Analytical and Numerical Study on the Fast Refill of
Compressed Natural Gas with Heat Removal

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Abstract

Heavy-duty vehicles powered by compressed natural gas (CNG) store the fuel in large onboard cylinders. Fast fill of depleted CNG cylinders is a common refueling method because it achieves refueling time comparable to liquid fuels. However, under-filling of CNG cylinders occurs due to the recompression work of CNG in the cylinder that heats the fuel. The heated fuel has a lower density at the rated pressure, and thus less mass of CNG can be stored than if it was at ambient temperature. While there are many previous works that have modeled or measured the pressure, temperature rise and the mass filled of the gas during filling, very few of them have investigated potential solutions to improve fill efficiency. Since heat generation during fast fill is inevitable, concepts that can actively or passively remove the generated heat during the fill process are required to achieve the needed improvements in fill efficiency.

In this study, analytical and numerical models of the filling process of CNG into a Type-III cylinder with and without heat removal are developed. In the analytical study, mass and energy conservation equations are coupled with an ideal-gas equation of state and orifice flow equations to predict the heat generation rates during fast fill. The influence of heat removal via a cooling coil inserted into the cylinder on the dispensed mass and fill time is quantified. The analytical study is compared to numerical simulations employing a two-dimensional axisymmetric computational fluid dynamics (CFD) model for unsteady, compressible turbulent flow without cooling, with active cooling and with pre-chilling. Dynamic average temperature, pressure and mass curves as well as the local temperature distribution in the cylinder are obtained at different time instances during the fill. The effect of the location of the heat removal coils is also investigated. The results illustrate the benefit of heat removal from the cylinder as a means of improving the fast fill
efficiency, which can help increase the penetration of CNG into the Canadian transportation sector and reduce greenhouse gas emissions.
Preface

The work outlined in this thesis was conducted by Guoyu, Zhang under the supervision of Dr. Sunny Ri Li and Dr. Joshua Brinkerhoff. It was supported by Agility Fuel Solutions and NSERC (Natural Sciences and Engineering Research Council of Canada). All the presented research work was finished in the Thermal Management and Multiphase Flows Laboratory and the Okanagan Computational Fluid Dynamics Laboratory in the School of Engineering at the University of British Columbia (Okanagan campus). Portions of this thesis have been published in journals as well as conference proceedings.


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My colleagues at Dr. Li and Dr. Brinkerhoff’s labs have provided me invaluable experience and insight into my research. I feel very grateful to them and the other friends of mine at UBC Okanagan who brought lots of convenience into my life and study.
Dedication

To my parents for your unconditional love and support in every day of my life.
Chapter 1: Introduction of CNG/NGVs

1.1 Natural gas as a necessary fuel

The necessity of developing and utilizing alternative fuels, natural gas and products of its processing in particular, is due to two interrelated basic causes: the rapid depletion of oil reserves on the planet and deterioration of the environmental situation in the whole world. The oil reserves in the Earth’s interior are finite while with the development of the modern society oil productions and transport costs become higher year after year. It is estimated that at the current rates of increasing in production and use, the proven oil reserves will totally deplete in between forty to fifty years, and in some countries, depletion of reserves is predicted to be even sooner according to OPEC data [1] (Fig.1.1).

Fig 1.1 Projected depletion of proven oil and gas reserves in basis producing countries: I) Algeria;
II) Indonesia; III) Uzbekistan; IV) Holland; V) Canada; VI) Iraq; VII) Saudi Arabia; VIII) Iran; IX) Venezuela; X) Mexico; XI) Russia; XII) China; XIII) Norway; XIV) USA; XV) England [1].

Up to the end of 2010, Almost 1.015 billion automobiles were operating (mostly fueled with gasoline and diesel fuel) in the world with an average annual growth rate of 2.6-3.1%. Operation of this automobile fleet deteriorates the environment primarily because of its emission of exhaust gases into the atmosphere. An alternative to using gasoline and diesel fuel is the use of natural gas. Natural gas is a clean burning fuel that emits far fewer emissions than gasoline or diesel fuel. The economic loss (in pound sterling per km) is 0.01 for use of gasoline, 0.026 for diesel fuel, and less than 0.002 for natural gas according to the new findings of English experts. Therefore, switching to natural gas especially in the transportation section is always at the heart of recent energy discussions.

1.2 Physiochemical properties of CNG vs gasoline and diesel

Physiochemical properties of natural gas are important facts to know in order to better compare the differences between natural gas and gasoline. The natural gas used in NGVs is the same as that used in domestic sector for cooking and heating, which typically consists of about 90% methane, less ethane, propane and even less hydrocarbons, nitrogen, carbon dioxide and water. Table 1.1 [2] shows the comparison between the physiochemical properties of CNG to that of gasoline and diesel.
<table>
<thead>
<tr>
<th>Properties</th>
<th>CNG</th>
<th>Gasoline</th>
<th>Diesel</th>
</tr>
</thead>
<tbody>
<tr>
<td>Octane/cetane number</td>
<td>120–130</td>
<td>85–95</td>
<td>45–55</td>
</tr>
<tr>
<td>Molar mass (kg/mol)</td>
<td>17.3</td>
<td>109</td>
<td>204</td>
</tr>
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<td>Stoichiometric (A/F)ₙ mass</td>
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<td>14.7</td>
<td>14.6</td>
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<td>1.42</td>
<td>1.46</td>
</tr>
<tr>
<td>L.H.V. (MJ/kg)</td>
<td>47.5</td>
<td>43.5</td>
<td>42.7</td>
</tr>
<tr>
<td>L.H.V. of stoichiometric mixture (MJ/kg)</td>
<td>2.62</td>
<td>2.85</td>
<td>2.75</td>
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<td>Combustion Energy (MJ/m³)</td>
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<td>42.7</td>
<td>36</td>
</tr>
<tr>
<td>Flammability limit in air (vol% in air)</td>
<td>4.3–15.2</td>
<td>1.4–7.6</td>
<td>1–6</td>
</tr>
<tr>
<td>Flame propagation speed (m/s)</td>
<td>0.41</td>
<td>0.5</td>
<td>–</td>
</tr>
<tr>
<td>Adiabatic Flame Temp. (°C)</td>
<td>1890</td>
<td>2150</td>
<td>2054</td>
</tr>
<tr>
<td>Auto-ignition Temp. (°C)</td>
<td>540</td>
<td>258</td>
<td>316</td>
</tr>
<tr>
<td>Wobbe Index (MJ/m³)</td>
<td>51–58</td>
<td>–</td>
<td>–</td>
</tr>
</tbody>
</table>

Table 1.1 Physiochemical properties of CNG vs gasoline and diesel [2].

1.3 Emission benefits of NGVs

The emission performance of alternative fuels is a vital area and one facing a wide range of analytical challenges. As the combustion of conventional fuel (i.e., gasoline and diesel) results in harmful emissions that impose a severe threat on the survival of life on the earth, nowadays natural gas as transportation fuel has become the subject of interest all around the world because the production from its burning contains significantly less pollutants than gasoline. From a “well-to-wheels” point of view, CNG is the cleanest burning transportation fuel available on the market today [3]. CNG burns cleaner than petroleum based products because of its lower carbon content, thus emissions from properly functioning NGVs are generally considered to be much lower than emissions from gasoline fuelled vehicles [4]. A case is that in Delhi (Indian capital and the 2nd most densely populated city around the world), the government switched over the entire on land public transportation to CNG fuelled vehicles from diesel and gasoline after the verdict of Indian Supreme Court at the beginning of 2002. As a result, there is a significant reduction in SO₂ (22%),
CO (10%), NO\textsubscript{x} (6%) and total suspended particles (14%) shown from the comparison between the levels of environment pollutants in pre and post years of NGVs implementation [5]. Compared to gasoline powered vehicles, there would be a reduction of 65% CO emission and 21% CO\textsubscript{2} emission by utilizing the 3\textsuperscript{rd} generation conversion kits in CNG retrofitted vehicles [6]. Reducing non-methane hydro carbon (NMHC) emissions could be another potential benefit of switching over to CNG from gasoline or diesel. Since methane, which is the biggest portion of CNG components, has no carbon to carbon molecular bonds, the CNG combustion brings a significantly lower probability of benzene emission, which by other way means a reduction in the formation of soot and carcinogenic polycyclic aromatic hydrocarbons. CNG has a higher hydrogen/carbon ratio and comprises less aromatic content, both of which are beneficial for the reduction of volatile organic compounds (VOCs) species in case of CNG fuelled vehicle [2].

1.4 Incentives of NGVs

Governments of different countries have introduced lots of policies to provide incentives of NGVs both to the infrastructure and the consumers. The principal factors that motivate governments to promote the adoption of NGVs include availability of natural gas resources and existing pipeline and delivery infrastructure, reduction of dependency on imported oil and environmental benefits of reducing local air pollution.

In China, the environmental concerns and energy security are the primary reasons for moving towards a larger NGV market. China’s growing demand for imported gasoline was evidenced when it surpassed Japan in 2003 to become the second largest crude oil consumer in the world. As a result, the Chinese government felt obliged to played a more important role in promoting CNG and liquefied petroleum gas (LPG) fuels in public transit through various R&D programs, loan
programs and direct investments. Similarly, strong government promotion of CNG to replace gasoline and diesel has stimulated rapid growth of NGV use in Latin American countries, primarily Brazil and Argentina. Recently, these two countries together account for more than half of the world’s total NGVs.

Things that has happened in New Zealand during the past 40 years turns out to be amazingly different and unique. By the mid-1980s there used to be a very successful NGV market as a result of government promotion, incentive programs (such as a 100% loan), and targets to incent the conversion to NGVs. However, after policy and political changes prompted the government to rescind favorable CNG loan conditions in 1985, the NGV market eventually disappeared, as shown in Fig 1.2. But overall, due to Yeh’s study [7], governments of different countries are still imposing incentives both to the consumers (fuel price ratio, payback period) and for improving alternative fuel infrastructure (vehicle-to-refueling-station index, VRI).

![Number of natural gas vehicles in case-study countries][1]

Fig 1.2 Number of natural gas vehicles in case-study countries [7].
1.5 NGV safety

Safety is always first concern for any application. The physical properties of CNG offer some safety benefits over diesel and gasoline. Physical properties of CNG which makes it an inherently safer than diesel or gasoline are as follows [2,8]:

(1) CNG cylinders are designed and fabricated to be much stronger than gasoline fuel tanks to withstand its corresponding high pressures, with a safety factor which is often greater than 1.5.

(2) Natural gas is non-toxic, non-corrosive and will not contaminate ground water.

(3) Comparing to gasoline/diesel fuels CNG has a narrower flammability range (4.3% to 15.2% by volume in air).

(4) CNG has a higher auto-ignition temperature of 540 °C compared to 258 °C of gasoline and 316 °C of diesel.

(5) Releasing aldehydes or other air toxins could be a concern for gasoline and some other alternative fuels, but natural gas combustion produces no significant amount of those harmful particles.

(6) Natural gas is lighter than air so once accidental leakage happens its lower density at atmosphere pressure will make it rise and disperse into the air rapidly, while gasoline pools on the ground and creates a fire hazard.

1.6 Motivation and thesis outline

This thesis studies the fast refuelling process of CNG cylinders without and with different types of heat removal by means of analytical and numerical models. The refuelling of a gasoline-
powered vehicle sets the standard for ease, complexity, safety and duration of fuelling. In order to gain consumer acceptability, refuelling of a natural gas powered vehicle should meet or exceed gasoline vehicles. People have been used to refuelling their gasoline tanks within a few minutes. Similar amount of time is expected for refuelling natural gas vehicles. However, fast refuelling of natural gas causes its temperature to increase, which results in less amount of gas filled. The fill efficiency is defined as the ratio of the actual filled mass to the capacity at the rated pressure and ambient temperature. How to achieve high-efficiency fast refuelling has become an engineering topic for suppliers of natural gas fuel systems including Agility Fuel Solutions.

