Determining the Optimal Performance of Compressed Natural Gas (CNG) Station Based on PSO Algorithm

H.YAZDANI[1] AND S.R. MOUSAVI[2]

[1,2] *1Department of Chemical Engineering, Payame Noor University, Tehran, Iran*
[*] *Corresponding author:moosavirahil@gmail.com*

Manuscript received 31 September, 2017; Revised 07 July, 2018, accepted 19 September,2018. Paper no. JEMT-1710-1043.

In this study, an attempt is made to model the compression and fast filling processes of the compressed natural gas (CNG) and their simulation in FORTRAN programming software. In this modeling, natural gas is considered as a real gas and AGA-8 equation of state used for computing the compressibility factor and other thermodynamic properties. In order to compute compressor work, the polytropic compression process of a real gas in a three stage compressor is considered. Also, fast filling process (FFP) is modeled based on mass conservation and thermodynamics first law in a non-adiabatic cylinder. Using the aforementioned proposed model, the compressor work, lost heat in the coolers, final temperature and accumulated mass of the gas in NGV tank, fill ratio and refueling process time are computed for different pressure arrangement of the station storage tanks at five ambient temperatures. Finally, to determine the optimal operational conditions, an optimization method is performed based on the Particle Swarm Optimization (PSO) algorithm. The pressure arrangement of 4-8.1-16-20.5 MPa for the station tanks and ambient temperature 273.15 K a reported as the optimal conditions.

keywords: *Fast filling process, Compression process, Modeling and simulation, Pressure Arrangement and PSO Algorithm.*

http://dx.doi.org/10.22109/jemt.2018.103355.1043

NOMENCLATURE

Symbol:

$\dot{M}_i$ inlet gas mass flow rate Kg/s

M Natural gas mass kg

ur the specific internal energy of the gas inside the cylinder kJ/kg

hs stagnation enthalpy kJ/kg

dQ/dt the heat transferred from the wall to the ambient kJ/s

h heat transfer coefficient kW/$(m^2.K)$

A surface areas of the NGV tank m^2

Cd orifice discharge coefficient

$AOrifice$ orifice cross section m^2

gc dimensionalizing factor $(kg.m)/(N.s^2)$

R' gas constant J/Kg.K

P pressure MPa

T temperature K

V volume m^3

Z Compressibility factor

n Polytropic exponent

B Second virial coefficient $m^3/kmol$

K Mixture size parameter $(m^3/kmol)^{1/3}$

ρ_r Reduced density

C_n^* Composition dependent functions

u_n AGA 8 constant

b_n AGA 8 constant

c_n AGA 8 constant

k_n AGA 8 constant

Subscripts:

cyl cylinder

amb ambient

icyl inside of the cylinder

ocyl outside of the cylinder

w cylinder wall

s station storage tanks

r inside the NGV cylinder

In Compressor Inlet gas

out Compressor outlet gas

1. INTRODUCTION

Despite industrial improvements towards human welfare, resulting environmental pollution is a critical issue which cannot be ignored. Transportation industry is one of the main resources of air pollution in urban areas which is growing at a high rate. Therefore, reducing air pollutants such as carbon monoxide, nitrogen oxides (NO_X), carbon dioxide, air toxins like benzene, Smog-forming volatile organic compounds and aerosols has attracted great attention in the last few decades [5]. Furthermore, increasing demand for petroleum products, their supply limitation and high import cost are other reasons that motivate the need for an alternative fuel. According to abovementioned items, natural gas (NG) can be considered as a suitable vehicle fuel tank [1, 5]. Generally, NG is stored in liquefied natural gas (LNG), dissolved natural gas, compressed natural gas (CNG) and adsorbed natural gas (ANG) forms among them CNG is one of the most commonly used form in transport industry [13]. Nowadays, millions of automobiles in the world utilize CNG as their fuel [4]. However, there are some problems that affect CNG widespread utilization as an alternative fuel.

