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# Compressed natural gas behavior in a natural gas vehicle fuel tank during fast filling process: Mathematical modeling, thermodynamic analysis, and optimization

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ABSTRACT

Every CNG station includes two main parts: a compressor equipped with inter- and after-coolers and a fast filling process (FFP). In this study, both processes were simulated in a FORTRAN based computer program. To model the compression process of real natural gas, the polytropic work of a three-stage compressor was considered. Moreover, the FFP was modeled based on mass conservation and first law of thermodynamics for a non-adiabatic cylinder. Due to high operating pressure, AGA-8 equation of state (EOS) was utilized for accurate computation of necessary thermodynamic properties. Both applied models for compression and FFP were compared with the real data. In particular, the FFP model was evaluated using experimental data obtained from an operating compressed natural gas (CNG) station in Sanandaj, Iran. The comparison showed a good agreement between model and experimental data. In the last part of this paper, the best operating condition for attaining either the minimum energy consumption in compressors and coolers or the maximum final accumulated mass of gas within NGV cylinders was determined using particle swarm optimization (PSO) algorithm.



## 1. Introduction

From the beginning of 1980s, natural gas as a vehicle fuel has attracted considerable attentions because of its low air pollutants emission, low cost, and availability (Lozano-Castello et al., 2002; Liang et al., 2012; Martins et al., 2014; Khan and Yasmin, 2014). In comparison with liquid fuel vehicles, natural gas vehicles (NGVs) produce 87% less nitrogen oxides, 89% less non-methane organic gas, and 70% less carbon monoxide (Liang et al., 2012). Therefore, natural gas is more environmentally friendly than liquid fuels. It seems that Iran is now the world's leader in terms of natural gas vehicles. The numbers of Iran CNG vehicles in 2011 was 2.86 million. Notably, the number of CNG filling stations active in Iran is 1976 stations up to April 2013. To store natural gas, four techniques namely liquefaction (Gadhiraju et al., 2008), compression (Lozano-Castello et al., 2002), hydrate formation (Englezos and Lee, 2005), and adsorption (Lozano-Castello et al., 2002; Molashahi and Hashemipour 2012; Balathanigaimani et al., 2006) have been utilized. Among these techniques, compression is the most widely used technique in transport industries. Nowadays, CNG is used as fuel for millions of automobiles (Lozano-Castello et al., 2002; Ma et al., 2013; Khan and Yasmin, 2014). However, there are some issues about CNG filling stations that limit its applications. These issues are high refueling time, lack of natural gas refueling stations, and low driving range in comparison with gasoline (Shipley, 2002).

Long refueling time is one of the problems within NGV refueling stations. In a CNG refueling station, the natural gas of distribution pipeline is compressed from 1.5–1.7 MPa to 20.7–25 MPa using a large multi-stage reciprocating compressor. Afterward, the prepared CNG is directly dispensed from compressor to NGV cylinders. This method, which is called slow filling process, has high refueling time in comparison with gasoline dispensers. Gas industries have remedied long refueling time problems using FFP (Shipley, 2002). Filling process occurs in less than 5 minutes in FFP (Farzaneh-Gord et al., 2008). In this method, prepared CNG in compressor is stored in large supply tanks. Then, due to the high pressure difference between CNG reservoirs and NGV cylinder, CNG flows quickly toward NGV tank. There are two techniques for storing CNG in supply tanks: single gas supply tank (single storage system (SSS)) and cascade gas supply tanks (cascade storage system (CSS)). In the first technique, only single pressure reservoir is used for storing CNG. However, CSS usually comprises of three gas reservoirs that are

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termed low, medium, and high pressure supply tanks (LPST, MPST, and HPST) (Farzaneh-Gord et al., 2011).