A method will be developed to allow 10% more natural gas to be injected during a fast fill process. The method is based on active heat rejection or pre-chilling, which is able to effectively remove the heat of gas recompression so that the fast fill process produces a smaller temperature increase upon reaching the cylinder’s service pressure. This method will be transferred to the industrial partner, Agility Fuel Solutions to integrate into Agility’s natural gas fuel systems. The new fuel systems will increase the driving range of natural gas powered vehicles. As a result, the penetration of natural gas into the transportation sector is expected to increase, bringing significant energy and environment benefits to Canadian transportation sector, which is the country’s second largest energy consumer and the highest source of greenhouse gas emissions.

The thesis is structured as follows: Chapter 2 includes a review of CNG/hydrogen refuelling literatures. In chapter 3, an analytical model incorporating real and ideal gas effects is developed to predict the transient thermal-fluid behaviour of natural gas during the fill with and without cooling. In chapter 4, 5 and 6, a two-dimensional axisymmetric CFD model incorporating real gas effects is developed to predict the transient thermal-fluid behaviours of natural gas for the filling process without cooling, with active cooling and with pre-chilling, respectively. A summary of
conclusions is made in chapter 7 to find the optimal cooling scenario which can provide the greatest filling efficiency increase.
Chapter 2: Review of CNG/Hydrogen Refuelling Literatures

For the past few years, natural gas has played a prominent role in energy discussions around the world [9, 10]. One reason is the emergence of abundant supplies of natural gas following the development of unconventional extraction methods. For example, the development of shale gas in USA has increased its production from 456 billion scf per year to 9198 billion scf per year from 2000 to 2012 [11]. Another driver is the lower carbon emissions of natural gas relative to other fossil fuels, which has important implications for the transportation section that is responsible for 20% of the global carbon dioxide emissions [12]. Given the increasing energy demand and high greenhouse gas (GHG) emissions associated with conventional fossil fuels, Yeh [7] concluded that shifting the transportation sector to natural gas can significantly reduce GHG emissions.

Due to the low volumetric energy density of natural gas relative to liquid fuels, transportation systems typically store fuel either as a low-temperature liquefied natural gas (LNG) or a high-pressure compressed natural gas (CNG), of which CNG currently has higher market share [13]. There are two kinds of fill methods for CNG: time fill and fast fill. Time fill dispensing is slower, but allows for the compression to occur at closer to isothermal conditions, which leads to fuller tanks. For most public stations and for fleets requiring quick refuelling, fast fill is required. As found by Kountz [14,15], underfilling of the cylinder is unavoidable during fast fill because of the heat generated during re-compression of CNG in the cylinder. During the fill process, high pressure CNG flows through the dispenser throttling device and enters the cylinder with reduced temperature because of the Joule-Thomson effect. The filled natural gas is then gradually heated via recompression by the continuously incoming gas, stopping when the internal pressure reaches the allowed cylinder pressure. Due to the recompression work, the temperature at the end of fast
fill is typically about 50ºF above the ambient temperature [14]. As a result, the charged mass of CNG is less than the rated storage capacity of the cylinder, and as the filled gas cools to ambient temperature, its pressure will decrease below the rated pressure. The fill efficiency—defined as the ratio of the actual filled mass to the capacity at the rated pressure and ambient temperature—is used to evaluate CNG filling. Fast fill of CNG cylinders at 20°C ambient temperature typically achieves a fill efficiency of 80% [15].

Fill efficiency of the fast fill process depends on several factors, including the CNG cylinder type and material, the CNG fill station pressure, and the transient heat transfer and gas transport inside the cylinder. Four types of CNG cylinders are commonly used for natural gas vehicles: Type-I cylinders are entirely metal. Type-II cylinders have a metal liner and hoop wrapped composite reinforcement. Type-III cylinders consist of a metal liner and full wrapped composite reinforcement. Type-IV cylinders have a non-metallic liner and a fully wrapped composite reinforcement [16]. The different materials have varying thermal-physical properties, particularly thermal conductivity, density and specific heat, which affect the heat transfer from the gas to the surroundings during the fill process. Diggins [17] and Newhouse et al. [18] compared the fill efficiency of different cylinder types, and found that metal cylinders have higher fill efficiency than all-composite cylinders due to the better heat absorption and conduction of the metal wall.

Many studies have been conducted to investigate the transient thermal behaviour during fast fill. A brief review about the previous analytical, numerical and experimental studies on the CNG/hydrogen fast filling process is as following.
2.1 Analytical studies

There have been a lot previous studies that focused on building analytical models of the filling process of compressed natural gas or hydrogen. In order to quantify the cylinder undercharging phenomena which occurs during rapid (< 5 min) refueling, Kountz [14] in his early study presented an analytical model and solution methodology which considered the effects of heat transfer from the cylinder gas to its constraining walls and ambient. The result shows that due to the recompression work, the temperature at the end of fast fill is typically about 50 °F above the ambient temperature, as shown in Fig 2.1 [14]. As a result, the charged mass of CNG is less than the rated storage capacity of the cylinder, and as the filled gas cools to ambient temperature, its pressure will decrease below the rated pressure. The fill efficiency defined as the ratio of the actual filled mass to the capacity at the rated pressure and ambient temperature is used to evaluate CNG filling. Fast fill of CNG cylinders at 20 °C ambient temperature typically achieves a fill efficiency of 80%. Usually, the final fill step is to over-pressurize the cylinder; for a Type-IV cylinder rated at 3600 psi, over-pressurization may exceed 4100 psi. “One opportunity, to alleviate the need for creating and storing such high pressures in the fuelling station, lies in the cooling of the supply gas, if a practical and cost effective way could be developed” [14]. For example, the required charged pressure can be reduced to about 3900 psi by cooling the supply gas to 60 °F to achieve a fully charged cylinder status. Future research is recommended in three areas associated with the fast refuelling topic. Firstly, further model development is needed to take finite supply reservoirs into consideration, in a commonly used cascade group of three, which might be designed and controlled during the fast refuelling operation to reduce the temperature rise in the NGV cylinder. Secondly, experimental efforts should be proposed to support the model development. Dynamic measurement of the mass entering the cylinder is needed to validate a proper model of gas flow
rate profile. Experiments need to be conducted with the supply reservoir ambient at lower temperatures, relative to a cylinder located in a lab environment, which can simulate the theoretically large supply gas cooling effect. Lastly, research and design studies are recommended to determine practical ways of cooling and storing the gas supply in a refuelling station. [14]

Fig 2.1 Average temperature in the cylinder during a 3000 psi refilling [14]

Khamforoush et al. [19] simulated the compressing and fast filling process in CNG stations with a FORTRAN based computer program. To model the compression process of real natural gas, the polytropic compression work of a three-stage compressor was considered. They simulated the fast refuelling process for a non-adiabatic cylinder based on mass conservation and first law of thermodynamics. Comparison was made between the experimental data obtained from an operating compressed natural gas station in Iran and the fast refuelling model and it showed a good agreement.

Farzaneh-Gord et at. [20] investigated an analytical model to study fast filling process of natural gas vehicle’s cylinder. This model has been applied for a single reservoir tank. They have derived a thermodynamic properties table for the case of ideal gas, which could be solved analytically. In
their results, the temperature rise during refuelling is estimated to be about 40 K when using real gas properties and more than 80 K when using ideal gas properties, with a corresponding effect on the fill efficiency. Therefore, the ideal gas assumption is not valid for natural gas filling process. Their results also indicated that ambient temperature has big effect on not only the final conditions in NGV cylinders but also the whole filling process.

![Graph showing effect of initial temperature on in-cylinder temperature rise](image.png)

**Fig 2.2** Effect of initial (ambient) temperature on in-cylinder temperature rise [20]

At a CNG filling station, compressed natural gas must be stored in a storage system in order to make the utilization of the station more efficient. There are two kinds of natural gas storage namely buffer and cascade storage systems. In buffer storage, only single high-pressure reservoirs are used to store CNG. However, the cascade storage system is usually divided into three reservoirs, generally termed low, medium, and high-pressure reservoirs. The pressures within these three reservoirs will have a big influence on the performance of a CNG fuelling station and a fast refuelling process of natural gas vehicle’s cylinder. A theoretical analysis based on the first and
the second law of thermodynamics, conservation of mass and ideal gas assumptions was developed by Farzaneh-Gord et al. to study the effects of the reservoirs temperatures and pressures on the performance of the CNG station [21]. The results indicate that no matter how the pressure within the filling station reservoirs is changed, the fill efficiency will almost remain constant; but as the reservoir temperature decreases, the fill efficiency will go up. The non-dimensional entropy generation and filling time profiles have an opposite trend. As entropy generation decreases, the filling time increases. In thermodynamic point of view, the optimized non-dimensional low and medium pressure-reservoir pressures are calculated to be 0.24 and 0.58, respectively.

Another theoretical analysis has been developed by the same group [22] to study the effects of reservoir type on performance of CNG filling stations and filling process. As the same final NGV fuel cylinder pressure for both storage systems is considered, from their conclusions we know that that each storage type has advantages over the other. The best configuration should be selected by balancing these advantages.

2.2 Numerical studies

Previous researchers have also paid lots of attention to study the state of charge (SOC) during hydrogen fast refuelling process. The final mass that can be filled is always the thing that will be focused the most on. However, identifying the most important factors and contribution of them to the final mass filled is still an open issue. The contributing factors are multiple, of which, the most important factors can be found out by thermodynamic analysis. The mass filling rate, the initial pressure in the cylinder and the inlet temperature of hydrogen have been confirmed to be the most important factors influencing the final mass filled from a computational fluid dynamic model established by Wang et al. [23]. The results show that there are linear or inverse proportional
relationships between the final mass and the above three factors. From their results a formula for the final mass with diverse filling conditions could be figured out, which can provide guidelines for the later investigations on the fill efficiency.

Another computational fluid dynamic (CFD) model for hydrogen refilling process has developed by Dicken and Merida [24] for predicting the distribution of in-cylinder gas temperature by discretizing the cylinder spatially. The model considered real gas effects, compressible unsteady viscous flow, heat transfer from gas to the cylinder walls and heat conduction through the cylinder walls to the ambient. By comparison with a set of experimental fast fills of a compressed gas cylinder instrumented with 63 thermocouples distributed within the cylinder, the model was validated to provide an accurate estimate of the in-cylinder gas temperature distribution. The validated model also helps to identify the best locations for the onboard temperature sensor such that local temperature best represents the mean gas temperature.

Navid [25] also investigated flow and heat transfer in natural gas vehicle’s onboard cylinder during filling. By using the commercial software Fluent which employs the finite-volume method to discretise the compressible form of the mass, momentum, and energy conservation equations, an axisymmetric computational model for unsteady, compressible turbulent flow has been built for predicting the temperature and pressure change during the refill. The working fluid in the CFD model consists of pure methane with real gas properties determined using the Redlich-Kwong equation of state. The k-ε turbulence model is applied with modified coefficients \( C_{1\varepsilon} = 1.52, C_{2\varepsilon} = 1.92, C_{\mu} = 0.09 \). The computation results have been compared with previous measured values and show good agreement. The results primarily indicate that the maximum temperature rise is about 35 K. Secondly, most of the heat dissipated from the in-cylinder gas is stored in the cylinder wall during the fill and the heat transfer to the ambient is negligible.
The refuelling process of a NGV fuel tank should be reasonably short but must be designed to avoid too high of temperature inside the tank. However, it has been found [26] that the shorter the fill would be, the higher the maximum average gas temperature in the tank climbs. For safety issues an upper temperature limit has been included in the requirements for refillable hydrogen tanks (ISO 15869) which sets a limit for any fill optimization. Therefore, it’s very crucial to understand the thermal behaviours during a tank fill to stay within the safety margins. Heitsch [26] described the fast filling process of hydrogen tanks by simulations based on the commercial CFD code CFX. The major result from these simulations is that the local temperature distribution, the maximum average gas temperature rise and the velocity distribution inside the cylinder strongly depends on the materials of the liner and outer thermal insulation.

