuser to a peak at the monolith inlet face due to pressure recovery and monolith resistance. The pressure then drops to about 0.5 kPa at the exit face of the monolith. The pressure stays constant at the exit cone because of compressing the flow coming towards the contraction. After the exit cone, the pressure drops to atmospheric pressure. The Cleanalytic™ monolith axial pressure follows the same trend as the baseline but has slightly higher pressure upstream the monolith with higher peak at the monolith face due to the smaller cross section area. Downstream the monolith, the pressure values for both Cleanalytic™ and baseline catalytic converters are identical due to the imposed atmospheric boundary condition.

The pressure drop across the 900 CPSI baseline and Cleanalytic™ catalytic converter followed the same trend represented for the 400 CPSI substrates and shown in Figure 5.27. Downstream of the monolith, the pressure is the same for both Cleanalytic™ and baseline catalytic converters. However, the pressure upstream the monolith is higher for the Cleanalytic™ when compared the baseline with a higher pressure at the monolith inlet face.

![Figure 5.27: The axial pressure across the simulation domain for the 900 CPSI monolith. z is the axial location and L is the length of the solution domain.](image-url)
From the discussion above, The Cleanalytic™ 400 CPSI substrate performed better thermally and hydraulically. Although the pressure drop for this configuration was higher than the baseline configuration, it would be recommended as the Canadian government are more interested in the emissions released more than the fuel economy. The Cleanalytic™ technology showed improvement in the thermal performance for both the 400 CPSI and the 900 CPSI substrate with enhancement in the flow distribution as well. Therefore, this technology can be further optimized using the current numerical model to improve the thermal hydraulic performance of catalytic converters.
Chapter 6 Concluding Remarks

6.1. Conclusion

Studying the thermalhydraulic performance of catalytic converters can be challenging due to limited capabilities of studying the flow behaviour inside the monolith substrate. Therefore, computational fluid dynamics models are utilized to enhance the understanding of the performance of the catalytic converters. However, these models require intensive calibration and validation to obtain reliable and realistic results.

This study utilized intensive experimental work to validate a CFD model used to study the performance of the catalytic converters. In addition, this study investigated the effect of the installing the new catalytic converter technology (Cleanalytic™) on the thermalhydraulic performance of baseline catalytic converters. Unlike other studies that are established in the literature which only uses velocity measurements
downstream the monolith for validation, the CFD model established in this study is validated using temperature, velocity and turbulence intensity profiles downstream the monolith. The study also investigated monolith cell densities of 400 CPSI and 900 CPSI. The main conclusions derived from this study are presented below for the different monolith substrates investigated. The validation and the performance investigation are done under steady state hot air flow with inlet mass flow rate and temperature of 0.0518 kg/s and 177 °C at Reynolds number equal to 43,000. Pressure drop measurements across the catalytic converters are also considered for hydraulic performance investigation.

6.1.1. 400 CPSI monolith substrate

1. The CFD model accurately predicted the temperature profile downstream both baseline and Cleanalytic™ catalytic converters with RMSE of 2.7 % and 2.5 % for baseline and Cleanalytic™, respectively.
2. The CFD model accurately predicted the velocity profile downstream both baseline and Cleanalytic™ catalytic converters with RMSE of 8.2 % and 5.7 % for baseline and Cleanalytic™, respectively.
3. The CFD model accurately predicted the turbulence intensity profile downstream both baseline and Cleanalytic™ catalytic converters with RMSE of 10.2 % and 7.4 % for baseline and Cleanalytic™, respectively.
4. The thermalhydraulic performance of the catalytic converter is improved when utilizing the Cleanalytic™ technology as the temperature inside the monolith is increased by 18 % in the smaller monolith compartment due to the enhancement of the flow uniformity index inside the catalytic converter from 0.79 to 0.83 (5 %).
5. Although the implementation of the Cleanalytic™ technology involves blocking few channels which leads to higher pressure drop, the pressure drop values obtained from experimentation and CFD modelling are insignificant and are compensated with the significant improvement of the thermal performance.
6.1.2. 900 CPSI monolith substrate

1. The CFD model accurately predicted the temperature profile downstream both baseline and Cleanalytic™ catalytic converters with RMSE of 3.7% and 3.2% for baseline and Cleanalytic™, respectively.

2. The CFD model accurately predicted the velocity profile downstream both baseline and Cleanalytic™ catalytic converters with RMSE of 5.2% and 4% for baseline and Cleanalytic™, respectively.

3. The CFD model accurately predicted the turbulence intensity profile downstream both baseline and Cleanalytic™ catalytic converters with RMSE of 6.9% and 7.2% for baseline and Cleanalytic™, respectively.

4. Using the 900 CPSI monolith substrate increased the temperature of the periphery region of the monolith by 5% when compared to the 400 CPSI monolith due to the higher flow uniformity index (0.87) obtained from the higher flow resistance provided by the 900 CPSI monolith.

5. Although the Cleanalytic™ improved the flow distribution inside the monolith, the temperature inside the smaller monolith compartment increased only by 5% which indicates a threshold beyond which the flow uniformity index improvement does not affect the temperature distribution.

6. The pressure drop accompanied by the 900 CPSI monolith was significantly higher than the pressure drop obtained from the 400 CPSI monolith (up to 33%) due to the significant increase in the flow resistance which implies that using the Cleanalytic™ 900 CPSI monolith would bring lower engine performance due to the higher fuel consumption that is expected to take place.

