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EFFECTS OF GAS TYPES AND MODELS ON OPTIMIZED GAS FUELLING STATION RESERVOIR'S PRESSURE

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Abstract - There are similar algorithms and infrastructure for storing gas fuels at CNG (Compressed Natural Gas) and CHG (Compressed Hydrogen Gas) fuelling stations. In these stations, the fuels are usually stored in the cascade storage system to utilize the stations more efficiently. The cascade storage system generally divides into three reservoirs, commonly termed low, medium and high-pressure reservoirs. The pressures within these reservoirs have huge effects on performance of the stations. In the current study, based on the laws of thermodynamics, conservation of mass and real/ideal gas assumptions, a theoretical analysis has been constructed to study the effects of gas types and models on performance of the stations. It is intended to determine the optimized reservoir pressures for these stations. The results reveal that the optimized pressure differs between the gas types. For ideal and real gas models in both stations (CNG and CHG), the optimized non-dimensional low pressure-reservoir pressure is found to be 0.22. The optimized non-dimensional medium-pressure reservoir pressure is the same for the stations, and equal to 0.58.
Keywords: Compressed Natural Gas; Compressed Hydrogen Gas; Fast-filling process; Cascade reservoirs; Thermodynamic analysis; Real gas model; Ideal gas model; Entropy generation.

INTRODUCTION

There are a lot of natural gas vehicles (NGV) in use, and the number is expanding every year. A number of national and international standards have been issued to ensure safe and efficient use of NGVs. Due to the relatively small number of hydrogen fuelled vehicles (HGV) currently on the roadway; there are limited regulations for these vehicles. The HGVs are currently using similar standards, regulations, infrastructures and fuelling stations to NGVs.

In these stations, the vehicles usually receive fuels from high pressure reservoirs during filling. The first problem with these fuel stations is the refuelling time. The NGV and HGV industries have made excellent advancements to provide a system to refuel a NGV or a HGV in a time comparable to that of a gasoline station. This fill time can be referred to as a fast fill or rapid charge.

The on-board storage capacity of natural gas and hydrogen vehicles is the other problem for the widespread marketing of these alternate fuelled vehicles. The on-board storage cylinders undergo a rise in storage gas cylinder temperature in the range of 40 K or more for CNG (Kountz, 1994) and 70 K or more for CHG (Dicken *et al*., 2007) during fast-filling. For both fuels (CNG and CHG), this temperature rise reduces the density of the gas in the cylinder, resulting in an under-filled cylinder relative to its rated specification. If this temperature rise is not compensated for in the fuelling station dispenser, by transiently over-pressurizing the tank, the vehicle user will experience a reduced driving range. Although NGV and HGV on-board cylinder volumes

*To whom correspondence should be addressed play the main role in the on-board storage capacity, but the fuelling station reservoir's pressure also has big effects on the amount of the filled mass of the on-board cylinder.

Natural gas from the distribution pipeline is compressed using a large multi-stage compressor into a "cascade" storage system. On the other hand, hydrogen must also be compressed by a compressing system and stored in a "cascade" storage system (Baur *et al*., 2004). The input work required by the compressor is the final problem with the fuelling stations, as the required work for compressing and storing the natural gas and hydrogen are then partially wasted through the filling process.

In order to make the utilization of the natural gas and hydrogen fuelling stations more efficient, these fuels are usually stored in a cascade storage system. The cascade storage system is commonly divided into three reservoirs, generally termed low (LPR), medium (MPR) and high-pressure reservoirs (HPR). The pressure within the reservoirs has big effects on 3 problems associated with the filling process and fuelling station as below:

1) Filling time;
2) The charged mass of the on-board cylinder after refuelling;
3) The compressor input work.

Considering the above three problems with a compressed gas fuelling station, one can conclude that, by reducing filling time, reducing compressor input work and (or) increasing the filled mass of the on-board cylinder, the performance of the compressed gas fuelling stations would be improved.

There is a strong possibility of using the current natural gas infrastructure as a starting point for hydrogen vehicle infrastructure. In this research, the effects of important parameters on the performance of CNG and CHG stations are studied. The principal aim is to show that the optimum algorithm for these stations is slightly different.

To understand the fast filling process and study the effect of the pressure and temperature within low, medium and high-pressure reservoirs on the performance of CNG and CHG fuelling stations, a theoretical analysis has been developed in this study. The fast fill process was assumed to be a quasi-static process and the natural gas presumed to be purely methane (as an ideal and real gas). The hydrogen is also treated as an ideal and real gas. A second law analysis has been employed to calculate the amount of entropy generations during the filling process. It is well known that a lower entropy generation is associated with less work required work by the compressor.

There have been limited researches in the field of filling process modelling in the literature. Kountz *et al*. (1997) were the first to model the fast filling process of a natural gas storage cylinder based on the first law of thermodynamics. They developed a computer program to model the fast filling process for a single reservoir. They have also developed a natural gas dispenser control algorithm that insures complete filling of NGV cylinders under a fast-fill scenario (Kountz *et al*., 1998; Kountz *et al*., 1998; Kountz *et al*., 1998). Research has also been carried out to model fast-filling of hydrogen-based fuelling infrastructure. Fast filling of a hydrogen cylinder using a number of experiments (Liss *et al*., 2002; Liss *et al*., 2003; Newhouse *et al*., 1999) resulted in a high temperature increase in the cylinder during the process. In another research, a control method optimized for a high utilization ratio and fast filling speed in hydrogen refuelling stations was reported (Zheng *et al*., 2010). The results of this research show that an optimized control method can significantly improve the utilization ratio and allows refuelling in an acceptable time.

A few experimental studies were also carried out to study fast filling of natural gas on-board cylinders (Thomas *et al*., 2002; Shiply, 2002). Shiply (2002) concluded that ambient temperature variation could affect the fast-fill process. He also concluded that the test cylinder is under-filled every time it is rapidly recharged. For the hydrogen fast fuelling process, there have been experiments on thermal characteristics during the hydrogen filling process of type IV cylinders (Chan Kim *et al*., 2010). In that study, a computational fluid dynamics (CFD) analysis was also employed to simulate the conditions of the experiments. The CFD results show reasonable agreement with the experiments. The discrepancy between the CFD and experimental values decreases as the initial gas pressure increases.