There are some other researches investigating the maximum gas temperature, which has a strict upper limit, within the cylinder during the hydrogen refuelling. Previous researchers have studied different filling strategies in terms of pressure and temperature of the gas injected into the cylinder and their effects on key parameters like maximum temperature, energy cooling demand, and fill efficiency by numerical models. It has been proved [27] that pre-cooling of the gas is very beneficial for improving fill efficiency and decreasing the maximum gas temperature but not necessary for the whole duration of the filling. Relevant energy savings can be achieved with pre-cooling only over a fraction of the time. The most convenient and cost-effective filling strategy was found to be with this scenario: pre-cooling on the inlet gas in the second half of the refuelling and a linear injecting pressure, a 60% reduction of the cooling energy requirement was achieved as compared pre-cooling for the whole filling.

Suryan et al. [28] reported the findings of the relationship between real gas models, inlet and initial conditions, and the maximum gas temperature by a three-dimensional numerical simulation of
hydrogen tank filling process. Comparison has been made with different real gas models in their research, which shows good agreement as shown in Fig 2.3. Inlet and initial temperature and pressure of the gas was varied to study the effect on the increase in temperature of the gas during filling while the cylinder liner and outer insulation were fixed. The key parameter, the maximum gas temperature did not exceed the 85 K prescribed safety limit while this permissible temperature was exceeded when they increase the initial gas temperature along with ambient temperature. As a vital conclusion, a 40 second fill is not to be recommended with the present material combination of aluminum and CFRP for liner and laminate.

Fig 2.3 Mean gas temperature with different gas models [28]. RKEoS: Redlich-Kwong equation of state; SRKEoS: Soave-Redlich-Kwong equation of state; ARKEoS: Aungier-Redlich-Kwong equation of state; PREoS: Peng-Robinson equation of state; IGEoS: Ideal-gas equation of state; Expt: experimental result.
2.3 Experimental studies

Experiments were conducted by Liu et al. [29] to study the thermal behaviors such as temperature rise and distribution inside 35 MPa, 150 L hydrogen storage cylinders during its refuelling. They varied the main factors affecting the temperature rise in the fast fill process such as the mass fill rate and initial pressure in the cylinder. Some important conclusions have been reported from the experimental results, like the mass fill rate remains constant when the ratio of the pressure in the tanks to the cylinder is greater than 1.7 due to flow choking, while as time goes by the mass fill rate decreases when the ratio becomes lower than 1.7(Fig 4); the maximum temperature will climb to a larger value with a lower initial pressure in the cylinder or a higher mass filling rate; the temperature inside the cylinder increases nonlinearly during the filling process and the maximum value of temperature at the interface of the cylinder exists in the caudal region.

Fig 2.4 Pressure in the cylinder and storage tank during refueling [29]
In order to achieve a desired time for the fill process of NGVs which, is a comparable time to a gasoline fill, a rapid charging system was developed by Shipley [8] using a three-stage high pressure compression system. A test manifold was built to better help in determining the characteristics of CNG during the filling process. “The test rig, which consists of a manifold with sensors (thermocouple, pressure transducer, and a flow meter with signal conditioner) and an NGV fuel storage cylinder with a thermos-couple/thermo-well setup, measures the exact time for the fast fill to be executed, temperature, pressure, and flow rate of natural gas” [13]. The information collected by the test manifold indicated that the filling process is affected by ambient temperature change in many aspects. It also concluded that the underfilling phenomenon exists in the test cylinder every time it was rapidly recharged. Shipley’s study does not intend to invent a new method of guaranteeing a 100% fill level to an NGV, but to provide a system to analyze any particular fast fill compressor station that is already online which may be able to aid in future NGV refueling station technology.

Zheng et al. [30] performed a series of hydrogen refuelling experiments within a 70 MPa, 74 L, Type-III cylinder to study the thermal behaviors. They found that the maximum gas temperature observed during the refueling process can be significantly reduced during refuelling by pre-cooling systems. The gas in the caudal region climbs to the highest temperature, whereas the region below the inlet achieved the minimum. The maximum temperature in the solid region appeared at the aft dome junctions of the cylinder. For linear pressure-rise with same refueling time, the final temperature decreases almost linearly with the increasing of initial pressure and the decreasing of the ambient temperature.
2.4 Research Objectives

While there are many previous works that have measured and modeled the time required, the temperature rise and the mass filled of the gas during filling, little research effort has been reported about potential solutions to improve fill efficiency that act on the cylinder being filled. Since heat generation during fast fill is inevitable, concepts that can actively or passively remove the generated heat during the fill process are required to achieve the needed improvements in fill efficiency. For modelling the conventional CNG fast refuelling process, previous researchers [21,24] have specified pressure and temperature boundary conditions that vary with time to match experimentally measured data, e.g. that of Shipley [8]. However, these conditions do not account for the incoming kinetic energy of the gas. Therefore, in this study a constant total enthalpy boundary condition is proposed corresponding to a total temperature of 300 K and a total pressure that linearly ramps from 4 to 20.6 MPa in the first 3 seconds of the fill and then is maintained at 20.6 MPa for the remainder of the fill. The ramped pressure condition is used to avoid very large pressure ratios at the beginning of the fill, for which convergence of the CFD solver is difficult. Since the ramping time is less than 10% of the total filling time, it’s reasonable to assume that it does not significantly impact the pressure and temperature history. At the gas inlet, a converging nozzle that has an entrance diameter of 0.01 m and an exit diameter of 0.005 m has been applied instead of those straight pipes used in previous numerical studies. When using the nominated constant enthalpy boundary condition, this converging nozzle can keep the incoming gas flow in the subsonic regime to assist in convergence of the numerical method.

The objective of the present study is to investigate the fast fill process of natural gas in Type-III cylinders without and with different ways of heat removal in order to identify the effectiveness of heat removal for improving fill efficiency. To achieve this objective the research will focus on
investigating the temperature field and the mass filled within a compressed gas cylinder during fast refuelling by analytical and numerical models, which are detailed in Chapter 3-6. The models will consider compressible unsteady viscous flow, real gas effects, heat transfer to the cylinder walls and conduction through the cylinder walls to ambient.

As a result of this project, new fast fill systems with active heat rejection or pre-chilling are developed. The new design will be transferred to Agility immediately, and it is expected that the new design will be integrated into Agility CNG fuel systems and become available on market in a short time after the completion of the project. The high-efficiency fuel systems will enhance Agility’s competitiveness and increase Agility’s market share. The research results will improve the viability of CNG fuel systems specifically and NGVs in general. It will also help reduce reliance on conventional fuels, thereby resulting in greenhouse gas (GHG) emissions.
Chapter 3: Analytical Study of CNG Refueling Process

Prior to numerical modelling, effort was put on analytical approaches to solve the thermal behaviors of natural gas during refuelling. In the analytical study, mass and energy conservation equations are coupled with ideal or real gas equation of state and orifice flow equations to predict the heat generation rates during fast fill. The influence of heat removal via a cooling coil inserted into the cylinder during fill on the dispensed mass and fill time is quantified.

3.1 Analytical refuelling model of ideal gas

3.1.1 Model system and assumptions

Natural gas is known as real gas but firstly, an analytical model of the filling process of ideal gas has been developed to see how much error the ideal gas model will bring comparing with the results in previous literatures. Figure 3.1 shows a schematic diagram of the system under consideration. Ideal gas first pass through a nozzle at a pressure of $P_0$, temperature of $T_0$ and mass flow rate of $\dot{m}$, which is considered as isentropic and isenthalpic expansion, then it starts to fill a tank with volume $V$. The gas inside the tank has an initial pressure of $P_i$ and temperature of $T_i$. 
3.1.2 Model development

Applying the First law of thermodynamics:

\[ \dot{m} c_p T_0 = \frac{dU}{dt} \]  

(3.1)

Where \( U \) is the internal energy, \( c_p \) is the specific heat for constant pressure and \( t \) is time.

For ideal gas:

\[ U = C_v \frac{PV}{R} \]  

(3.2)

Where \( C_v \) denotes the specific heat for constant volume and \( R \) denotes the gas constant.

Substitute Equation (3.2) into (3.1) we will obtain:
\[
\dot{m} = \frac{1}{kRT_0} \frac{dP}{dt}
\]  
(3.3)

Also, the mass flow rate can be expressed as:

\[
\dot{m} = \rho v A
\]  
(3.4)

Where \( k, \rho \) are the specific heat ratio and density, respectively.

Assuming the filling process to be isentropic expansion:

\[
\left( \frac{\rho}{\rho_0} \right)^k = \left( \frac{P}{P_0} \right) , \rho = \rho_0 \left( \frac{P}{P_0} \right)^{\frac{1}{k}}
\]  
(3.5)

\[
\left( \frac{T}{T_0} \right)^{\frac{k}{k-1}} = \left( \frac{P}{P_0} \right) , T = T_0 \left( \frac{P}{P_0} \right)^{\frac{k-1}{k}}
\]  
(3.6)

\[
T_0 - T = \frac{v^2}{2C_p}
\]  
(3.7)

From Equation (3.5) to (3.7) the gas velocity at the inlet \( v \) can be solved as:

\[
v = \sqrt{2C_p T_0 \left[ 1 - \left( \frac{P}{P_0} \right)^{\frac{k-1}{k}} \right]}
\]  
(3.8)

Substitute Equation (3.5) and (3.8) into (3.3) we get:

\[
\dot{m} = A \rho_0 \left( \frac{P}{P_0} \right)^{\frac{1}{k}} \sqrt{2C_p T_0 \left[ 1 - \left( \frac{P}{P_0} \right)^{\frac{k-1}{k}} \right]}
\]  
(3.9)

Combining Equations (3.3) and (3.9) we will obtain:

\[
\frac{V}{Ak\sqrt{2C_p T_0}} \frac{d\left( \frac{P}{P_0} \right)}{dt} = \sqrt{2C_p T_0 \left[ 1 - \left( \frac{P}{P_0} \right)^{\frac{k-1}{k}} \right]}
\]  
(3.10)

To simplify the derivation, let \( \frac{V}{Ak\sqrt{2C_p T_0}} \) be equal to \( \beta \), and \( \frac{P}{P_0} \) be equal to \( X \), the equation above reduces to:
\[ \beta \frac{dX}{dt} = X^\frac{1}{k} \sqrt{1 - X^{1 - \frac{1}{k}}} \] (3.11)

\[ \frac{\beta k}{1-k} \frac{d(1-X^{1 - \frac{1}{k}})}{dt} = \sqrt{1 - X^{1 - \frac{1}{k}}} \] (3.12)

Let Y be equal to \( 1 - X^{1 - \frac{1}{k}} \), Equation (3.12) can be further reduced to:

\[ \frac{dY}{Y^{\frac{1}{2}}} = \frac{1-k}{\beta k} \frac{dt}{dt} \] (3.13)

By doing integration from \( Y_i \) to \( Y \) we get:

\[ Y^{\frac{1}{2}} = \frac{1-k}{2\beta k} t + Y_i^{\frac{1}{2}} \] (3.14)

where \( Y_i = 1 - \left( \frac{P_i}{P_0} \right)^{1 - \frac{1}{k}} \)

Replacing \( Y \) and \( \beta \) back to Equation (3.14) and solve for \( \frac{P}{P_0} \):

\[ \frac{P}{P_0} = \{ 1 - [Y_i^{\frac{1}{2}} - \frac{A\sqrt{2C_pT_0}}{2V} t]^2 \}^{k-1} \] (3.15)

Since \( P \) should almost be equal to \( P_0 \) when \( t = t_{max} \), We know that \( Y_i^{\frac{1}{2}} - \frac{A\sqrt{2C_pT_0}}{2V} t_{max} = 0 \)

Therefore, the explicit solution for the time require for the ideal gas filling process is as following:

\[ t_{max} = Y_i^{\frac{1}{2}} \frac{2V}{A\sqrt{2C_pT_0}(k-1)} \] (3.16)
3.1.3 Model validation

As a typical ideal gas, the properties of air have been substituted into the expressions above (Eqs. 3.15 and 3.16) to get relationship between the gas average pressure $P$ and the filling time as well as the total filling time required. However, this result shows very big difference from the CNG filling time numerically acquired by previous researchers [25]. The dynamic average gas pressure curve is shown in Fig. 3.2 when considering filling a tank with volume of 23.4 L and orifice diameter of 0.005 m. The filling time of natural gas reported by Navid [25] is around 34 s with the same tank and orifice, while the filling of ideal gas in the above analytical model is unreasonably too fast, which only takes 2.2 s. Therefore, an analytical model for the refuelling process using real gas model needs to be built to get more accurate understandings, which will be discussed in the following sections of this chapter.