One of the reasons for the lack of CNG stations in different areas is the high cost of exploitation. Compressors, which are the heart of CNG stations, contain more than one third of the whole station cost [1, 2]. These compressors are three stage reciprocating compressors compressing NG to its desired pressure. Due to temperature increment during compression, two inter-coolers and one after-cooler are used. Therefore, consumed work and energy in these compressors and their coolers are extremely high. Hence, determining the optimal consumed energy for injecting some gas into the NGV fuel tank at a certain pressure (20.5 MPa in this study) is important [10].

NGVs low driving range considered to be another hurdle for the widespread application of CNG. Although several factors interfere in CNG popularity as an alternative fuel, under-filling phenomenon of a NGV fuel tank during fast filling process (FFP) mainly leads to low driving range [5, 23]. FFP is a process in which NGV fueling is carried out in less than five minutes. Due to short refueling period, the gas temperature will increase to 45K, resulting in under-filling of NGV tank [12, 14, 23]. Accordingly, modeling compression and cooling processes along with FFP may be a useful tool to improve the optimal conditions of a CNG station or create new systems that can provide a complete filling in each refueling [2]. Due to high pressure in NGV and storage tanks, exact experimental investigation of CNG behavior during FFP is very hard although some experimental studies have been carried out in this field [24]. Therefore, many researchers have been interested in modeling NGV refueling process since 1994. For the first time, Kountz [14] simulated FFP based on a proposed model and evaluated the effect of different factors such as the initial pressure of a NGV fuel tank, the pressure and temperature of the storage tanks on the cylinder charging process. He used Peng-Robinson equation of state to calculate NG thermodynamic properties. In this research, he considered single control volume for the station storage tanks during filling process. Kountz et al. [15–18] also proposed a control algorithm for the natural gas distributer, which can guarantees the complete filling during FFP [19, 20]. This research group has also modeled hydrogen FFP at the stations with hydrogen fuel. Among other performed researches on FFP is the hydrogen tank FFP simulation done by E.Werlen et al. [**?**]. In their work, hydrogen considered as an ideal gas. Comparing the simulation results with experimental ones, showed that the cylinder temperature may reach 358.2 K. L. N. Newhouse et al. [21] conducted some brief experimentally researches on the filling of CNG tanks by evaluating the filling efficiency of different tanks. Thomas et al. [22] evaluated the CNG distributers in a comprehensive research. Farzaneh-Gord et al. studied the effects of single and cascade storage tanks on the performance of a CNG storation theoretically [8–10]. Farzaneh et al. [19] continued the simulations done by Kountz by evaluating FFP in the case of cascade storage tanks. For simplicity, they considered NG as pure methane and used Peng-Robinson equation of state to calculate thermodynamic properties. Since FFP is performed at high pressures up to 25 MPa and the obtained results are not valid at high pressures, a more accurate equation of state such as AGA-8 should be used. This equation of state proposed by the gas association of America and the gas research center in 2003 is an accurate and complex equation of state used to calculate the natural gas compressibility factor at extremely high pressures [25]. Moosavi et al. [5] investigated CNG behavior in NGV fuel tank during FFP based on AGA-8 equation of state. In their research, NG compression and FF processes have been modeled and simulated. Finally, the optimum performance of CNG station is predicted in two individual cases; minimizing the consumed energy and maximizing the charged mass in the NGV cylinder [5]. Recently, new theoretical studies have been carried out in this field [1–5].

The main objective of this research is to find an optimal temperature and pressure arrangement of storage tanks in which the consumed work and energy of the compressor and the coolers are minimized and the accumulated gas in NGV cylinder is maximized simultaneously. To the best of our knowledge, this kind of optimization has not been carried out yet. To this end, compression and FF processes are modeled by improving previously proposed models. AGA-8 equation of state is utilized to calculate all thermodynamic properties of NG considered as pure methane.

2. MODELING

A. Fast Filling Process

Fast filling process is modeled based on two fundamental laws of mass and energy conservation. Considering some simplifying assumptions, the mass and energy conservation equations are expressed as equations (1) and (2). The assumptions are described in detail in our previous work [5].