The authors of the current study have also modelled the CNG fast filling process (Farzaneh-Gord *et al*. 2007; Farzaneh-Gord, 2008, Farzaneh-Gord *et al*. 2013, Deymi-Dashtebayaz *et al*., 2013). They developed a computer programme based on the Peng-Robinson state equation and methane properties for a single reservoir fuelling station. They investigated the effects of ambient temperature and initial cylinder pressure on the final cylinder conditions. In another study, they (Farzaneh-Gord *et al*. 2008) presented thermodynamics analysis of the cascade reservoir filling process of natural gas vehicle cylinders. The results indicated that ambient temperature has a big effect on the filling process and final NGV cylinder conditions. Farzaneh-Gord *et al*.

(2011) have employed a theoretical analysis to study the effects of buffer and cascade storage systems on performance of a CNG fuelling station. It was found that the time (filling time) required for bringing up the NGV on-board cylinder to its final pressure in the buffer storage system is about 66% less than the cascade storage system. The charged mass for the cascade system is about 80% of the buffer system, which gives an advantage to the buffer system over the cascade system. The biggest advantage of the cascade system over the buffer system is 50% less entropy generation for this configuration, which probably causes much lower required compressor input work for this configuration compared to the buffer system. Farzaneh-Gord *et al*. (2012a, 2012b) have also studied effects of natural gas compositions on fast filling process for buffer and cascade storage banks. In these researches, the conditions of storage bank were considered constant. Farzaneh-Gord *et al*. (2012c) have examined two storage systems for compressed hydrogen stations. The important parameters such as filling time, filled mass and compressor input work have been examined in detail. The results show that the filling time of the buffer storage system is much less than that of the cascade storage system. However, the filled mass related to the buffer system for the same conditions is approximately equal to that of the cascade system. Furthermore, the buffer system is accompanied by much higher entropy generation as compared to the cascade storage system, which is directly reflected in the amount of compressor input work required.

As mentioned previously, the second law has been employed in this study to calculate the entropy generation theoretically. Entropy generation is associated with thermodynamic irreversibilities, which are common in all types of thermal systems. There have been numerous investigations in the field of entropy generation. A researcher has concentrated on the different mechanisms responsible for entropy generation in applied thermal engineering (Bejan, 1982; 1996). Generation of entropy dissipates work into heat. Therefore, it makes good engineering sense to focus on irreversibilities of heat transfer and fluid flow processes and try to understand the function of the related entropy generation mechanisms (Bejan, 1972). Since then, a lot of investigations have been carried out to compute the entropy generation and irreversibility profiles for different geometric configurations, flow situations, and thermal boundary conditions (Sordi *et al*., 2009; Diaz *et al*., 2007). Here, entropy generation has been employed as a main tool to determine the amount of work destruction during filling.

CNG AND CHG FILLING STATIONS

Figure 1 shows a typical CNG filling station. Gas from the distribution pipeline, usually “low” pressure at <4bar (0.4 MPa) or possibly “medium” pressure (1.6 MPa), is compressed using a large multi-stage compressor into a “cascade” storage system. The pressure within the storage system is kept at a higher value than in the vehicle’s on-board cylinder so that gas transfers to the vehicle under differential pressure. Commonly, the cascade storage will operate in the range of 20.5 MPa to 25 MPa, while the vehicle’s maximum on-board cylinder pressure is 20 MPa. For more efficient use of the compressor and the storage system, the CNG stations commonly operate using a three-stage “cascade” storage system.

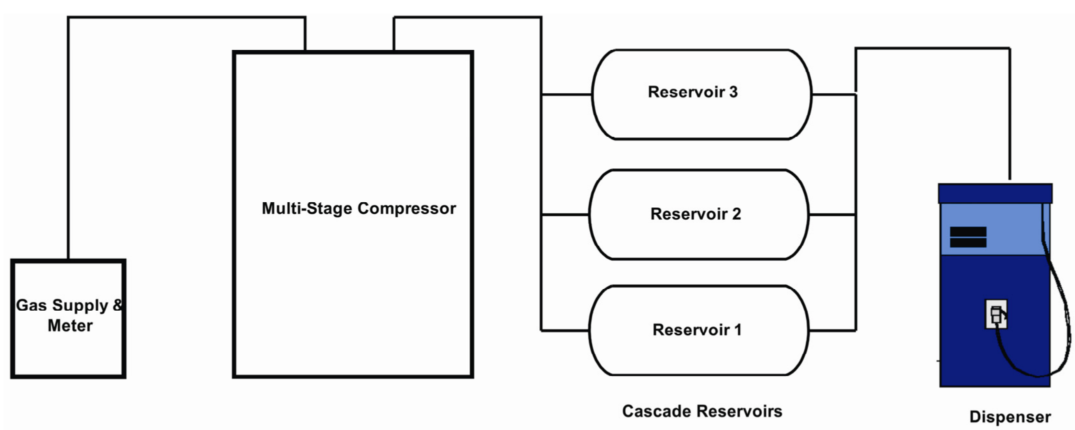

Figure 1: A schematic diagram of a NGV filling station.

In a CHG fuelling station, there is a similar algorithm as in a CNG fuelling station. The hydrogen can be supplied using various methods (Sordi *et al*., 2009). The common method for supplying hydrogen is by using an electrolyser (Baur *et al*., 2004). In this method, hydrogen can be produced through the electrolysis of water. The hydrogen is then compressed to a high pressure similar to a CNG station. In CHG stations, the cascade storage operates in the range of 35-44 MPa (or 70-80 MPa), while the vehicle's maximum on-board cylinder pressure is 35 MPa (or 70 MPa) (Zheng *et al*., 2010).