Fig 3.2 Dynamic average gas pressure curve by ideal gas filling model
3.2 Analytical refuelling model of real gas

As compared to section 3.1, real gas equation of state is applied here instead of ideal gas. A computer program called STRAPP written by National Institute of Standards and Technology has been used to calculate the compressibility factor, the internal energy, the enthalpy and the specific heat ratio of nature gas at different temperature and pressure. The natural gas flow into the cylinder is only considered as isenthalpic expansion through the orifice. A series of more complex equations describing the orifice flow rate is applied in this section.

3.2.1 Model system and assumptions

Figure 3.3 shows a schematic diagram of the system under consideration consisting of a Type-3 cylinder with a volume of $V = 23.4$ L filled with natural gas. The natural gas composition in Kountz’s study [14] (CH$_4$ 92.87%; C$_2$H$_6$ 3.34%; N$_2$ 2.07%; CO$_2$ 0.78%; C$_3$H$_8$ 0.63%; less than 0.1% of i-butane, n-butane, i-pentane, n-pentane, and n-hexane, by molar percentages), which is the mean U.S. natural gas composition, has been used in our model. The gas has an initial pressure of $P_i = 2$ MPa and temperature of $T_i = 300$ K. The gas source and the cylinder are connected by a tube with orifice diameter of $d = 5$ mm and length $l = 98$ mm. At the inlet to the tube, a gas total pressure of $P_s = 20.6$ MPa and temperature of $T_s = 300$ K are imposed so that the corresponding total enthalpy $h_s$ is fixed. The effect of actively removing the heat generated during the fill is incorporated into the model by assuming that the heat removal system consists of a coiled tube with circulating coolant inserted from the other end of the cylinder. By assuming a high heat transfer coefficient of the coolant flow and high thermal conductivity of the cooling tube, a constant temperature condition of $T_c = 300$ K can be assumed on the coil outer surface. The
convective heat transfer coefficient between the gas and the tube wall, $h$, and area of the tube, $A_c$, are expected to play major roles in the active cooling.

Fig 3.3 Schematic diagram of the system considered in the real gas filling model

The following assumptions are made in this model:

1. The gas pressure and temperature are spatially uniform, i.e. the filling process can be viewed as quasi-steady;
2. The natural gas flow into the cylinder can be considered as isenthalpic expansion through the orifice;
3. The temperature and pressure of the supply gas are constant;
4. Heat transfer between the cylinder outer surface and the ambient is negligible, as per Kountz’s analysis [14].
5. When considering adding cooling coils, the $hA_c$ value is assumed to be constant during the fill.

3.2.2 Model development

Applying conservation of energy to the system in Fig 3.3 yields:
\[ \dot{m}h_s - hA_c(T_g - T_c) = \frac{d}{dt}(m_gu_g) \]  

(3.17)

where \( \dot{m} \) is the mass flow rate, \( T_g \) denotes the gas average temperature, and \( m_g \) and \( u_g \) are the total mass and the specific internal energy of the gas inside the cylinder. The term \( hA_c \) equals to 0 when active heat removal is not considered. Because the cylinder only has one inlet and no outlets, conservation of mass is:

\[ \frac{dm_g}{dt} = \dot{m} \]  

(3.18)

The equation of state is given by:

\[ p_g v_g = R z_g m_g T_g \]  

(3.19)

where \( p_g \), \( v_g \) and \( z_g \) are the pressure, specific volume and compressibility factor of the gas, and \( R \) denotes the gas constant.

Finally, the equations describing the orifice flow rate [14] are provided as:

\[ \dot{m} = C_d A \frac{p_s}{\sqrt{v_s}} f \left( \frac{p_g}{p_s} \right) \]  

(3.20)

Here \( C_d \) is the orifice discharge coefficient, and \( A \) is the orifice cross-section area. The coefficient \( C \) is given by:

\[ C = \sqrt{\frac{g k}{R \left( \frac{k+1}{2} \right)^{\frac{k}{k-1}}} \frac{k+1}{k+1}} \]  

(3.21)

Here \( g \) denotes the dimensionalizing factor, and \( k \) denotes the ratio of specific heat of the gas.

The function \( f \) in Eq. (3.20) depends on pressure ratio \( \frac{p_g}{p_s} \) in comparison to a critical value, which is
\[
\left( \frac{P_g}{P_s} \right)_{crit} = \left( \frac{2}{k+1} \right)^{\frac{k}{k-1}}
\]

If \( \frac{P_g}{P_s} \leq \left( \frac{P_g}{P_s} \right)_{crit} \),
\[
f \left( \frac{P_g}{P_s} \right) = 1
\]  \hspace{1cm} (3.23)

If \( \frac{P_g}{P_s} > \left( \frac{P_g}{P_s} \right)_{crit} \),
\[
f \left( \frac{P_g}{P_s} \right) = \sqrt{\left( \frac{2}{k-1} \right) \left( \frac{k+1}{k-1} \right)^{\frac{k+1}{k-1}} \left( \frac{P_g}{P_s} \right)^{\frac{1}{k}} \sqrt{1 - \left( \frac{P_g}{P_s} \right)^{\frac{k-1}{k}}}}
\]  \hspace{1cm} (3.24)

The fill is considered to be completed at time \( t \) when the average gas pressure \( p_g(t) \) satisfies the following equation:
\[
\frac{p_g(t) - p_i}{p_s - p_i} = 95\%
\]  \hspace{1cm} (3.25)

Previous studies have shown that non-ideal gas properties of CNG affect the final in-cylinder conditions. For instance, Farzaneh-Gord and Branch [20] estimate a temperature rise during refuelling of about 40 K when using real gas properties and more than 80 K when using ideal gas properties, with a corresponding effect on the fill efficiency. Therefore, the ideal gas assumption is not valid for natural gas filling process. When dealing with a real gas (natural gas), the gas does not obey ideal gas laws. The molecules of natural gas behave in a manner that is more complex than a typical ideal gas. A compressibility factor for natural gas must be applied to correct the ideal gas law for use with natural gas. An effective means of computing the compressibility factor for CNG is important for this study. The compressibility factor has to be determined to help evaluate the theoretical amount of natural gas dispensed to the fuel storage cylinder used in this study. A computer program called STRAPP which is written by the National Institute of Standards and
Technology (NIST) is used here to calculate the compressibility factor, the internal energy, the enthalpy and the specific heat ratio of natural gas at several different temperature and pressure.

STRAPP is executed after a few required pieces of information are entered during the input section of the program. The information required is the mole fraction of each component or compound present in natural gas and the temperature (Kelvin) and the pressure (bar) of the natural gas. The components of the natural gas are assumed to be equivalent to that of the national average for natural gas composition. An illustration of the U.S. average of each component present in natural gas is shown in Table 3.1.

<table>
<thead>
<tr>
<th>Constituent</th>
<th>Mole %</th>
</tr>
</thead>
<tbody>
<tr>
<td>Methane</td>
<td>92.87</td>
</tr>
<tr>
<td>Ethane</td>
<td>3.34</td>
</tr>
<tr>
<td>Propane</td>
<td>0.63</td>
</tr>
<tr>
<td>I-Butane</td>
<td>0.07</td>
</tr>
<tr>
<td>N-Butane</td>
<td>0.12</td>
</tr>
<tr>
<td>I-Pentane</td>
<td>0.04</td>
</tr>
<tr>
<td>N-pentane</td>
<td>0.03</td>
</tr>
<tr>
<td>N-Hexane</td>
<td>0.05</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>2.07</td>
</tr>
<tr>
<td>Carbon Dioxide</td>
<td>0.78</td>
</tr>
</tbody>
</table>

Table 3.1 The composition of the mean U.S. natural gas mixture

STRAPP calculated the compressibility factor, the internal energy, the enthalpy and the specific heat ratio of natural gas for each temperature and pressure combination entered into the program.

These thermophysical properties calculated above have been curve-fitted to yield functions of temperature and pressure. These functions together with the above governing equations yield a
system of ordinary differential equations that is solved using a fourth-order Runge-Kutta method to obtain the transient solutions for the average gas temperature, pressure and the total mass inside the cylinder.

3.2.3 Transient solutions and the effects of adding cooling coils

Figures 3.4-3.6 show the average gas pressure, temperature and mass without cooling and with a cooling coil that has a high value of $hA_c = 280$ W/K. Figure 3.4 shows that the fill process is completed when the average pressure reaches 19.6 MPa, and the time required to complete the fill increases with active heat removal. Figure 3.5 shows that the average gas temperature at the end of the fill can be lowered significantly with active heat removal, and Fig 3.6 shows the corresponding increase in the mass of filled CNG for the case with the largest heat removal rate. The effect of the heat removal rate is shown in Fig 3.5 through dynamic temperature curves with multiple cooling scenarios ($hA_c = 0, 70, 140, 210$ and $280$ W/K). Overall, as the cooling effect becomes stronger, the mean gas temperature is lower at the same filling time. The temperature increases at the beginning due to the heat generated by compression work. Only the gas near the inlet is cooled by the Joule-Thomson effect, and because this portion is only a small fraction of the total mass of gas in the cylinder, there is no noticeable temperature dip in Fig 3.5 early in the fill; this is also observed in the CFD results in the following section.
Fig 3.4 Dynamic change in gas average pressure

Fig 3.5 Dynamic change in gas average temperature
Several additional observations can be made from Fig 3.6. The mass increases linearly in the first 20 seconds because the pressure ratio \( \frac{P_d}{P_s} \) has not reached the critical value expressed by Eq. (3.20), so the mass flow rate is determined primarily by the pressure and temperature of the supply gas according to Eqs. (3.20) and (3.23). The mass of the in-cylinder gas will be 3.2 kg after a fill without cooling and 4.45 kg after a fill with cooling regardless of the \( hA_c \) value because the gas temperature eventually equalizes with the temperature of the coolant. The \( hA_c \) value merely changes the time required for the in-cylinder temperature to reach the coolant temperature, with higher \( hA_c \) values resulting in shorter times to completely finish the fill. Figure 3.7 shows the effect of \( hA_c \) value on the fill time required to reach equilibrium. When the \( hA_c \) value is 14W/K, the time needed to finish the fill will be 30 minutes, which is impractical. When the \( hA_c \) value is 70W/K, 10 minutes is needed, which is reasonable compared to liquid fuels. Around 70 s is required for the fill when the \( hA_c = 280 \)W/K.