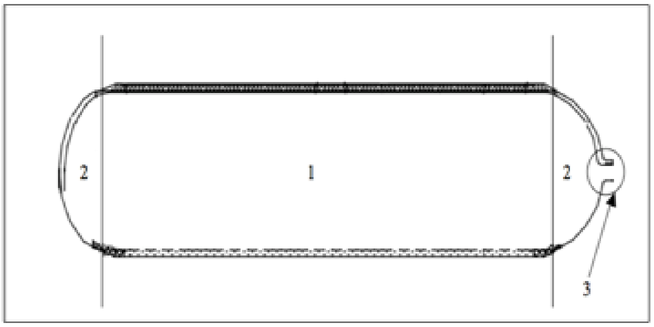

Fig. 1. CNG tank 1- Shell, 2- Concave end or cap, 3- Nozzle [20].

$$\overset{\bullet}{M}_i = \frac{dM_r}{dt} \tag{1}$$

$$\overset{\bullet}{M}_i\, h_s + \frac{dQ_r}{dt} = M_r(\frac{du_r}{dt}) + \overset{\bullet}{M}_i\, u_r \tag{2}$$

Heat transferred from CNG to the cylinder walls are calculated according to the following equations [5]:

$$\frac{dQ_r}{dt} = -h_{cyl}A_{icyl}(T_r - T_w) \tag{3}$$

$$\frac{dQ_{amb}}{dt} = h_{amb}A_{ocyl}(T_w - T_{amb}) \tag{4}$$

According to Fig. 1, a CNG cylinder is composed of a cylindrical shell, two concave or semi spherical ends and a nozzle. However, the volume of a NGV tank occupied by CNG is the volume of the cylindrical shell and two hemispheres. The relevant equations are explained in detail in our previous work [5].

Inlet gas flow rate to the NGV tank has been determined by the isentropic relations of compressible gases [5].

$$\overset{\bullet}{M}_i = CC_dA_{orifice}\left(\frac{P_s}{\sqrt{T_s}}\right) f\left(\frac{P_r}{P_s}\right) \tag{5}$$

$$C = \sqrt{\frac{g_c\gamma}{R'\left(\frac{\gamma+1}{2}\right)^{\left(\frac{\gamma+1}{\gamma-1}\right)}}} \tag{6}$$

$$\left(\frac{P_r}{P_s}\right)_{crit} = \left(\frac{2}{\gamma+1}\right)^{\left(\frac{\gamma}{\gamma-1}\right)} \tag{7}$$

$$f\left(\frac{P_r}{P_s}\right) = 1 \text{for} \frac{P_r}{P_s} \leq \left(\frac{P_r}{P_s}\right)_{crit} \tag{8}$$

$$f\left(\frac{P_r}{P_s}\right) = \left(\frac{P_r}{P_s}\right)^{\left(\frac{1}{\gamma}\right)} \sqrt{\left(\frac{2}{\gamma-1}\right) \quad \left(\frac{\gamma+1}{2}\right)^{\left(\frac{\gamma+1}{\gamma-1}\right)}} \sqrt{1-\left(\frac{P_r}{P_s}\right)^{\left(\frac{\gamma-1}{\gamma}\right)}} \quad for \quad \frac{P_r}{P_s} > \left(\frac{P_r}{P_s}\right)_{crit} \tag{9}$$

By solving the main differential equations (1) and (2) by Runge-Kutta fourth-order method [5,27] along with the above-mentioned relations, the internal energy and molar specific volume of the gas have been determined. Knowing these two thermodynamic properties, the gas pressure and temperature are also determined.

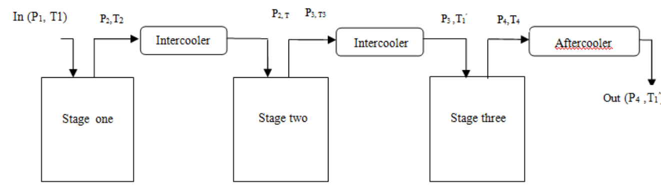

Fig. 2. Three stage compressors with inter- and after-coolers.