The cascade storage system is usually divided into three reservoirs, commonly termed low, medium and high-pressure reservoirs (Thomas *et al*., 2002). During fast filling, the on-board cylinder is first connected to the low-pressure reservoir. As the pressure in the reservoir falls and that in the on-board cylinder rises, the flow of gas decreases. When the flow rate has declined to a pre-set level, the system switches to the medium pressure reservoir, then finally to the high-pressure reservoir to complete the fill. It is expected that the cascade system results in a more complete "fill" than if the whole storage were maintained at one pressure and utilises the compressor and storage with maximum efficiency. In addition, when the compressor is automatically turned on to refill the reservoirs it fills the high pressure reservoir first, and then switches to the medium and the low reservoirs. This ensures that the high pressure reservoir (employed to complete the fill) is kept at maximum pressure all the time, ensuring that vehicles are always supplied with the maximum amount of gas available. Correct specification of the compressor capacity and the volume of cascade storage is necessary to ensure that the CNG and CHG stations can cope with the type (passenger cars, buses or trucks) and frequency (peak periods) of vehicles using the facility.

Compressed Natural Gas and Hydrogen Cylinders

The natural gas and hydrogen cylinders have various design types based on the construction materials used. Design types include Type 1, which are all-metal, Type 2, which have a metal liner and a hoop-wrapped composite reinforcement, Type 3, which have a metal liner and a full-wrapped composite reinforcement, and Type 4, which have a non-metallic liner and a full-wrapped composite reinforcement. Metal containers and liners are typically steel or aluminium. Composite reinforcements are typically carbon or glass fibbers in an epoxy resin matrix. These cylinders are designed for a specified nominal service pressure at a specified temperature, essentially a specified density (kg/m^3) of fuel. This will result in a given mass of natural gas or hydrogen stored in the fuel container (cylinders). The actual pressure in the fuel container will vary from the nominal service pressure as the temperature of the fuel in the cylinder varies. Under-filling of the on-board cylinders can occur at fuelling stations during fast-fill charging operations at ambient temperatures greater than 30 °C. The resulting reduced driving range of the vehicle is a serious obstacle that the gas industry is striving to overcome, without resorting to unnecessarily high fuelling station pressures, or by applying extensive over-pressurization of the cylinder during the filling operation. Undercharged cylinders are a result of the elevated temperature that occurs in the CHG and CNG storage cylinder.

Chemical Compositions of Natural Gas

Natural gas composition (mixture) varies with location, climate and other factors. The gas is refined before flowing into the pipe lines. Methane is the component that is a very high percentage of natural gas. As a result and for the sake of simplicity, it is assumed that methane is the only substance in the natural gas.

Cascade Reservoir Parameters

For a cascade storage system, there are a few important parameters that affect the filling. These parameters are introduced in this section.

Figure 2 shows a schematic diagram of a cascade reservoir system. Thermodynamic properties in cascade reservoirs play important roles in the filling process. Two main properties are pressure and temperature. As shown in Figure 2, each reservoir has its own temperature (T_R) and pressure (P_R). These are assumed to be unchanged while the pressure and temperature in the on-board NGV and HGV cylinders varies during filling.

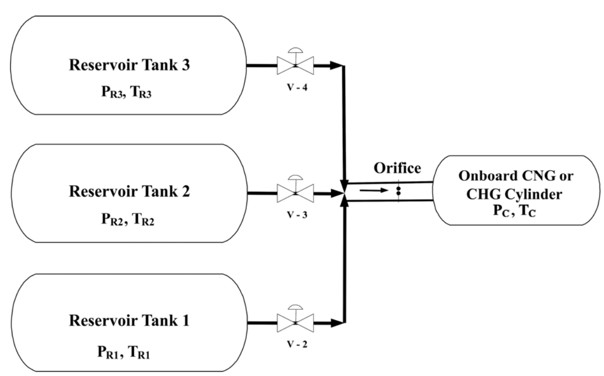

Figure 2: A schematic diagram of cascade reservoirs.

To maintain the final pressure within the on-board cylinder at its rated value, the pressure within the HPR assumed to be constant (20.5 MPa for CNG and 37 MPa for CHG) throughout this study. The effects of medium and low reservoir pressures on performance of the fuelling station have been studied by introducing the two dimensionless parameters. The ratio of the medium and low pressure reservoirs to the high-pressure one, defined as below, are these two parameters:

$$NP1 = P_{R1} / P_{R3} \qquad NP2 = P_{R2} / P_{R3} \tag{1}$$

The final dimensionless number is the "fill ratio". The cylinder "fill ratio" is defined as the mass of charged gas after refuelling divided by the mass which the cylinder could hold at the rating condition (300 K, 20 MPa for CNG and 300 K, 35 MPa for CHG). This parameter is directly related to the driving range of the NGV and HGV, defined as:

$$FR = \frac{m_c \text{ (at end of filling)}}{\rho(300K, 20MPa \text{ for CNG and } 300K, 35MPa \text{ for CHG})V_c} \tag{2}$$

It should also be noted that the cylinder volumes (V_c) for NGV and HGV were considered to be 67 and 150 liters (Zheng *et al*., 2010), respectively, throughout this study.

THERMODYNAMIC ANALYSIS

First Law Analysis

In this study, in order to model the fast filling process and develop a mathematical method, the on-board cylinder was considered to be an open thermodynamic system which undergoes a quasi-steady process.

To develop a theoretical analysis, continuity and the first law of thermodynamics have been applied to the cylinder to find 2 thermodynamic properties. Considering the onboard cylinder as a control volume based on Figure 3 and knowing that it has only 1 inlet, the continuity (conservation of mass) equation may be written as follows:

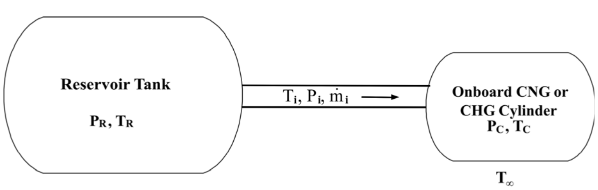

Figure 3: A schematic diagram of the thermodynamic system.