Fig 3.6 Dynamic change in mass of gas filled
Fig 3.7 The effect of the $hA_c$ value on the fill time

3.3 Summary

In this chapter, analytical models considering ideal gas and real gas effects have been built to solve the thermal behaviors of natural gas during refuelling. Mass and energy conservation equations are coupled with ideal or real gas equation of state and orifice flow equations to predict the heat generation rates during fast fill. The results indicate that ideal gas model provides inaccurate prediction on the dynamic gas pressure, temperature and filling time. By using the real gas model the transient solutions and the benefits of adding heat removal on the dispensed mass have been obtained and quantified.
Chapter 4: Numerical Study of CNG Refueling Process

The analytical study suffers from the following assumptions: the cylinder contents are approximated as a single lumped mass, spatial variation in the cylinder conditions are neglected, and the convective heat transfer coefficient of the cooling coil is not calculated, but is assumed constant. To quantify the effect of these simplifications on the results of the analytical study and to validate the results against a higher-order method, a CFD model is developed of the fast fill process. ANSYS Fluent®, a commercial CFD package employing the finite-volume method to discretise the compressible form of the mass, momentum, and energy conservation equations is used. During the hydrogen filling process studied by Zhao et al. [31] and Itou [32], the influences of gravity and buoyancy forces were found to be negligible if the mass flow rate exceeded 9 g/s. Since the mass flow rate in this case will be many times greater than 9 g/s, the flow inside the cylinder is modelled as an axisymmetric flow without buoyancy forces due to gravitational acceleration. The working fluid in the CFD model consists of pure methane with real gas properties determined using the Redlich-Kwong equation of state [33]. The k-ε turbulence model is applied with modified coefficients ($C_{1\varepsilon} = 1.52, C_{2\varepsilon} = 1.92, C_{\mu} = 0.09$), as suggested by Ouellette et al. [34].

4.1 Governing equations

During the refuelling the flow within the cylinder and heat transfer through the wall to the ambient vary with time. Therefore, all the governing equations should be solved in their unsteady form. The compressibility effects have to be considered in the numerical model primarily due to the very
high velocity of the gas at the inlet. Viscous effects are also of vital importance for accurately calculating the convective heat transfer between the gas and the cylinder liner because the increase in average gas temperature is dominated by the heat of compression. A real gas equation of state is used instead of the ideal gas law because of the high density of the gas during the filling at high pressure. As discussed in previous literatures [24, 25], the flow at the inlet is turbulent throughout the almost the entire fill hence for closure of the turbulent viscosity terms the model solves the Reynolds averaged governing equations using a turbulence model.

For the fluid region in the numerical model, applying the conservation of mass and Reynolds averaging techniques, the following equation yields:

\begin{equation}
\frac{\partial}{\partial t} \bar{\rho} + \frac{\partial}{\partial x_i} (\bar{\rho} \bar{u}_i) = 0 \tag{4.1}
\end{equation}

Where \( t \) is time, \( \bar{\rho} \) is average density of the gas and \( \bar{u}_i \) is the Farve average of velocity. The conservation of momentum yields the following equations.

\begin{equation}
\frac{\partial}{\partial t} (\bar{\rho} \bar{u}_i) + \frac{\partial}{\partial x_j} (\bar{\rho} \bar{u}_i \bar{u}_j) = - \frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} (\bar{\tau}_{ij} - \rho \bar{u}_i' \bar{u}_j') \tag{4.2}
\end{equation}

\begin{equation}
\tau_{ij} = - \frac{2}{3} \mu \varepsilon_{ij} \frac{\partial u_k}{\partial x_k} + \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \tag{4.3}
\end{equation}

Applying the conservation of energy produces the equations below.

\begin{equation}
\frac{\partial}{\partial t} (\bar{\rho} \bar{H}) + \frac{\partial}{\partial x_j} (\bar{\rho} \bar{H} \bar{u}_j) = - \frac{\partial p}{\partial t} + \frac{\partial}{\partial x_j} \left( - \bar{q}_j - \rho \bar{h}' \bar{u}_j' + \bar{u}_i \bar{\tau}_{ij} + \bar{u}_i' \bar{\tau}_{ij} \right) \tag{4.4}
\end{equation}

\begin{equation}
q_j = -k \frac{\partial r}{\partial x_j} \tag{4.5}
\end{equation}

\begin{equation}
H = h + \frac{1}{2} u_i u_i \tag{4.6}
\end{equation}
The terms, \(-\overline{\rho u'_i u'_j}\) and \(\overline{u'_i \tau_{ij}}\) are the enclosed terms related to turbulent fluctuating component which could be modeled by using the k-\(\varepsilon\) turbulence model, of which the governing equations are as following:

\[
\frac{\partial}{\partial t}(\rho k_i) + \frac{\partial}{\partial x_j}(\rho k_i u_j) = \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k_i}{\partial x_j} \right] - \rho \overline{u'_i u'_j} \frac{\partial u_j}{\partial x_i} - \rho \varepsilon - 2 \rho \varepsilon \frac{k_i}{c_s^2} \quad (4.7)
\]

\[
\frac{\partial}{\partial t}(\rho \varepsilon_i) + \frac{\partial}{\partial x_j}(\rho \varepsilon_i u_j) = \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \frac{\partial \varepsilon_i}{\partial x_j} \right] + C_{1\varepsilon} \frac{\varepsilon_i}{k} \left( -\rho \overline{u'_i u'_j} \frac{\partial u_j}{\partial x_i} \right) - C_{2\varepsilon} \rho \frac{\varepsilon_i^2}{k} \quad (4.8)
\]

With the suggestion by Ouellette et al. [34], the value of the constants in the k-\(\varepsilon\) turbulence model are modified, which are presented in Table 4.1

<table>
<thead>
<tr>
<th>Constant</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>(C_{1\varepsilon})</td>
<td>1.52</td>
</tr>
<tr>
<td>(C_{2\varepsilon})</td>
<td>1.92</td>
</tr>
<tr>
<td>(C_\mu)</td>
<td>0.09</td>
</tr>
</tbody>
</table>

Table 4.1 The modified coefficients of the k-\(\varepsilon\) turbulence model used in this study [34]

Within the solid regions (domain of the aluminum liner and carbon fiber wrap) the conservation of momentum and mass do not apply since the materials are solid. For these regions in this numerical model, applying the conservation of energy the following equation yields:

\[
\frac{\partial}{\partial t}(\rho_w h_w) = k_w \frac{\partial^2 T_w}{\partial x_j^2} \quad (4.9)
\]

### 4.2 Gas equations

Natural gas is used as working fluid in this study. As discussed above, it has been pointed out [20,25] that assuming working fluid to be ideal gas brings huge error into the dynamic temperature
and mass curves of the filling process due to its very high working pressure. Therefore, the gas is considered as real gas. For simplicity, natural gas is assumed to contain only methane.

Since the real gas properties are not included in Fluent, the Redlich-Kwong (RK) equation of state (EOS) [25] is applied in this model for computing the thermodynamic properties of the working fluid. Many real gas models exist and are available in Fluent. Comparison has been made [28] with different real gas equations of state in their real gas filling research and it shows good agreement. The reasons why the Redlich-Kwong equation was chosen are as it provides acceptable accuracy in the ranges of temperature and pressure in this study, and is computationally inexpensive [24]. Some other real gas models could be more accurate but require way more computation resources, which will significantly limit the computation speed.

The RK EOS is presented in the following form [25]:

\[
P = \frac{RT}{(V-b)} - \frac{a(T)}{V(V+b_0)} \quad \text{and} \quad V = \frac{1}{\rho}, \quad a(T) = a_0 \left(\frac{T_c}{T}\right)^n
\]

\[n = 0.4986 + 1.1735w + 0.475w^2 \quad (4.10)\]

\[a_0 = 0.42747 \frac{RT_c^2}{P_c}, \quad b_0 = 0.8664 \frac{RT_c}{P_c} \quad (4.11)\]

\[\tilde{b} = b_0 - c_0 \quad \text{and} \quad c_0 = \frac{RT_c}{p_c + \frac{a_0}{\rho_0(v_0+b_0)}} + b_0 - V_c \quad (4.12)\]

Where the subscript \(c\) means the value of the property at the critical point.

Based on the RK EOS, the thermodynamic properties could be calculated by the equations summarized in Table 4.2. A user-defined function (UDF) in Fluent is created and compiled to calculate all these thermodynamic properties required by the solver.
<table>
<thead>
<tr>
<th>Property</th>
<th>Equation</th>
</tr>
</thead>
<tbody>
<tr>
<td>$h = h^0(T) + PV - RT - \frac{a(T)}{b_0}(1 + n)\ln\left(\frac{V + b_0}{V}\right)$</td>
<td></td>
</tr>
<tr>
<td>$h^0(T) = \int_{T_0}^{T} C_p^0(T) dT$</td>
<td></td>
</tr>
<tr>
<td>$C_p^0(T) = C_1 + C_2 T + C_3 T^2 + C_4 T^3 + C_5 T^4$</td>
<td></td>
</tr>
<tr>
<td>$h^0(T) = C_1 T + \frac{1}{2} C_2 T^2 + \frac{1}{3} C_3 T^3 + \frac{1}{4} C_4 T^4 + \frac{1}{5} C_5 T^5 - h^0(T^0)$</td>
<td></td>
</tr>
<tr>
<td>$V^3 + a_1 V^2 + a_2 V + a_3 = 0$</td>
<td></td>
</tr>
<tr>
<td>$a_1 = C_0 - \frac{RT}{\rho}$</td>
<td></td>
</tr>
<tr>
<td>$\rho$</td>
<td>$a_2 = -(\bar{b} b_0 + \frac{RT b_0}{p} - \frac{a(T)}{p})$</td>
</tr>
<tr>
<td>$a_3 = -\frac{a(T) \bar{b}}{p}$</td>
<td></td>
</tr>
<tr>
<td>$\rho = \frac{1}{V}$</td>
<td></td>
</tr>
<tr>
<td>$C_p = C_p^0(T) + \left(\frac{\partial V}{\partial T}\right)_p R - \frac{d}{dT} \left[\frac{a(T)}{b_0}(1 + n)\ln\left(\frac{V + b_0}{V}\right) + a(T)(1 + n)\left(\frac{d}{dT}\right)\ln\left(\frac{V + b_0}{V}\right)\right]$</td>
<td>(4.16)</td>
</tr>
<tr>
<td>$S = S^0(T, P_0) + R\ln\left(\frac{V - \bar{b}}{V^0}\right) + \frac{d}{dT} \left(\frac{a(T)}{b_0}\right)\ln\left(\frac{V + b_0}{V}\right)$</td>
<td>(4.17)</td>
</tr>
<tr>
<td>$S^0(T, P_0) = S^0(T^0, P_0^0) + \int_{T_0}^{T} \frac{C_p^0(T)}{T} dT$</td>
<td></td>
</tr>
</tbody>
</table>
\[ S^0(T, P^0) = S^0(T^0, P^0) + C_1 \ln(T) + C_2(T) + \frac{1}{2} C_3 T^2 + \frac{1}{3} C_4 T^3 \]

**c**
\[ c = V \sqrt{-\frac{C_p}{C_p - C} \frac{1}{\left(\frac{\partial V}{\partial P}\right)_T}} \quad (4.18) \]

**μ**
\[ \mu(T) = 6.3 \times 10^7 \frac{M_w^{0.5} P_c^{0.6666}}{T_e^{0.1666}} \frac{T_r^{1.5}}{T_r + 0.8} \quad (4.19) \]