7. The catalytic converter design that showed the most promising results in this study is the Cleanalytic™ 400 CPSI converter. As the emission regulations became more strict, lower emissions levels are favourable over fuel economy as the pressure drop for this configuration was higher than the baseline converter. However, the improvement in both the flow distribution and the thermal performance can enhance allow for a faster light-off and less production of harmful emissions.
6.2. Recommendations

The following remarks suggest potential future work that could be done to improve the understanding of the performance and operation of the catalytic converters:

1. Applying real engine tests and implementing intensive experimental work on the thermal and chemical interactions inside the Cleanalytic™ catalytic converter using non-intrusive instrumentation.

2. Including chemical kinetics in the current model to investigate the effect of the chemical and thermal interactions on the flow inside the Cleanalytic™ catalytic converters and examine the emissions level produced.

3. Expand the current model to study the unsteady fluid flow through the Cleanalytic™ catalytic converters in order to improve the performance during the cold start period.
Chapter 7 References


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Appendix A

A.1 Cleanalytic™ 400 CPSI Inlet Pipe Temperature and Velocity Development Profiles

Figure A.1: Temperature development in the inlet pipe for the 400 CPSI Cleanalytic™ monolith substrate

Figure A.2: Velocity development in the inlet pipe for the 400 CPSI Cleanalytic™ monolith substrate
A.2 Baseline 900 CPSI Inlet Pipe Temperature and Velocity Development Profiles

Figure A.3: Temperature development in the inlet pipe for the 900 CPSI Baseline monolith substrate

Figure A.4: Velocity development in the inlet pipe for the 900 CPSI Baseline monolith substrate
A.3 Cleanalytic™ 900 CPSI Inlet Pipe Temperature and Velocity Development Profiles

Figure A.5: Temperature development in the inlet pipe for the 400 CPSI Cleanalytic™ monolith substrate

Figure A.6: Temperature development in the inlet pipe for the 400 CPSI Cleanalytic™ monolith substrate
A.4 The 400 CPSI Monolith Inside Temperature Profiles

Figure A.7: 400 CPSI monolith substrate temperature profiles at the front for baseline and Cleanalytic™

Figure A.8: 400 CPSI monolith substrate temperature profiles at the rear for baseline and Cleanalytic™
A.5 The 900 CPSI Monolith Inside Temperature Profiles

Figure A.9: 900 CPSI monolith substrate temperature profiles at the front for baseline and Cleanalytic™

Figure A.10: 900 CPSI monolith substrate temperature profiles at the rear for baseline and Cleanalytic™
## Appendix B

### B.1 Electric Heater Specifications

<table>
<thead>
<tr>
<th>Attribute</th>
<th>Unit</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Voltage</td>
<td>V~</td>
<td>3 x 480</td>
</tr>
<tr>
<td>Power</td>
<td>W</td>
<td>11000</td>
</tr>
<tr>
<td>Max. air outlet temperature</td>
<td>°C</td>
<td>650</td>
</tr>
<tr>
<td>Max. air inlet temperature</td>
<td>°C</td>
<td>65</td>
</tr>
<tr>
<td>Max. ambient temperature</td>
<td>°C</td>
<td>65</td>
</tr>
<tr>
<td>Relative humidity (non condensing)</td>
<td>%</td>
<td>5 – 95</td>
</tr>
<tr>
<td>Max. inlet pressure</td>
<td>kPa</td>
<td>100</td>
</tr>
<tr>
<td>Heating pipe diameter $\phi$</td>
<td>mm</td>
<td>92</td>
</tr>
<tr>
<td>Size ($L \times W \times H$)</td>
<td>mm</td>
<td>363 $\times$ 114 $\times$ 138</td>
</tr>
<tr>
<td>Weight</td>
<td>kg</td>
<td>3.65</td>
</tr>
<tr>
<td>Conformity mark</td>
<td></td>
<td>CE</td>
</tr>
<tr>
<td>Approval mark</td>
<td></td>
<td>¥</td>
</tr>
<tr>
<td>Protection class I</td>
<td></td>
<td>IP 1</td>
</tr>
</tbody>
</table>

*Figure B.1: Leister LHS 61L 11kW specifications*
Appendix C

C.1 Turbulent Flow Calculations

The flow inside the inlet pipe is considered to be turbulent based on the supplied mass flow rate and free stream temperature. The calculations below represent the Reynolds number in this region based on inlet diameter.

\[ \dot{m} = \rho VA \quad (C.1) \]

The mass flow rate is \( 5.18 \times 10^{-2} \) kg/s, the density of air at 177 °C and atmospheric pressure is 0.784 kg/m\(^3\) and the cross-section area for the inlet pipe is \( 2.03 \times 10^{-3} \) m\(^2\). This yield average flow velocity of 32.5 m/s.

\[ Re = \frac{\rho AV}{\mu} \quad (C.2) \]

The pipe diameter is 2 inches (50.8 mm) and the dynamic viscosity 2.945 \( \times 10^{-6} \) Pa.s. Substituting the velocity obtained from Equation C.1 to Equation C.2, Reynolds number is approximately 43,000 which indicates a turbulent flow in this pipe.

C.2 Laminar Flow Calculations

The mass flow rate going through each channel for both the 400 CPSI and 900 CPSI substrate assuming uniformly utilized substrate was calculated. For the 400 CPSI substrate the number of channels are equal to the cell density multiplied by the cross-section area. For a diameter of 3 inch (76 mm), the number of channels is 2800 cells. If the total mass flow rate is \( 5.18 \times 10^{-2} \) kg/s, the mass flow rate passing through a single channel will be about \( 1.8 \times 10^{-5} \) kg/s. Using Equations C.1 and C.2 and a hydraulic diameter of 1 mm, Reynolds number will be about 600. The same procedure is applied for the 900 CPSI substrate and Reynolds number is 350. The values of Reynolds number obtained indicate that the flow in the substrate region is laminar.