$$\frac{dm_C}{dt} = \dot{m}_i \tag{3}$$

In Equation (3), $\dot{m}_i$ is the inlet mass flow rate and can be calculated by considering an isentropic expansion through an orifice. Applying gas dynamics laws:

$$\dot{m}_i = C_d \rho_R A_{orifice} \left(\frac{P_C}{P_R}\right)^{\frac{1}{\gamma}} \left\{ \left(\frac{2\gamma}{\gamma-1}\right)\left(\frac{P_R}{\rho_R}\right)\left[1-\left(\frac{P_C}{P_R}\right)^{\frac{\gamma-1}{\gamma}}\right]\right\}^{\frac{1}{2}} \quad \text{if } \frac{P_C}{P_R} \le \left(\frac{2}{\gamma+1}\right)^{\frac{\gamma}{\gamma-1}} \tag{4}$$

$$\dot{m}_i = C_d \sqrt{\gamma P_R \rho_R}\, A_{orifice} \left(\frac{2}{\gamma+1}\right)^{\frac{\gamma+1}{2(\gamma-1)}} \quad \text{if } \frac{P_C}{P_R} > \left(\frac{2}{\gamma+1}\right)^{\frac{\gamma}{\gamma-1}} \tag{5}$$

In Equations (4)-(5), C_d is the discharge coefficient of the orifice.

The first law of thermodynamics in general form can be written as:

$$\dot{Q}_{cv} + \sum \dot{m}_i (h_i + V_i^2/2 + gz_i) = \sum \dot{m}_e (h_e + V_e^2/2 + gz_e) + d/dt[m(u + V^2/2 + gz)]_{cv} + \dot{W}_{cv} \tag{6}$$

The work term is zero in the filling process and the change in potential and kinetic energy can be neglected. The equation can then be simplified as below:

$$\frac{dU_C}{dt} = \dot{Q} + \dot{m}_i\left(\frac{V_i^2}{2} + h_i\right) \tag{7}$$

Since $h_R = \frac{V_i^2}{2} + h_i$, the above equation can be further simplified as:

$$\frac{dU_C}{dt} = \dot{Q} + \dot{m}_i h_R \tag{8}$$

The heat lost from the onboard cylinder to the environment can be calculated as

$$\dot{Q} = -U_{HC}A_C\left(T_C - T_\infty\right) \tag{9}$$

Combining (3), (8) and (9), one can write the above equation as:

$$\frac{d(m_C u_C)}{dt} = -U_{HC}A_C\left(T_C - T_\infty\right) + \frac{dm_C}{dt}h_R \tag{10}$$

Or in the following form:

$$\frac{d(m_C u_C)}{dt} - \frac{d(m_C h_R)}{dt} = -U_{HC}A_C\left(T_C - T_\infty\right) \tag{11}$$

The above equation can be rearranged to the following form:

$$d(m_C u_C - m_C h_R) = -U_{HC}A_C\left(T_C - T_\infty\right)dt \tag{12}$$

The above equation can be integrated from the "start" of filling up to the "current" time as:

$$\int_s^c d(m_C u_C - m_C h_R) = -\int_o^t U_{HC}A_C\left(T_C - T_\infty\right)dt \tag{13}$$

The integration of the above equation for a single reservoir fuelling station results in:

$$m_C(u_C - h_R) - m_{Cs}(u_{Cs} - h_R) = -U_{HC}A_C\Delta T_{av}t \tag{14}$$

Where m_c, m_{cs} are the mass of charged gas at the "current" and "start" of the filling process, ΔT_{av} is the average temperature difference between the cylinder and environment, which is defined as:

$$\Delta T_{av} = \frac{1}{t}\int_o^t \left(T_C - T_\infty\right)dt \tag{15}$$

The first law of thermodynamics for the onboard cylinder can finally be written as:

$$u_C = h_R - \frac{U_{Hc}A_C\Delta T_{av}t}{m_C} + \frac{m_{Cs}}{m_C}(u_{Cs} - h_R) \tag{16}$$

The Equation (3), (4) and (16) can be employed to calculate the two thermodynamic properties of the in-cylinder natural gas and hydrogen at any time. By knowing two thermodynamics properties (here the specific internal energy and specific volume), the other in-cylinder properties could be found.

Adiabatic System

For an adiabatic system, Equation (16) can be further simplified as:

$$u_C = h_R + \frac{m_{Cs}}{m_C}(u_{Cs} - h_R) \tag{17}$$

And if $m_{cs} = 0$, the following relation is valid at any time:

$$u_C = h_R \tag{18}$$

Ideal Gas Model for An Adiabatic System

For the case of ideal gas behaviour, the governing equation can be substantially simplified. Considering the following ideal gas assumptions:

$$u = c_v T,\ h = c_p T,\ m = \frac{PV}{RT} \tag{19}$$

and knowing that the volume of the cylinder, specific heats, and reservoir temperature are constant, then Equation (8) can be simplified as follows:

$$\begin{aligned} &\frac{d(mu)_{cv}}{dt} = \dot{m}_i h_R \Rightarrow \frac{d\left(\frac{PV}{RT}c_v T\right)_{cv}}{dt} = \dot{m}_i c_p T_R \\ &\Rightarrow \frac{V_{cv}c_v}{R}\frac{d(P_{cv})}{dt} = \dot{m}_i c_p T_R \end{aligned} \tag{20}$$

By replacing the inlet mass flow rate from Equations (4) and (5), the following simple equation can be obtained:

$$d(P_C)/dt = \dot{m}_i(\gamma R/V_{cv})T_r = \begin{cases} (\gamma R/V_{cv})T_R C_d \rho_R A_{orifice}\left(\frac{P_C}{P_R}\right)^{\frac{1}{\gamma}}\left\{\left(\frac{2\gamma}{\gamma-1}\right)\left(\frac{P_R}{\rho_R}\right)\left[1-\left(\frac{P_C}{P_R}\right)^{\frac{\gamma-1}{\gamma}}\right]\right\}^{\frac{1}{2}} & \text{if } \frac{P_C}{P_R} \le \left(\frac{2}{\gamma+1}\right)^{\frac{\gamma}{\gamma-1}} \\ (\gamma R/V_{cv})T_R C_d\sqrt{\gamma P_R \rho_R}\,A_{orifice}\left(\frac{2}{\gamma+1}\right)^{\frac{\gamma+1}{2(\gamma-1)}} & \text{if } \frac{P_C}{P_R} > \left(\frac{2}{\gamma+1}\right)^{\frac{\gamma}{\gamma-1}} \end{cases} \tag{21}$$

The Second Law Analysis

The second law of thermodynamics and the flow processes occurring in the "cascade" storage system of the gas filling station adopted in this study makes it possible to evaluate the entropy generation rates, $\dot{S}_{gen}$, for the characteristic nodes of the system.