**k**
\[ k = \mu(C_p + \frac{5}{4}R) \quad (4.20) \]

\[ \left(\frac{\partial V}{\partial P}\right)_T = -\frac{(a_1)_p' V^2 + (a_2)_p' V + (a_3)_p'}{3V^2 + 2a_1 V + a_2} \quad (4.21) \]

\[ (a_1)_p' = \frac{RT}{p^2}, (a_2)_p' = \frac{RTb_0 - a(T)}{p^2}, (a_3)_p' = \frac{RT\tilde{b}}{p^2} \]

\[ \left(\frac{\partial V}{\partial T}\right)_P = -\frac{(a_1)_T' V^2 + (a_2)_T' V + (a_3)_T'}{3V^2 + 2a_1 V + a_2} \quad (4.22) \]

\[ (a_1)_T' = \frac{R}{p}, (a_2)_T' = \frac{Rb_0 + \frac{da(T)}{dT}}{p}, (a_3)_T' = \frac{da(T)\tilde{b}}{dT} \frac{1}{p} \]

\[ \left(\frac{\partial p}{\partial p}\right)_T = \left(\frac{\partial p}{\partial p}\right)_T = -\rho^2 \left(\frac{\partial V}{\partial p}\right)_T \quad (4.23) \]

\[ \left(\frac{\partial p}{\partial T}\right)_p = -\rho^2 \left(\frac{\partial V}{\partial T}\right)_P \quad (4.24) \]

\[ \left(\frac{\partial H}{\partial T}\right)_P = C_p \quad (4.25) \]

\[ \left(\frac{\partial H}{\partial P}\right)_T = V - T \left(\frac{\partial V}{T}\right)_P \quad (4.26) \]

Table 4.2 The derived equations for calculating the thermodynamic properties of natural gas based on RK EOS [25]
4.3 Boundary and initial conditions

The heat transfer outside the cylinder is considered as free convection. In our model, a convection boundary condition is imposed on the outer wall of the cylinder with a constant heat transfer coefficient of 10 W/m²·K, and the ambient air temperature is kept constant at 300 K throughout the filling process. At the inner wall, a no-slip boundary condition is imposed. The initial pressure of the gas inside the cylinder is 2 MPa. Previous researchers [21,24] have specified pressure and temperature boundary conditions that vary with time to match experimentally measured data, e.g. that of Shipley [8]. However, these conditions do not account for the incoming kinetic energy of the gas. Therefore, in this study a constant total enthalpy boundary condition is applied corresponding to a total temperature of 300 K and a total pressure that linearly ramps from 4 to 20.6 MPa in the first 3 seconds of the fill and then is maintained at 20.6 MPa for the remainder of the fill. The ramped pressure condition is used to avoid very large pressure ratios at the beginning of the fill, for which convergence of the CFD solver is difficult. Since the ramping time is less than 10% of the total filling time, it’s reasonable to assume that it does not significantly impact the pressure and temperature history. Figure 4.1 compares the numerical results and boundary conditions of this study against the experimentally-matched boundary conditions and results of Navid [25]. The milder pressure boundary condition in that study results in a slower fill compared to the present study. At the gas inlet, a converging nozzle that has an entrance diameter of 0.01 m and an exit diameter of 0.005 m has been applied instead of those straight pipes used in previous numerical studies. When using the nominated constant enthalpy boundary condition, this converging nozzle can keep the incoming gas flow in the subsonic regime to assist in convergence of the numerical method. Figure 4.2 shows the velocity distribution near the converging nozzle at time of 5 s.
Fig 4.1 Comparison between the pressure boundary conditions and dynamic pressure curves by current study and Navid [25]

Fig 4.2 Velocity distribution near the converging nozzle at filling time of 5 s
4.4 Computational domain and spatial grid

The computational domain for conventional fast filling process is illustrated in Fig 4.3. The gas enters the cylinder through a converging nozzle that has an entrance diameter of 0.01 m and an exit diameter of 0.005 m. The geometry is divided into the gas domain and the solid domain consisting of the aluminium liner and the carbon fiber wrap. Table 4.3 includes the thermal properties of these two kind of materials. Since the thermal resistance of aluminium is much smaller than that of carbon fiber, only the carbon fiber wrap is considered as cylinder wall for simplicity when building the geometry. The dimensions of the cylinder (length, \( L = 0.893 \) m; outer diameter, \( D = 0.234 \) m; wall thickness, \( \delta = 0.019 \) m) follow the model by Nahavandi [25]. During the hydrogen filling process studied by Zhao et al. [31] and Itou [32], the influences of gravity and buoyancy forces were found to be negligible if the mass flow rate exceeded 9 g/s. Since the mass flow rate in this case will be many times greater than 9 g/s, the flow inside the cylinder is modelled as an axisymmetric flow with respect to the centreline of the cylinder without buoyancy forces due to gravitational acceleration.

![Fig 4.3 The computational domain for conventional fast filling process](image-url)
### Table 4.3 Thermal properties of aluminum and carbon fiber

<table>
<thead>
<tr>
<th>Materials</th>
<th>Density (kg/m³)</th>
<th>Specific heat (J/kg·m)</th>
<th>Thermal conductivity (W/m·k)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Aluminum</td>
<td>900</td>
<td>2730</td>
<td>238</td>
</tr>
<tr>
<td>Carbon fiber</td>
<td>930</td>
<td>1500</td>
<td>3.7</td>
</tr>
</tbody>
</table>

Figure 4.4 shows the unstructured mesh applied in conventional fast filling case. Mesh refinement is utilized near the inlet region where the biggest gas property changes and flow gradients are expected.

![Mesh](image1.png)

Fig 4.4 The computational mesh used: the grid for the case without cooling coils and a zoomed-in view of the refined mesh in inlet region.

### 4.5 Results and discussion

Figures 4.5 - 4.7 present the temporal variation of the average gas pressure, temperature, and mass within the cylinder during conventional fast refuelling process. As shown in Fig 4.5, the average gas pressure increases quickly and almost linearly at the initial stages of the fill. It then gradually slows down due to the decreasing pressure difference. However, it could be realized from Fig 4.1
that the pressure [25] almost increases linearly throughout the whole fill. This is due to the
difference between the constant total enthalpy boundary condition applied in this study and the
pressure boundary condition nominated in [25].

Fig 4.5 Dynamic change in gas average pressure

Fig 4.6 shows the dynamic change in average gas temperature during the fill. A significant
temperature rise occurs in the first 5 seconds. This is then followed by a more gradual monotonic
temperature rise for the remainder of the fill as the in-cylinder gas is compressed by the incoming
gas. The maximum average gas temperature increase during the conventional fast refuelling is
approximately 29 K. This is much lower than that of hydrogen case. Daniele Melideo and Daniele
Baraldi [27] have modelled fast-filling process of hydrogen tanks with different strategies. The
temperature rise for their cases ranges from 60 K to 90 K. The mass of gas filled during the
refuelling process is plotted in Fig 4.7, which has a similar trend with the pressure curve. At the
end 3.35 kg mass of natural gas can be filled into the cylinder. Potential of increasing the final mass has been found by different heat removal scenarios proposed in the following chapters.

Fig 4.6 Dynamic change in gas average temperature

Fig 4.7 Dynamic change in the mass of gas filled
4.6 Summary

A CFD model has been developed of the conventional fast refuelling process to quantify the effect of some simplifications on the results of the analytical study. The Redlich-Kwong equation of state and the k-ε turbulence model with modified coefficients have been applied for the compressibility effect and turbulence modelling. Using the constant enthalpy boundary condition designed in current study, more accurate predictions on the dynamic gas pressure, temperature and filling mass have been obtained via numerical modelling.
Chapter 5: Increasing CNG Fill Efficiency by Active Cooling

In this chapter, numerical simulations employing a two-dimensional axisymmetric computational fluid dynamics (CFD) model for unsteady, compressible turbulent flow in a Type-III cylinder with active cooling coils placed in the front and back have been performed. Dynamic average temperature, pressure and mass curves as well as the local temperature distribution in the cylinder are obtained at different time instances during the fill. The effect of the location of the heat removal device is also investigated. The results provide guidance on the future optimization of the heat removal device.

5.1 Computational domain and spatial grid

The computational domain for fast filling process with active cooling is illustrated in Fig 5.1. Comparing to the conventional filling, active heat removal is achieved by adding three coils near the front or back side of the cylinder. The locations of these coils are also shown in Fig 5.1. The active heat removal system is expected to consist of cooling coils installed inside the cylinder and connected to the coolant pump and heat exchanger outside the cylinder (similar with the cooling system presented in Fig 3.3). The outside heat exchanger rejects heat to the ambient. For the current study, only the inside cooling coils are considered, and the surfaces of these coils are assumed to maintain a uniform and constant temperature, which is lower than the surrounding gas, so they transfer heat outside the cylinder. The total heat transfer area is designed to be 0.06 m². Figure 5.2 shows the unstructured mesh applied in the case with active cooling in the back. Refined meshes
are utilized near the inlet region and the coils where the biggest gas property changes and flow gradients are expected.

Fig 5.1 The computational domain for filling process with active cooling in the front and back

Fig 5.2 The computational mesh used: the grid for the case with cooling coils near the back and a zoomed-in view of the refined mesh near the cooling coils.
5.2 Boundary and initial conditions

The same constant enthalpy boundary condition at the gas inlet, cylinder wall boundary condition and the initial condition of the gas inside the cylinder as section 4.3 are applied in this section. The cooling coils will maintain their surface temperature to be constant at 300 K, which equals to the coolant temperature imposed in the analytical model in chapter 3.

5.3 Results and discussion

Figures 5.3 - 5.5 present the temporal variation of the average gas pressure, temperature, and mass within the cylinder during the fill, respectively, with active heat removal via the cooling coils in the front and back. Comparisons have been made with conventional fast refuelling without cooling. As shown in Fig 5.3, the average gas pressure increases quickly and almost linearly at the initial stages of the fill. It then gradually slows down due to the decreasing pressure difference. When the active heat removal is added, the average gas pressure increases more slowly due to the fact that the cylinder can hold more mass of natural gas with its relatively lower gas temperature at the same pressure level. The placement of the cooling coils also impacts the fill time; when the cooling coils are located towards the back, the fill time is 5 seconds longer than when the cooling coils are located towards the front. The differences in the cooling coil cases is due to differences in the heat transfer rates the two coil locations can achieve. This is illustrated in Fig 5.4 by plotting the temporal variation in the average gas temperature. A significant temperature rise occurs in the first 3 seconds for all simulated cases. In the uncooled case, this is followed by a more gradual monotonic temperature rise for the remainder of the fill as the in-cylinder gas is compressed by the incoming gas. In the cooled cases, however, the initial temperature increase is followed by a decrease in the average gas temperature as the cooling effect overcomes the compression heating
and conversion of supply enthalpy to cylinder internal energy. Differences in the cooling rate with coil location are noted; the average gas temperature inside the cylinder with cooling coils in the back is consistently lower than when the cooling coils are located in the front. The maximum average gas temperature increase during the fill without cooling is approximately 29 K, compared with 13.3 K and 10 K for cooling coils located in the front and back of the cylinder, respectively.

![Graph showing dynamic change in gas average pressure](image)

Fig 5.3 Dynamic change in gas average pressure
Fig 5.4 Dynamic change in gas average temperature

The impact of heat removal on the filled mass of CNG inside the cylinder is shown in Fig 5.5, which plots the temporal variation of the mass of in-cylinder gas during the filling process. Removal of the recompression-generated heat allows 7% more mass of gas can be filled into a cylinder when the cooling coils are located in the back. This number reduces to 4.5% if the cooling coils are located in the front. These improvements in fill efficiency come at the cost of increased fill times, but the longer fill times are still reasonable compared to liquid fuels. These results provide guidance on the future optimization of the cooling coil placement and heat transfer rates.
The mass increase achievable in the two cooling coil cases is driven by the final average gas temperature, which is a product of the spatiotemporal temperature distribution of the gas within the cylinder. To illustrate the spatiotemporal temperature variation, Fig 5.6 shows the spatial temperature distribution inside the cylinder at different time intervals during the fill. The same contour levels can be used for each time instance in Fig 5.6 (b) and (c) because the range of spatial temperature variation in the cooled cases is comparable to the range in the temporal temperature variation. In contrast, the temporal temperature range for the uncooled case is much larger than the spatial temperature range, and so to better illustrate the spatial temperature variation in Fig 5.6 (a), different contour levels are used at each time instance.