The second problem with CNG as an alternative fuel is the unavailability of enough numbers of CNG stations due to the high exploitation costs to construct a station (Lozano-Castello et al., 2002; Shipley, 2002). On the other hand, CNG compressors are multi-stage reciprocating compressors that compress natural gas to very high pressure. As gas temperature increases during compression, a cooler is arranged after each stage. Hence, in addition to the high cost for constructing a CNG station, the compression process consumes a lot of energy (Lozano-Castello et al., 2002).

Low driving range of NGVs relative to liquid fueled vehicles is the other problem for the marketing of these vehicles (Lozano-Castello et al., 2002; Shipley, 2002). One reason for this low driving range is the low density of CNG relative to gasoline (Lozano-Castello et al., 2002). Additionally, the pressure of gas supply tanks in CNG stations is very effective on the on-board cylinder charged mass (Farzaneh-Gord et al., 2011). However, the main reason for the low driving range of NGVs lies behind the under-filling phenomenon which occurs during FFP in CNG stations. During FFP, the gas temperature within NGV fuel tank increases by 45 K (Kountz, 1994). This temperature increment stops charging process before the cylinder be really fulfilled, and consequently reduces driving range.

According to the above explanations, by reducing the filling time, compressor work, and consumed energy in coolers, and increasing the final accumulated mass of CNG in an on-board cylinder, the performance of CNG refueling stations can be significantly improved (Farzaneh-Gord et al., 2011). FFP modeling for analyzing the gas behavior in NGV cylinder provides valuable information for this purpose. This information can be useful in design or improvement of existing systems or creating new systems to ensure 100% full fill in each refueling. Modeling and simulation of compression and FFP can also be utilized as a suitable tool to obtain optimal conditions in the designing of CNG stations.

Up to now, a few experimental and theoretical studies have been carried out in the field of current study (Shipley, 2002; Farzaneh-Gord et al., 2008, 2011; Kountz, 1994). Shipley (2002) studied the FFP for a natural gas cylinder. Shipley (2002) studied the effect of ambient temperature on the FFP. He found that NGV cylinder was under filled when it was rapidly recharged. Kountz (1994) modeled the FFP of a NGV cylinder using a single gas supply tank and quantified the cylinder undercharging phenomenon. He used Peng-Robinson EOS to calculate the compressibility factor of natural gas. Farzaneh-Gord et al. (2008) developed Kountz's model for cascade gas supply tanks. They considered natural gas as pure methane in order to simplify their calculations. It must be mentioned that FFP operation accomplishes at very high pressures up to 25 MPa. In Such condition, Peng-Robinson EOS and other customary cubic EOSs are not valid. Therefore, a suitable and more accurate EOS, such as AGA-8, must be used to predict the required thermodynamic properties at this condition. AGA-8 is an accurate and complex EOS which was developed by Gas Research Institute and American Gas Association (Starling and Savidge, 2003) for calculating the Z-factor of natural gas at very high pressure conditions.

The main objective of this study was to apply a reliable mathematical model for a CNG station including compressor, coolers, and FFP. This paper also aimed to determine the best operating conditions in order to attain either the minimum consumed energy in compressor or the maximum accumulated mass in NGV fuel tank. For this purpose, the proposed study by Kountz (1994) and Farzaneh-Gord et al. (2008) were improved by developing a FORTRAN based computer program using AGA-8 EOS. To validate the FFP model, the required experimental data was obtained from a working CNG station.

## 2. Mathematical model

### 2.1. FFP

FFP was modeled based on mass conservation law together with the first law of thermodynamic. These laws were applied to a NGV fuel tank considered as a control volume with no chemical reaction involved. As NGV fuel tank had no outlet flow, output terms in applied equations were ignored. During FFP, no mechanical power was generated, and the kinetic and potential energy were neglected. On the basis of the above assumptions, mass conservation and the first law of thermodynamic were simplified as follows (Farzaneh-Gord et al., 2008; Kountz, 1994);