The second law of thermodynamics for the filling process of the on-board cylinder can be expressed as:

$$\dot{S}_{gen} = dS_C / dt - \dot{Q} / T_\infty - \dot{m}_i s_i \geq 0 \tag{22}$$

Here, all irreversibility is assumed to occur at the inlet to in-cylinder position. There is an isentropic expansion from the reservoir to the inlet position, which means $s_i = s_R$. Considering this assumption and combining Equation (3), (9) and (22), the following equation can be obtained:

$$\begin{aligned}\dot{S}_{gen} = &\frac{d(m_C s_C)}{dt} - \frac{dm_C}{dt} s_R \\ &+ U_{Hc} A_C \left(T_C - T_\infty\right) / T_\infty\end{aligned} \tag{23}$$

in the following form:

$$\begin{aligned}\dot{S}_{gen} dt = &\, d(m_C s_C - m_C s_R) \\ &+ U_{HC} A_C \left(T_C - T_\infty\right) / T_\infty dt\end{aligned} \tag{24}$$

the above equation can be integrated from "start" of filling to the "current" time as below:

$$\begin{aligned}S_{gen} = &\int_s^c d(m_C s_C - m_C s_R) \\ &+ \int_s^c \frac{U_{HC} A_C \left(T_C - T_\infty\right)}{T_\infty} dt\end{aligned} \tag{25}$$

For a fuelling station with a single reservoir in which s_R remains constant throughout the filling process, the integration of the above equation results in a simple equation:

$$\begin{aligned}S_{gen} = &\, m_C(s_C - s_R) - m_{Cs}(s_{Cs} - s_R) \\ &+ \frac{U_{HC} A_C \left(T_{av} - T_\infty\right)}{T_\infty}\end{aligned} \tag{26}$$

Adiabatic System

Equation (26) can be further simplified for an adiabatic system as:

$$S_{gen} = m_C(s_C - s_R) - m_{Cs}(s_{Cs} - s_R) \tag{27}$$

and if the cylinder is empty at the start of the filling process ($m_{cs} = 0$), the following relation can be obtained:

$$S_{gen,max} = m_C(s_C - s_R) \tag{28}$$

Ideal Gas Model for an Adiabatic System

For the case of ideal gas behaviour, the second law is much simplified. Considering the following ideal gas assumptions:

$$\begin{aligned}&s_C - s_R = c_p \ln\frac{T_C}{T_R} - R \ln\frac{P_C}{P_R}, \\ &m_c = \frac{P_C V_C}{R T_C}\end{aligned} \tag{29}$$

and knowing that the volume of the cylinder, V_c, specific heat, c_p, and reservoir temperature are constant, then Equation (27) can be simplified as follows:

$$\begin{aligned}S_{gen} = &\, m_C(c_p \ln\frac{T_C}{T_R} - R \ln\frac{P_c}{P_R}) \\ &- m_{Cs}(c_p \ln\frac{T_{Cs}}{T_R} - R \ln\frac{P_{Cs}}{P_R})\end{aligned} \tag{30}$$

For the case of $m_{cs} = 0$ and assuming that the pressure within the on-board cylinder reaches its reservoir pressure $(p_C \approx p_R)$, then Equation (30) gives the maximum entropy generation for a fuelling station as follows:

$$S_{gen,max} = S_{gen} = m_C c_p \ln\frac{T_c}{T_R} \tag{31}$$

Considering Equations (18) and (19), the above equation can be further simplified as follows:

$$S_{gen,max} = S_{gen} = \frac{c_v P_R V_c}{R T_R} \ln\gamma \tag{32}$$

It should be noted that Equations (29) to (32) are only valid for a single reservoir fuelling station. Calculating the entropy generation for a fuelling station with a cascade reservoir system demands more effort. Here the non-dimensional entropy generation is introduced to compare the results for various configurations as follows:

$$NS = S_{gen} / S_{gen,max} \tag{33}$$

It is worth mentioning that NS expresses the irreversibility in the system. The minimization of NS means reducing the part of input work which dissipates into heat in the system. As all work required by the system is provided by the station compressor, one can conclude that the minimum of NS indicates the least input work by the compressor.

SIMULATION METHODOLOGY

The set of equations presented in the previous section constitutes the model for the filling. The solution of these equations is, however, not straight-forward. The simulation proceeds in the following steps:

1. Initial reservoir and on-board cylinder thermodynamic properties are known.
2. Equation (4) (or (5)) is employed to calculate the mass flow rate.
3. By assuming a small time increment, Equation (2) is solved numerically to calculate the in-cylinder mass (and specific volume) at the new time step.
4. The energy equation is solved numerically to calculate the specific internal energy at the new time step.
5. By knowing the specific volume and specific internal energy and utilizing the properties table, other thermodynamic properties will be found by trial and error.
6. If the in-cylinder pressure has reached its target value, the simulation is stopped, otherwise go to step 2.

RESULTS AND DISCUSSION

In this study, the NGV and hydrogen cylinders have been considered to be adiabatic. Consequently, the orifice diameter will affect the final state in the cylinder. The orifice diameter will affect the filling time and inlet mass flow rate. The orifice diameter and the cylinder volume for NGV and HGV were considered to be 1 mm and 67 and 150 liters (Zheng *et al*., 2010), respectively. Also in this study ambient temperature was fixed at 300 K. The results are presented here for the commonly used cascade group of three, as shown in Figure 2.

Figure 4 shows dynamic pressure profiles for CNG and CHG cylinders during filling for the real and ideal gas models. The LPR, MPR, HPR pressures are assumed to be respectively 5.5, 10.5 and 20.5 MPa for CNG and 11, 21 and 37 MPa for CHG. Discontinuity in the pressure profile is due to switching to another reservoir tank. As expected, the final in-cylinder pressure for CNG and CHG cylinders for both gas models is constant, respectively 20 and 35 MPa.