The discussion of Figure 5.6 will first describe the thermal behaviour of the uncooled case in Fig 5.6 (a), and then discuss the impact of the cooling coils. Throughout the fill, a region of cool gas exists near the inlet due to the Joule-Thompson effect that cools the incoming gas as it expands in
the cylinder. High temperature gas exists immediately above the cooled gas at the front of the cylinder. This high-temperature gas is that which has been compressed by the incoming gas stream and has been heated, and is initially located near the front of the cylinder. As the fill progresses, the temperature steadily increases from the front of the cylinder towards the rear. By the end of the fill, the largest temperature occurs at the back of cylinder, where the compressed gas stagnates and the highest recompression heating takes place.

When cooling coils are located in the front of the cylinder, Fig 5.6 (c) shows that the spatial temperature distribution is much more uniform. This is because the cooling coils remove heat from the hot gas that accumulates near the front of the cylinder, leading to a relatively more spatially-uniform temperature distribution in the cylinder throughout the fill. In contrast, when the cooling coils are located in the back, Fig 5.6 (b) shows that heating is much more spatially non-uniform, with high temperatures occurring behind the cooling coils at the back of the cylinder. These high temperatures yield the larger heat transfer rates achieved by the coils in the back, as noted in Fig 5.4, and contribute to the better fill efficiency for the case with cooling in the back.

Fig 5.6 Temperature distribution with and without cooling at time of 5 s, 10 s and 20 s
To explain why higher temperatures are observed behind the cooling coils when the coils are located near the rear of the cylinder, the forced convection velocity surrounding the coils needs to be considered. This is illustrated in Fig 5.7 by plotting the flow streamlines colored by the velocity magnitude at $t = 5$ s. The uncooled case in Fig 5.7 (a) shows that the high-speed fluid occurs near the centerline and a single large recirculation pattern develops in the cylinder. When the cooling coils are located near the front (Fig 5.6 (b)), the cooling coils have a minimal impact on the flow streamlines. The high-speed flow near the centerline convects around the cooling coils and the large recirculation zone in the cylinder in Fig 5.7 (a) is largely preserved, although there are two smaller recirculation zones created near the coils. When the cooling coils are located near the back (Fig 5.7 (c)), the flow pattern is significantly altered. The momentum of the incoming gas has reduced sufficiently and the area of the high-speed region has broadened to the point that the cooling coils present a significant flow obstruction. As a result, the dominant recirculation pattern is established only within the space between the inlet and the coils, while downstream of the coils the gas velocity is very low. The nearly stagnant gas surrounding the coils is not mixed with the cooler gas elsewhere in the cylinder, allowing high temperature gas to accumulate in the stagnant zone near the rear of the cylinder, which corresponds the temperature distribution plotted in Fig 5.6 (b). The resulting large temperature difference between the coil surface and the gas produces the larger heat removal rates noted in Fig 5.4 when the coils are located near the back of the cylinder.
A further reason for the decreased fill efficiency in the case with cooling coils located near the front of the cylinder is visible in Figures 5.6 and 5.7. From Fig 5.7 (b), it is apparent that the coil nearest the centreline will have the highest convective heat transfer coefficient because the velocity past the cylinder is the highest. However, Fig 5.6 (c) shows that the temperature difference between the coil surface and the gas will be small and perhaps even negative during the early stages of the fill. The impact of these flow features on the local heat transfer rate for the three coils (averaged over the coil circumference) is shown in Fig 5.8. Initially, the heat transfer rate is positive, i.e. the coils are actually heating the gas, which is of course opposite to their intended purpose. The largest total heating rate occurs at $t = 2.5$ s, which is approximately when the ramped inlet pressure reaches its maximum value. The coils transition from heating to cooling the gas first for Coil #3, which is farthest from the inlet, and lastly for Coil #1, which is nearest to the inlet. The highest total cooling rate occurs at about $t = 12$ s for Coil #3 due to the balance in gas temperature and velocity; with reference to Fig 5.6 (c) and Fig 5.7 (b), while Coil #3 has lower velocities than Coil #1, it has a larger local temperature difference that yields higher heat transfer rates. In contrast, for the case...
with cooling coils near the back of the cylinder (not shown), the local heat transfer rates are consistently negative (i.e. cooling) throughout the fill duration.

Fig 5.8 The heating/cooling rate of the three coils when placed in the front side. Coil #1 is nearest to the cylinder inlet, and coil #3 is farthest.

Finally, to compare the analytical model to the numerical results, Fig 5.9 compares the CFD results and the analytical model. To ensure a consistent comparison, the analytical model is corrected by imposing the same ramped inlet pressure as the CFD and the convective heat transfer coefficient of the cooling coils calculated from Fig 5.8 instead of the constant $hA$ value assumed in chapter 3. The comparison in Fig 5.9 shows that the corrected analytical model over-predicts the temperature rise and the fill time required compared to the CFD. This over-prediction is likely due to neglecting spatial variations in the analytical model (i.e. the lumped mass assumption), as the CFD results show that spatial variations in the temperature and velocity occur and affect the considered active heat removal strategies for improving the fill efficiency.
5.4 Summary

In this chapter, numerical simulations employing a two-dimensional axisymmetric computational fluid dynamics (CFD) model for unsteady, compressible turbulent flow in a Type-III cylinder with active cooling coils placed in the front and back have been performed. Dynamic average temperature, pressure and mass curves as well as the local temperature distribution in the cylinder are obtained at different time instances during the fill. The results show that adding active cooling can significantly lower the average gas temperature, thereby resulting in more mass filled. Placing the cooling coils near the back of the cylinder achieves higher fill efficiency increase than near the front. The results can provide guidance on the future optimization of the heat removal device.
Chapter 6: Increasing CNG Fill Efficiency by Pre-chilling

In this chapter, numerical simulations employing a two-dimensional axisymmetric computational fluid dynamics (CFD) model for unsteady, compressible turbulent flow in a Type-III cylinder with pre-chilling have been performed. Dynamic average temperature, pressure and mass curves as well as the local temperature distribution in the cylinder are obtained at different time instances during the fill. The benefits of adding pre-chilling have been quantified. A method of pre-chilling has been introduced with its effectiveness proved. The results provide guidance on the future optimization of the heat removal device.

6.1 Fast refuelling process with pre-chilling

6.1.1 Pre-chilled temperature calculation and material selection

Considering adding pre-chilling, a pre-chilled mass is designed to be placed in the back side (which has been proved to provide a more significant cooling than in the front in section 5.3) of the cylinder. Commercial bronze and aluminum alloy 2024-T6 are selected as the material since as compared to the other materials listed in Table 6.1, they have higher thermal inertia (shown in Table 6.2) and are easier to get. This pre-chilled mass is cooled by the coolant circulation to a lower temperature than the surrounding gas prior to starting the filling process so they will keep bringing heat generated outside during the refill.
Fig 6.1 Schematic diagram of the pre-chilling model

<table>
<thead>
<tr>
<th>Composition</th>
<th>Melting point (K)</th>
<th>$\rho (kg/m^3)$</th>
<th>$C_p (J/kg K)$</th>
<th>k(W/m K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pure aluminum</td>
<td>933</td>
<td>2702</td>
<td>903</td>
<td>237</td>
</tr>
<tr>
<td>Aluminum alloy 2024-T6</td>
<td>775</td>
<td>2770</td>
<td>875</td>
<td>177</td>
</tr>
<tr>
<td>Germanium</td>
<td>1211</td>
<td>5360</td>
<td>322</td>
<td>59.9</td>
</tr>
<tr>
<td>Commercial bronze</td>
<td>1293</td>
<td>8800</td>
<td>420</td>
<td>52</td>
</tr>
<tr>
<td>Chromium</td>
<td>2118</td>
<td>7160</td>
<td>449</td>
<td>93.7</td>
</tr>
<tr>
<td>Cadmium</td>
<td>594</td>
<td>8650</td>
<td>231</td>
<td>96.8</td>
</tr>
<tr>
<td>Boron</td>
<td>2573</td>
<td>2500</td>
<td>1107</td>
<td>27</td>
</tr>
<tr>
<td>Bismuth</td>
<td>545</td>
<td>9780</td>
<td>122</td>
<td>7.9</td>
</tr>
<tr>
<td>Beryllium</td>
<td>1550</td>
<td>1850</td>
<td>1825</td>
<td>200</td>
</tr>
</tbody>
</table>

Table 6.1 Thermal properties of some materials at temperature of 300 K
The pre-chilled temperature is very important to determine since it can’t be too high in order to guarantee its cooling effect, or too low for the energy saving issue. Some calculations regarding this pre-chilled temperature are as following.

It is assumed that the copper has the same temperature with the gas at the end of the filling process. Applying conservation of energy and the equation of state to the system yields:

\[
C_{p,NG} \frac{(1+\eta)P V_{tank}}{1000RT_1 z_1} M (T_1 - T_2) = C_{p,d} \rho_d V_d (T_2 - T_i) \tag{6.1}
\]

Where P is the final average gas temperature (20 MPa), \(V_{tank}\) and \(V_d\) are the volume of the test cylinder (23.4 L) and pre-chilled devices, \(T_1\) and \(T_2\) are the final average gas temperature without cooling (329 K obtained from section 4.5) and with cooling, \(T_i\) denotes the temperature of the pre-chilled devices, \(C_{p,NG}\) and \(C_{p,d}\) are the specific heat of natural gas and pre-chilled devices, \(M\) is the Molecular mass of natural gas, \(R\) is the universal gas constant, \(\rho_d\) denotes the density of the pre-chilled devices, and \(\eta\) is the proposed increase of the fill efficiency.
Conservation of mass is given by:

\[(1 + \eta) \times \frac{P_{V_{\text{tank}}}}{T_{1}z_{1}} = \frac{P_{(V_{\text{tank}}-V_{d})}}{T_{2}z_{2}} \quad (6.2)\]

Where \(z_{1}\) and \(z_{2}\) are the average gas compressibility factor without and with cooling gained from NIST database.

By solving Eqs. (6.1) and (6.2), correlations between \(V_{d}/V_{\text{tank}}\) and \(T_{i}\) can be obtained for different materials of the pre-chilled device if \(\eta\) is given. Fig 6.2 shows their relationships when \(\eta\) is fixed as 10%. When selecting aluminum alloy 2024-T6 as the material, it does not have to be pre-chilled to the same temperature as using commercial bronze so its temperature curve is consistently higher. This is due to that aluminum alloy 2024-T6 has a larger \(\rho C_{p}\) value. It can be observed that in order to achieve a 10% increase on the fill efficiency, the temperature to which the pre-chilled device has to be pre-chilled increases significantly with the volume percentage of it over the cylinder when this ratio is between 0% to 5%. The pre-chilled temperature almost remains constant if this ratio keeps increasing beyond this range. Therefore, pre-chilling the devices made of commercial bronze (or aluminum alloy 2024-T6) which accounts for 5% of the cylinder volume to 252 K (or 266 K) are selected to be the most effective and cost-optimal heat removal scenario.
Fig 6.2 The pre-chilled temperature vs the volume percentage of the pre-chilled devices over the test cylinder

6.1.2 Computational domain and spatial grid

Two kinds of geometry of the pre-chilled device are considered in this section. The computational domains are illustrated in Fig 6.3. Both of them are designed to account for 5% of the tank volume, which has been proved above to be the most effective and cost-optimal as the pre-chilled device volume. Figure 6.4 shows the refined unstructured mesh applied near these pre-chilled devices where the biggest gas property changes and flow gradients are expected.
Fig 6.3 The computational domain of the filling process with pre-chilling

Fig 6.4 Zoomed-in views of the refined mesh near the pre-chilled devices
6.1.3 Boundary and initial conditions

The same constant enthalpy boundary condition at the gas inlet, cylinder wall boundary condition and the initial condition of the gas inside the cylinder as section 4.3 are applied here. As discussed above, in case (a) and (b) the pre-chilled devices made of commercial bronze and aluminum alloy 2024-T6 are pre-chilled to 252 K and 266 K prior to the natural gas filling process, respectively.

