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Analytical and numerical study on the fast refill of compressed natural gas with active heat removal

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A B S T R A C T

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 during fast fill due to the recompression work of CNG in the cylinder that heats the fuel during the fill. 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. To increase the mass of dispensed CNG during fast fill, an active heat removal method is proposed. In this study, analytical and numerical models of the filling process of CNG into a Type-III cylinder with and without active 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 during fill 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 in a Type-III cylinder with and without active heat removal. 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 of the analytical/numerical study illustrate the benefit of heat removal from the cylinder as a means of improving fast-fill efficiency in natural gas fueled heavy-duty vehicles.

1. Introduction

For the past few years, natural gas has played a prominent role in energy discussions around the world (Paltsev et al., 2011; Moniz et al., 2011). 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 (Stephenson, 2016). 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 (Greene and Plotkin, 2011). Given the increasing energy demand and high greenhouse gas (GHG) emissions associated with conventional fossil fuels, Yeh (2007) 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 (Economides et al., 2006). 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 refueling, fast fill is required. As found by Kountz (1994, 1996), 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-

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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 50 °F above the ambient temperature (Kountz, 1994). 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% (Kountz, 1996).

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 re-enforcement. Type-IV cylinders have a non-metallic liner and a fully wrapped composite reinforcement (Murray et al., 1992). 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 (1998) and Newhouse and Liss (1999) 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 (Kountz, 1994, 1996; Newhouse and Liss, 1999; Shipley, 2002; Thomas et al., 2002; Farzaneh-Gord, 2008; Farzaneh-Gord et al., 2007). Kountz (1994) and Farzaneh-Gord (2008) focused on mathematical theory and modelling of CNG fast fill. Shipley (2002) experimentally measured the temperature rise of CNG with different ambient temperatures, and observed under-fill of test cylinders for all the fast fill tests. Farzaneh-Gord et al. (2007) studied the effect of initial conditions on the fill efficiency of CNG cylinders by varying the initial pressure between 1 bar and 100 bar and initial temperature between 280 K and 320 K. The same group (Farzaneh-Gord et al., 2014) also found that the composition of natural gas affects the filling process and final in-cylinder conditions, where gas with lower methane percentage in its composition yields higher fill efficiencies. Some researchers have investigated the transient thermal behaviour during gas filling by numerical methods. Dicken and Merida (2007) used computational fluid dynamics (CFD) to simulate the transient temperature distribution in the cylinder during filling of hydrogen cylinders. Nahavandi et al. also carried out CFD simulations of fast fill, comparing the temperature rise, pressure curves, and fill efficiency for natural gas (Nahavandi et al., 2013) and hydrogen (Farzaneh-Gord et al., 2012, 2013).

There have been several approaches to address fill efficiency by focusing only on the fueling station side. Kountz et al. (1997, 1998a, 1998b, 1998c) proposed a temperature-compensated procedure that minimizes the heat of re-compression by optimizing the CNG station and reservoir pressures. However, Farzaneh-Gord and Deymi-Dashtebayaz (2013) showed that this procedure requires proper fill equipment and control systems, limiting its practicality. Moreover, selecting either a buffer or cascade filling strategies does not make much different, as Deymi-Dashtebayaz (Deymi-Dashtebayaz et al., 2014) showed that while filling time of buffer systems is much less than cascade systems, the filled mass is approximately the same. Owing to the inability of these station-side approaches to improve fill efficiency, most fill procedures over-pressurize the cylinder to compensate; for a Type-IV cylinder rated at 3600 psi, over-pressurization may exceed 4100 psi, which certainly presents safety implications.

Very few of the above studies have investigated potential solutions to improve fill efficiency that act on the cylinder being filled. Because 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. The objective of the present study is to investigate the fast fill process of natural gas in Type-III cylinders with and without active heat removal in order to identify the effectiveness of heat removal for improving fill efficiency in heavy-duty vehicles. The active heat removal system involves placing cooling coils inside the cylinder through which a coolant is circulated to remove heat from the cylinder and eject it to the surroundings. The passive heat removal system involves pre-chilling thermal heat sinks in the cylinder.

The paper is structured as follows: in Sections 2 and 3, an analytical model and a two-dimensional axisymmetric CFD model incorporating real gas effects are respectively developed to predict the transient thermal-fluid behaviour of natural gas during the fill. In Section 4, the models are used to investigate the effects of heat removal rate and the location of the cooling coils on the fill efficiency. Local and average gas temperatures, pressure, and velocity distributions in the cylinder are presented at several instances during the fill to explain the physical mechanisms governing the heat removal effectiveness and the resulting fill efficiency.

2. Analytical model

2.1. Model system and assumptions

Fig. 1 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 (Kountz, 1994) (CH_4 92.87%; C_2H_6 3.34%; N_2 2.07%; CO_2 0.78%; C_3H_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

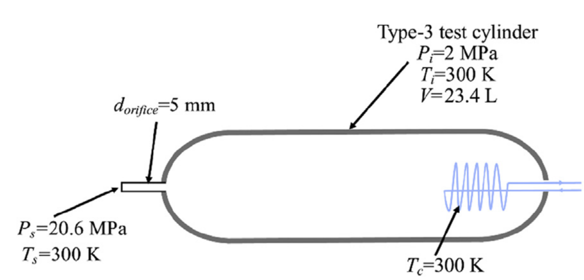

Fig. 1. Schematic diagram of the system considered in the analytical model.