Figure 5 shows dynamic in-cylinder mass profiles for CNG and CHG cylinders during filling. In this figure, the thermodynamic conditions of reservoirs are similar to Figure 4. Discontinuity in the profiles is due to switching to another reservoir tank. Note from the figure that the final CHG in-cylinder mass for the ideal gas model is much higher than for the real gas model, whereas the final CNG in-cylinder mass for the real gas model is much higher than for the ideal gas model. The reason is due to variations in the final in-cylinder temperature. As the final in-cylinder pressure reaches its targeted value, the in-cylinder mass is higher for the cylinder in which the final temperature is lower. Yang (2009) carried out a theoretical analysis and calculated the final in-cylinder temperature to initial temperature ratio for a single reservoir system for CHG. The ratio was found to be 1.48. In the present study, the ratio was found to be 1.42 and 1.45 for the ideal and real CHG gas models, respectively.

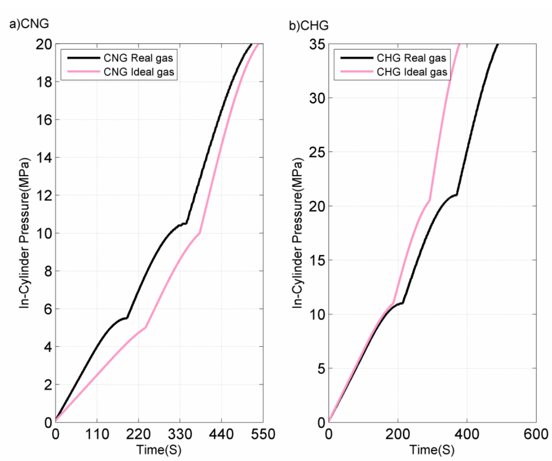

Figure 4: CNG and CHG dynamic in-cylinder pressures for the real and ideal gas models.

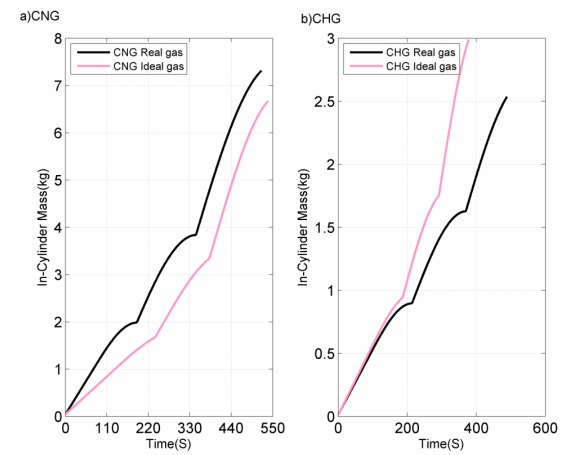

Figure 5: CNG and CHG dynamic in-cylinder masses for the real and ideal gas models.

Figure 6 shows dynamic in-cylinder temperature profiles for CNG and CHG during filling for the real and ideal gas models. Note from this figure that, for CNG, there is no dip in the temperature profile at early filling times; however, two dips in the temperature profile occur when the supply tank changes. This behaviour can indicate that the Joule-Thompson cooling effect is not high enough in the early stage of the filling process and is not able to overcome the conversion of reservoir enthalpy energy into cylinder internal energy. When the supply system switches to the higher pressure reservoir tank, the higher Joule-Thompson cooling effect, with the help of the low temperature inlet gas, causes small dips in the temperature profile. Because the Joule-Thompson coefficient for CHG is positive throughout the filling, the temperature will rise as the pressure drops. This causes the final in-cylinder temperature for real CHG to be higher than that of ideal CHG.

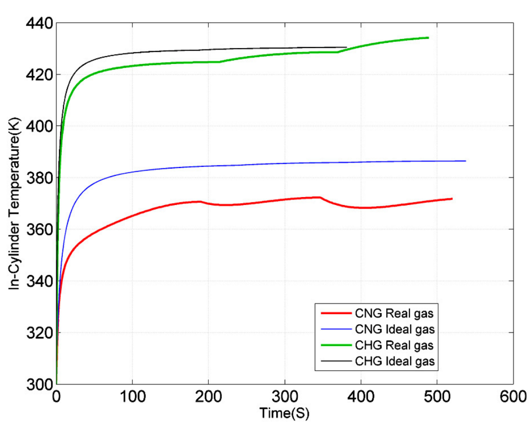

Figure 6: CNG and CHG dynamic in-cylinder temperatures for the real and ideal gas models.

Note from Figure 6 that the rise in temperature only occurs when the CNG and CHG cylinders are connected to the lowest pressure reservoir tank and the temperature profile is nearly monotonic otherwise. Note that the discontinuity in the temperature profile in Figure 6 is due to switching to another reservoir tank.

As expected for the ideal gas model, there is no dip in the temperature profile due to the fact that the Joule-Thompson cooling effect is not present. Comparing the real and ideal models in Figure 6, it can be realized that the temperature profiles are highly different and the temperature rise for CHG is much higher than for CNG cylinders. So it can be concluded that the thermodynamic properties of the gas have a big effect on the temperature profile.

The results presented here are only valid for adiabatic on-board cylinders. In real conditions, the on-board cylinders are not adiabatic. This makes the final in-cylinder temperature lower than the values reported in the present study due to the heat lost during the filling. The actual final in-cylinder temperature depends on the charging time, but for safety considerations it should be lower than 85 °C. To avoid this problem, the charging time is controlled by the station dispenser algorithm through regulating the inlet mass flow rate.

Figure 7 shows how the fill ratio varies with initial temperature (in the cylinders), which could represent the effect of ambient temperature. It can be seen that as the initial temperature increases the fill ratio decreases. This means that the driving range of CNG and CHG vehicles will decrease if filling is carried out in hot weather compared to the colder conditions. The ambient temperature has opposite effects on the final in-cylinder temperature. The final in-cylinder temperature increases as ambient temperature increases. Note again from Figure 7 that the fill ratio is higher for the real gas model in the CNG cylinder. For CHG, the fill ratio is higher for the ideal gas model.