6.1.4 Results and discussion

Figure 6.5 presents the temporal variation of the average gas temperature within the cylinder during the fill for the two pre-chilling cases. As shown in Fig 6.5, the temperature rise in the first 3 s is less significant than the two active cooling cases. A reason is that those pre-chilled devices are pre-chilled to much lower temperature (depending on the material) comparing with the active cooling coils (maintained at 300 K). This temperature rise is followed by a decrease in the average gas temperature as the pre-chilling effect starts to overcome the compression heating and conversion of supply enthalpy to cylinder internal energy. However, as the in-cylinder gas keeps transferring heat to the pre-chilled device which will finally make it unable to absorb that much heat at a time, the compression heating and conversion of supply enthalpy to cylinder internal energy become dominant again, which result in another rise in the average gas temperature.
Fig 6.5 Dynamic change in average gas temperature

The impact of heat removal on the filled mass of CNG inside the cylinder is shown in Fig 6.6, which plots the temporal variation of the mass of in-cylinder gas during the filling process. Removal of the recompression-generated heat allows 3.3% for case (a) and 8.1% for case (b) more mass of gas can be filled into a cylinder. These improvements in fill efficiency come at the cost of increased fill times, but the longer fill times are still comparable to liquid fuels.
The mass increase achievable in the pre-chilling cases is driven by the final average gas temperature, which is also a product of the initial and final temperature distribution within the pre-chilled device. A low and non-uniform final average temperature of the cooling device shows that there’s still huge cooling potential, which in turn means the gas hasn’t got sufficient or efficient cooling. Figures 6.7 and 6.8 show the spatial temperature variation within the cooling device of these two cases. At the end of the filling process, the temperature distribution of the cooling device which is made of commercial bronze is found to be more spatially non-uniform. Due to its lower thermal inertia, the heat from the gas is hard to transfer into the center of the cooling device, which results in a low temperature region there. This is the main reason why the two cases are designed to achieve the same increase on fill efficiency but the results turn out to be different.
6.2 A method to achieve pre-chilling: through truck AC system refrigerant circulation

This section presents a way by which the cooling devices can be pre-chilled. The liquid refrigerant from truck air conditioning system at low temperature are used to cool down the cooling devices prior to the natural gas filling process. A basic description of automotive air condition system and how it works are given below [35].
Fig 6.9 Schematic diagram of car AC system [35]

(1) Starting at the compressor, the gaseous refrigerant enters the compressor, gets compressed and becomes high pressure (typically about 200 psi), high temperature refrigerant gas.

(2) From there it immediately flows into the condenser, loses some heat and turns to high pressure and temperature refrigerant liquid.

(3) After passing through the expansion valve it becomes low pressure and temperature liquid.

(4) Finally, it goes into the evaporator, absorb heat from ambient air (the air that needs to be cooled) by evaporation.

Currently, R134A is the mainly used refrigerant in automotive air conditioning systems which boils at -26.3 °C when its pressure is 1 bar. Ideally it is designed to come into the evaporator at
0 °C (273K). We use the low temperature liquid refrigerant here to generate a close-loop coolant circulation for pre-chilling the devices. A schematic diagram of the current design is shown in Fig 6.10.

**Fig 6.10 Schematic diagram of pre-chilling achieved by refrigerant circulation**

### 6.2.1 Computational domain and spatial grid

In comparison with section 6.1.2, the geometry of the pre-chilled device has been redesigned with thinner but longer fins while maintaining its total volume to help enhance heat transfer performance. Its dimension, location and computational grid applied are presented in Fig 6.11 and 6.12.
6.2.2 Boundary and initial conditions

Some work has been reported on the performance of truck air conditioning systems. Bagheri et al. [36] determined the relationship between refrigerant mass flow rate and condenser air inlet temperature by experiments when the evaporator air inlet temperature equals to 20 °C, 30 °C and
40 °C, which is shown in Fig 6.13. The mass flow rate to be imposed on the refrigerant inlet marked in Fig 6.18 is roughly estimated based on this result. Assuming that the air to be cooled in the car is 30 °C and the condenser inlet air temperature to be 5-10 °C higher, we know from Fig 6.20 that the refrigerant mass flow rate is 0.007 kg/s.

![Graph showing Refrigerant mass flow rate vs. condenser air inlet temperature](image-url)

Fig 6.13 Refrigerant mass flow rate vs. condenser air inlet temperature [36]

Saturated liquid refrigerant flow with temperature of -1.2 °C and pressure of 40 psi [36] are imposed on the inlet to test its ability of cooling the pre-chilled device. Using secondary loop the mass flow rate can be easily increased. By doing numerical simulations of a 30-min pre-chilling process prior to the natural gas filling, average temperature curves of the pre-chilled device when imposing different refrigerant mass flow rates are plotted in Fig 6.14. A constant temperature boundary condition with the inlet refrigerant temperature is applied at the wall of the channel when considering infinite mass flow rate.
Fig 6.14 Average temperature of the pre-chilled device vs. pre-chilling time

The same constant enthalpy boundary condition at the gas inlet, cylinder wall boundary condition and the initial condition of the gas inside the cylinder as section 4.3 are applied here. The pre-chilled device made of aluminum alloy 2024-T6 is set as 300 K prior to the pre-chilling process.

6.2.3 Results and discussion

Two simulations have been performed to illustrate the effectiveness of using liquid refrigerant from truck air conditioning system to pre-chill prior to the natural gas filling process. Since the temperature and pressure are fixed for the refrigerant obtained before entering the evaporator, the mass flow rate turns out to be the only important factor. In case (c) mass flow rate of 0.0035 kg/s
is imposed on the refrigerant inlet, while a constant temperature boundary condition with the inlet refrigerant temperature is applied at the wall of the channel in case (d) which considers an infinite mass flow rate.

![Graph showing temperature vs time for different cooling scenarios](image)

**Fig 6.15 Dynamic change in average gas temperature**

The differences in case (c) and case (d) is due to difference in the heat transfer rates the two pre-chilled devices can achieve. This is illustrated in Fig 6.15 by plotting the temporal variation in the average gas temperature. The curves start from a temperature lower than ambient temperature due to its decrease during the pre-chilling process. The same trend can be observed in case (b), (c) and (d), which are using similar geometry and the same material for the pre-chilled devices but pre-chilled to different temperatures. The temperature profile of case (d) is consistently lower than that of case (c) due to the impact of a lower pre-chilled temperature coming from a greater mass flow rate.
Temporal variation of the mass of in-cylinder gas during the filling process, for all the cases performed in this study, has been plotted in Fig 6.16. At the end of the filling process, 6.6% more mass of gas can be filled in case (c). This number reduces to 5% if the pre-chilling scenario in case (d) is applied. These improvements in fill efficiency come at the cost of increased filling time but prove the effectiveness of the current pre-chilling design.
Further potential on optimizing the geometry of the pre-chilled device can be found through temperature distribution plotted in Fig 6.17 and 6.18. As we can see, the good thermal contact between fins and gas results in a much higher final temperature of the fins than the rear of the pre-chilled device. Therefore, cutting down some thermal mass from the rear and adding to the fins could be a method to enhance its cooling performance. Another indication we can get from the two figures above is that although the gas temperature near the rear is very high, not a lot heat has
been transferred into the rear of the pre-chilled device because the gas there is nearly stagnant. Ways to improve gas circulation near the rear of the cylinder should be beneficial for cooling. Lastly, avoiding heat transfer from the cylinder wall (or the ambient air) to the pre-chilled device will also contribute to its higher heat absorption rate.

6.3 Summary

In this chapter, numerical simulations employing a two-dimensional axisymmetric computational fluid dynamics (CFD) model for unsteady, compressible turbulent flow in a Type-III cylinder with pre-chilling have been performed. Dynamic average temperature, pressure and mass curves as well as the local temperature distribution in the cylinder are obtained at different time instances during the fill. The effectiveness and benefit of adding pre-chilling has been proved and quantified via numerical modelling. Refrigerant from truck air conditioning system can be obtained for generating a circulation, which provides a way to pre-chill the cooling device prior to the natural gas filling process. Further improvement on fill efficiency could be achieved by optimizing the geometry of the cooling device, gas circulation near the rear and heat insulation from the cylinder wall.
Chapter 7: Summary, Conclusions and Future Work

7.1 Summary and conclusions

A combined analytical/computational study of the fast fill of compressed natural gas was performed to investigate the effect of active heat removal on improving the fill efficiency. Active heat removal was introduced by adding three coiled tubes inside the cylinder, and the tube surface temperature was assumed to be uniform and constant. The influence of coil placement location was assessed by placing coils either in the front or in the back of the cylinder. The transient and spatial development of temperature, pressure, and dispensed mass of gas were analyzed for the cases with and without heat removal.

Both the numerical and analytical results demonstrate that active heat removal lowers the average gas temperature of the dispensed gas so that more mass of natural gas can be dispensed into the cylinder without a significant increase in fill time. Moreover, the location of the cooling coils affects the heat removal due to the relative effects of the gas temperature and velocity distributions inside the cylinder. Placing the coils in the back of the cylinder achieves the largest improvement in fill efficiency, as the high gas temperatures near the rear of the tank yield the largest heat transfer rates for the heat removal system.

The effectiveness and benefit of adding pre-chilling has been proved and quantified via numerical modelling. Refrigerant from truck air conditioning system can be obtained for generating a circulation, which provides a way to pre-chill the cooling device prior to the natural gas filling process. Further improvement on fill efficiency could be achieved by optimizing the geometry of the cooling device, gas circulation near the rear and heat insulation from the cylinder wall.
Fig 7.1 shows the average gas temperature at the end of every filling process considered in this study. As compared to the conventional fast refill, the cooled cases can achieve significantly lowered final gas temperatures ranging from 302.9 K to 307.5 K, which result in higher gas density. Imposing active cooling in the back brings a better cooling performance than in the front. The lowest gas temperature is obtained in pre-chilling case (b) which has lower pre-chilled temperature than case (c) and (d), and better material and geometry selection of the cooling device than case (a).

![Bar chart showing final average gas temperature for different cases](image)

**Fig 7.1 The final average gas temperature of all cases under investigation**

The comparison in Fig 7.2 shows the mass that can be filled at the end and the corresponding fill efficiency increase, which are primarily driven by the gas volume, the final gas temperature and its distribution. Removal of the recompression-generated heat allows 3.3% - 8.1% more mass of gas can be filled into a cylinder. The most gas filled is observed in pre-chilling case (b).
7.2 Limitations and future work

While this study was successful in improving the fill efficiency by different kinds of heat removal, limitations still exist due to some uncertainties that may occur during refuelling. For example in cold winter, the ambient temperature can be much lower than the constant temperature assumed in both the analytical and numerical models, which may have a strong influence on the heat transfer and fill efficiency. This study only focused on the filling process of a cylinder which has an initial pressure of 2 MPa, while the drivers may want to start filling their fuel tanks at other pressures. Another point is that due to the lack of information for further analysis, the cost, economic benefits and driving range improvement of adding heat removal are not investigated in detail, which is actually out of the scope of this study. Some recommendations can be made here for future researchers. It should be noted that the geometry of cooling devices and the gas circulation can be
significantly optimized to further enhance the heat transfer rate. Some assumptions have been made in both the analytical model and the numerical model. Although several have been proved to be feasible by previous researchers, there are still some of them which need experimental verification. When conducting experiments, proper locations for thermocouples need to be identified in order to accurately measure the average in-cylinder gas temperature. Therefore, future work should focus on optimal cooling scenarios and experiments in order to predict the natural gas filling process more accurately.
Bibliography