$$\dot{M}_i = \frac{\mathrm{d}M_\mathrm{r}}{\mathrm{d}t} \tag{1}$$

$$\dot{M}_i h_s + \frac{\mathrm{d}Q_\mathrm{r}}{\mathrm{d}t} = M_\mathrm{r}\left(\frac{\mathrm{d}u_r}{\mathrm{d}t}\right) + \dot{M}_i u_r, \quad h_\mathrm{s} = h_\mathrm{i} + \frac{V_i^2}{2} \tag{2}$$

where $\dot{M}_i$, $M_\mathrm{r}$, $h_i$, $h_s$, $V_i/2$, $u_\mathrm{r}$, and $\mathrm{d}Q_\mathrm{r}/\mathrm{d}t$ denote inlet mass flow rate to the cylinder, accumulated mass within the cylinder, specific inlet enthalpy, specific stagnation enthalpy, specific inlet kinetic energy, specific internal energy of the mass within the cylinder, and the rate of heat transfer, respectively.

Applying gas dynamics laws together with isenthalpic expansion of compressible gases through an orifice, the mass flow rate was determined as follows (Kountz, 1994):

$$\dot{M}_i = C_\mathrm{d} A_\mathrm{orifice}\left(\frac{2}{\gamma+1}\right)^{\frac{\gamma+1}{2(\gamma-1)}}\sqrt{\gamma P_\mathrm{s}\rho_\mathrm{s} Z_\mathrm{s} g_\mathrm{c}} \quad \text{if} \quad \frac{P_\mathrm{r}}{P_\mathrm{s}} \le \left(\frac{2}{\gamma+1}\right)^{\left(\frac{\gamma}{\gamma-1}\right)} \tag{3}$$

$$\dot{M}_i = C_\mathrm{d} A_\mathrm{orifice}\rho_\mathrm{s}\left(\frac{P_r}{P_s}\right)^{\frac{1}{\gamma}}\left\{g_\mathrm{c}\left(\frac{2\gamma}{\gamma-1}\right)\left(\frac{P_\mathrm{s}Z_\mathrm{s}}{\rho_\mathrm{s}}\right)\left[1-\left(\frac{P_\mathrm{r}}{P_\mathrm{s}}\right)^{\frac{\gamma-1}{\gamma}}\right]\right\}^{\frac{1}{2}} \quad \text{if} \quad \frac{P_\mathrm{r}}{P_\mathrm{s}} > \left(\frac{2}{\gamma+1}\right)^{\left(\frac{\gamma}{\gamma-1}\right)} \tag{4}$$

where, $C_\mathrm{d}$ is orifice discharge coefficient, $A_\mathrm{orifice}$ is orifice area, $\gamma$ is the ratio of specific heats, $g_\mathrm{c}$ is dimensionalizing factor, $P$ is pressure, $Z$ is compressibility factor, and $\rho$ is density. In addition, the subscripts $r$ and $s$ refer to the NGV cylinder and supply tanks, respectively.

The heat transferred from gas to the cylinder wall, $Q_\mathrm{r}$, and from the cylinder wall to ambient, $Q_\mathrm{amb}$, were calculated as follows (Kountz, 1994);

$$\frac{\mathrm{d}Q_r}{\mathrm{d}t} = -h_\mathrm{cyl}A_\mathrm{icyl}(T_\mathrm{r}-T_\mathrm{w}) \tag{5}$$

$$\frac{\mathrm{d}Q_\mathrm{amb}}{\mathrm{d}t} = h_\mathrm{amb}A_\mathrm{ocyl}(T_\mathrm{w}-T_\mathrm{amb}) \tag{6}$$

where, $h$ is heat transfer coefficient, $A$ is surface area of the cylinder, and $T$ is temperature. The subscript cyl, amb, icyl, ocyl, and w refer to cylinder, ambient, inside of the cylinder, outside of the cylinder, and the cylinder wall, respectively. Using Eqs. (5) and (6) along with the energy balance for the cylinder wall, which was imagined as a