Figure 8 shows the effect of initial cylinder and reservoir tank temperature on the filling time for the real and ideal gas models in CNG and CHG stations. As can be seen, as initial temperature increases, filling time decreases. Note from the figure that, for CNG, the filling time for the real gas model is less than for the ideal gas model. This is mainly due to less mass filled into the cylinder (see FR in Figure 7). For CHG, the FR is higher for the real gas model, so it is expected that the filling time will be higher for the ideal gas model. This can be seen in the figure.

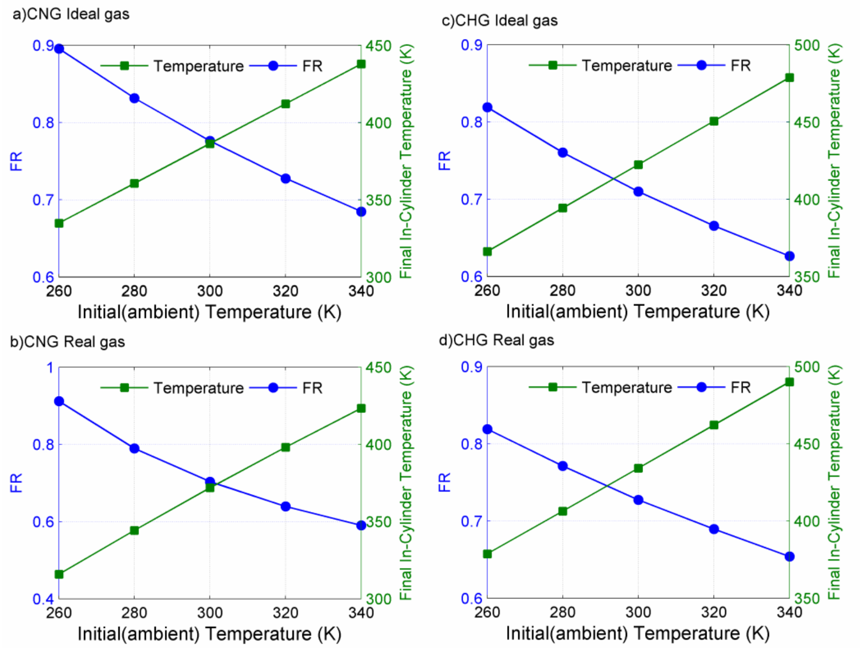

Figure 7: Effect of initial (ambient) temperature on fill ratio and final in-cylinder temperature for the ideal and real gas models.

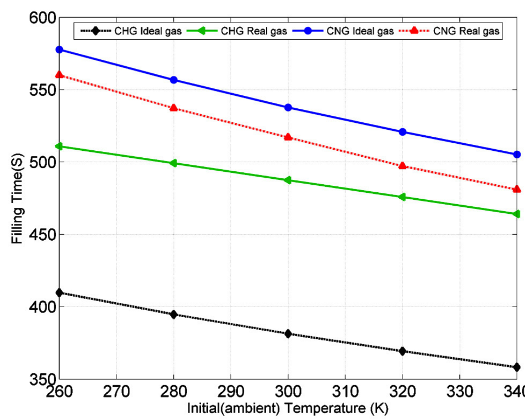

Figure 8: Effect of initial (ambient) temperature on filling time ($NP2 = 0.53$) for the ideal and real gas models in the two stations (CNG and CHG).

Figure 9 shows the effects of LPR pressure on filling time when the MPR pressure is kept constant ($NP2 = 0.53$) for the real and ideal gas models in CNG and CHG stations. As the LPR pressure ($NP1$) increases, the filling time decreases except for the ideal CNG case. For the ideal gas model in a CNG station, the maximum filling time occurs at $NP1 \approx 0.17$. As the LPR pressure ($NP1$) increases, the filling times approach each other for all cases.

Figure 10 shows the effects of MPR pressure on filling time when the LPR pressure is kept constant ($NP1 = 0.275$) for the real and ideal gas models in CNG and CHG stations. Considering the fact that reducing the filling time is a way to enhance filling station performance, a designer should seek a combination of NP1 an NP2 in which the filling time is minimized. For a constant value of $NP1 = 0.275$, there are specific values of NP2 for the models in which the filling time is maximized. So one can conclude for the real and ideal gas models in both stations (CNG and CHG) that the maximum values of the filling time are obtained as

$NP2 = 0.65$ and $NP2 = 0.55$ respectively.

It should also be noted that the filling time could also be reduced by appropriate sizing of the piping equipments (e.g., the orifice diameter).

As mentioned previously, entropy generation is associated with thermodynamic irreversibilities. Irreversibilities dissipate work into heat in the filling station. The available work is provided by the compressor, so one can conclude that, as entropy generation is decreased, available work destruction is decreased too.

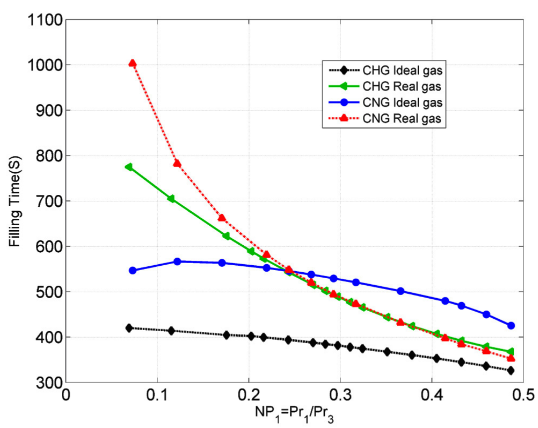

Figure 9: Effect of varying LPR pressure ($NP1$) on filling time ($NP2 = 0.53$) for the ideal and real gas models in the two stations (CNG and CHG).