B. Compression Process

NG compression process is carried out through a three-stage compressor. The block diagram of CNG compressors is illustrated in Fig. 2 [5]. According to Fig. 2, total consumed work is the sum of the works done in each stage as follows:

$$W = \frac{n_1Z_1RT_1}{n_1-1}\left[\left(\frac{P_2}{P_1}\right)^{\frac{n_1-1}{n_1}} - 1\right] + \frac{n_2Z_2RT'_1}{n_2-1}\left[\left(\frac{P_3}{P_2}\right)^{\frac{n_2-1}{n_2}} - 1\right] + \frac{n_3Z_3RT'_1}{n_3-1}\left[\left(\frac{P_4}{P_3}\right)^{\frac{n_3-1}{n_3}} - 1\right] \tag{10}$$

To determine equation (10), some simplifying assumptions have been considered which explained in our previous work [5].

In order to find minimum consumed work, the best values for inter-stage pressures (P_2, P_3) should be determined [?, 5]. Hence, equation (10) which is differentiated relative to inter-stage pressures, must be equal to zero. Considering $a_1 = \frac{n_1-1}{n_1} a_2 = \frac{n_2-1}{n_2}, a_3 = \frac{n_3-1}{n_3}$, spartial derivative calculated by equations (11) and (12):

$$\frac{\partial W}{\partial P_2} = Z_1RT_1\left[\left(P_1{}^{(-a_1)}\right)\left(P_2{}^{(a_1-1)}\right)\right] - Z_2RT'_1\left[\left(P_3^{a_2}\right)\left(P_2^{(-a_2-1)}\right)\right] + \frac{RT'_1}{a_2}\left[\left(\frac{P_3}{P_2}\right)^{a_2} - 1\right]\left(\frac{\partial Z_2}{\partial P_2}\right)_{T'_1} = 0 \tag{11}$$

$$\frac{\partial W}{\partial P_3} = Z_2RT'_1\left[\left(P_2{}^{(-a_2)}\right)\left(P_3{}^{(a_2-1)}\right)\right] - Z_3RT'_1\left[\left(P_4{}^{a_3}\right)\left(P_3^{(-a_3-1)}\right)\right] + \frac{RT'_1}{a_3}\left[\left(\frac{P_4}{P_3}\right)^{a_3} - 1\right]\left(\frac{\partial Z_3}{\partial P_3}\right)_{T'_1} = 0 \tag{12}$$

The aforementioned equations are solved numerically by Newton-Raphson [27] method via trial and error.

C. Cooling Process

According to the first law of thermodynamics, the lost heat in coolers is equal to the difference between the inlet and outlet enthalpies. Neglecting the pressure drop in coolers, the total wasted heat in a three stage compressor is simplified as follows:

$$Q_{cooling} = Q_{cooling_1} + Q_{cooling_2} + Q_{cooling_3} = -\int_{T'_1}^{T_2} c_{m,P}dT - \int_{T'_1}^{T_3} c_{m,P}dT - \int_{T'_1}^{T_4} c_{m,P}dT \tag{13}$$

Since the specific heat capacity is not constant, equation (13) is solved numerically by Romberg [27] method.

D. Thermodynamic Properties

D.1. AGA-8 equation of state

AGA-8 equation of state is a semi-empirical equation used to calculate compressibility factor, density, heat capacity, internal energy and isentropic power of natural gas. It is necessary to mention that this equation of state can be utilized based on two different computational methods namely detail and gross characterization methods. In this research, the detail characterization method has been used for which the value of the compressibility factor is determined according to equation (14):

$$Z = 1 + \frac{B\rho_r}{K^3} - \rho_r \sum_{n=13}^{18} C_n^* T^{-u_n} + \sum_{n=13}^{58} C_n^* T^{-u_n} (b_n - c_n k_n \rho_r^{k_n}) \rho_r^{b_n} \exp(-c_n \rho_r^{k_n}) \quad (14)$$

ρ_r K B and C_n^* are also determined by some equations [24]. In order to determine other thermodynamic properties, different partial derivatives of compressibility factor have been calculated. The derivatives along with other required equations are represented in literature [30–32].