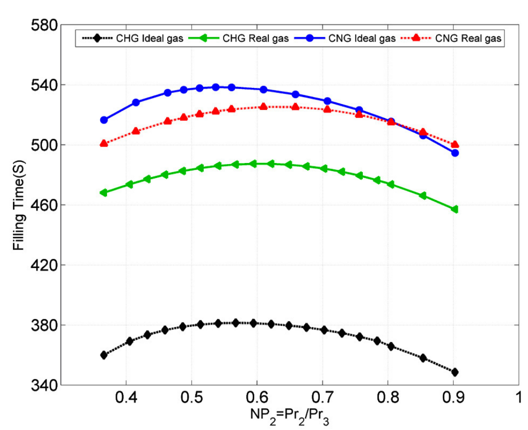

Figure 10: Effect of varying MPR pressure ($NP2$) on filling time ($NP1 = 0.275$) for the ideal and real gas models in the two stations (CNG and CHG).

Figure 11 shows the effects of LPR pressure on non-dimensional entropy generation when the MPR pressure is kept constant ($NP2 = 0.53$) for various gas models. For any gas model and station, the minimum values of non-dimensional entropy generation occur near $NP1 = 0.22$.

Figure 12 shows the effects of MPR pressure on non-dimensional entropy generation when the LPR pressure is kept constant ($NP1 = 0.275$). In both stations (CNG and CHG) the non-dimensional entropy generation for real gas is less than for the ideal gas model. Note from the figure that there is an optimum near $NP2 = 0.6$ where minimum entropy generation occurs.

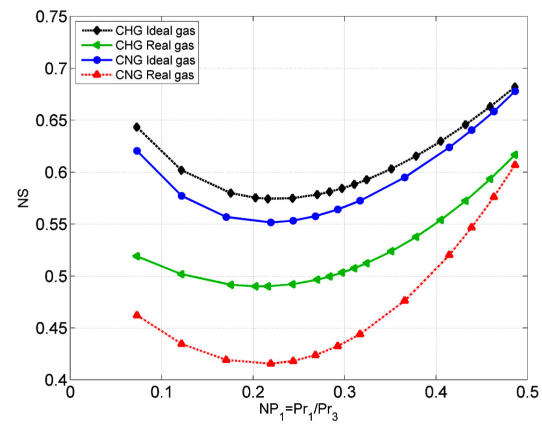

Figure 11: Effect of varying LPR pressure ($NP1$) on non-dimension entropy generation ($NP2 = 0.53$) for the ideal and real gas models in the two stations (CNG and CHG).

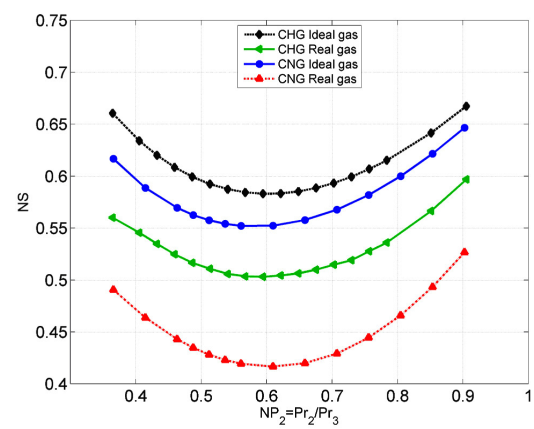

Figure 12: Effect of varying MPR pressure ($NP2$) on non-dimension entropy generation ($NP1 = 0.275$) for the ideal and real gas models in the two stations (CNG and CHG).

Considering Figures 9-10 and 11-12, it could be realized that, for each of the models in various stations, non-dimensional entropy generation and filling time profiles have opposite trends. So as entropy generation in the system decreases, the filling time increases. Because the filling time could be reduced by appropriate sizing of the piping equipment, one can conclude that an optimized thermodynamic point should be selected to enhance performance of a fuelling station.

CONCLUSION

The first and second laws of thermodynamics have been employed as theoretical tools to compare performance of cascade reservoir natural gas and hydrogen fuelling stations based on ideal and real gas models. A theoretical analysis has been developed to study and compare effects of reservoir temperature and pressure on fill ratio, filling time and entropy generation during the fast-fill process of on-board CNG and CHG cylinders.

It is found that, for both stations (CNG and CHG), as the reservoir temperature decreases, the fill ratio increases. The pressure within the filling station has no effect for ideal gas assumptions. The final in-cylinder temperature for CHG is much higher than for CNG, so for developing standards for CHG cylinders, this has to be considered.

For the real and ideal gas models in both stations (CNG and CHG), the maximum values of filling time are obtained when $NP2 = 0.65$ and $NP2 = 0.55$, respectively. This is the case when the LPR pressure is kept constant ($NP1 = 0.275$).

Non-dimensional entropy generation and filling time profiles have opposite trends and, as entropy generation in the system decreases, the filling time increases. Since the filling time could be reduced by appropriate sizing of piping equipments, one could conclude that the optimized thermodynamic point should be selected for enhancing the performance of a fuelling station.

For these filling stations (CNG and CHG), the optimized non-dimensional LPR and MPR pressures are found to be $NP1 = 0.22$ and $NP2 = 0.6$, respectively.

In the present study, some simplifications have been employed such as the adiabatic assumption for the on-board cylinder and fixed conditions of the reservoirs, which will be studied in our future work.

NOMENCLATURE

A	area	m^2
C_d	orifice discharge coefficient	
c_p , c_v	Constant pressure and constant volume specific heats	kJ/kg K
g	Gravitational acceleration	m/s^2
h	Specific enthalpy	kJ/kg
$\dot{m}$	Mass flow rate	kg/s
M	Molecular weight	kg/kmol
P	Pressure	bar or Pa
$\dot{Q}$	Heat transfer rate	kW
T	Temperature	K or °C
u	Internal energy	kJ/kg
h	Enthalpy	kJ/kg
s	Entropy	kJ/ K
t	time	S
v	Specific volume	m^3/kg
V	Volume	m^3
W	Actual work	kJ/kg
$\dot{W}$	Actual work rate	kW or MW
z	Height	m)
ρ	Density	kg/m^3
NP	Pressure Ratio	
NS	Entropy Ratio	
γ	Specific heat ratio	

Subscripts

C	NGV on-board cylinder
R	reservoir tank
i	initial or inlet condition
s	start of filling process
a, ∞	ambient
av	average
gen	generation
1	Reservoir tank 1
2	Reservoir tank 2
3	Reservoir tank 3

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