3. RESULTS AND DISCUSSIONS

Validation of the proposed models for compression and FF processes have been investigated. Despite some errors, the simulation results have had good agreement with experimental data. So, the models are applied to determine the parameters required for optimization. The comprehensive evaluations of the models are represented in our previous work [5]. As explained in our previous work, 144 and 588 pressure arrangements have been determined for three and four cascade storage tanks (CSTs), respectively [5]. The parameters of compression and FF processes are calculated for each pressure arrangement, considering NG as pure methane. The results are obtained at 5 ambient temperatures of 273.15 K, 288.15 K, 298.15 K, 313.15 K and 318.15K.

As stated earlier, the main objective of this research is to achieve the optimum conditions for CNG station i.e. the optimum pressure arrangement of the storage tanks and ambient temperature under which the least consumed work and energy in compressor and coolers and the most accumulated CNG in NGV tank are obtained simultaneously. In our previous work, minimizing the total energy consumption in compressors and coolers and maximizing the final accumulated mass of gas within the NGV tank have been evaluated in two individual cases.

Optimum point is determined using the Particle Swarm Algorithm (PSO). PSO is an algorithm in which a group of particles are appeared randomly at the beginning. These random particles then search for the optimal solution by updating the generations. At each step, each particle is updated by the best two values. The first case is the best location that the particle has reached. This location is recognized and kept. The other best value used by the name pbest is the best location that is reached by the particle swarm. This location is represented by gbest. After finding the best values, each particle velocity and location is updated using equations (15) and (16).

$$V[] = V[] + c_1 * rand() * (pbest[] - position[]) + c_2 * rand() * (gbest[] - position[]) \quad (15)$$

$$position[] = position[] + V[] \quad (16)$$

A. Optimization results

The results of optimization are presented in Tables 1 and 2 for three and four CSTs, respectively. According to the results presented in these tables, it can be observed that the optimal pressure arrangement for each of the five ambient temperatures is similar (4-9.1-20.5 and 4-8.1-16-20.5 for three and four CSTs, respectively). In this optimal pressure arrangement, lower ambient temperatures lead to better results. Moreover, the consumed work and energy of the compressors and coolers are less at lower ambient temperatures. Comparing the results obtained for the amount of mass charged in the NGV tank and the consumed energy at different ambient temperatures, it can be derived that a desired result can be achieved at 273.15 K ambient temperature. Furthermore, the consumed work and energy in compressors and coolers have increased with ambient temperature. The reason lies behind the increment of gas temperature during inter-stage compression. The inlet gas with high temperature consumes more energy in the coolers. As the inlet gas temperature is considered the same as ambient temperature, the consumed work and energy in compressors and coolers has increased with ambient temperature.

Table 1. The optimum results for three CSTs

$T_{amb}(k)$	273.15	288.15	298.15	313.15	318.15
$P_{s_1}(MPa)$	4.0	4.0	4.0	4.0	4.0
$P_{s_2}(MPa)$	9.1	9.1	9.1	9.1	9.1
$P_{s_3}(MPa)$	20.5	20.5	20.5	20.5	20.5
$t_m(s)$	66.8	63.4	61.5	59.1	58.4
$T_r(k)$	325.273	344.791	357.663	376.625	382.84
$M_r(Kg)$	3.1509	2.8565	2.6943	2.4913	2.4331
FR	0.7931	0.719	0.6782	0.6271	0.6124
$Rwork(kJ/Kg)$	300.752	320.906	333.859	352.76	359.006
$Tecooling(kJ/Kg)$	403.824	410.163	415.323	424.231	427.548

According to these tables, the results follow a similar trend for both three and four CSTs. Final temperature of the gas in NGV tank increases with ambient temperature. Because the kinetics energy of high speed inlet gas converts to the internal energy during FFP, a significant temperature rise occurs which leads to pressure increment before fulfilling the tank. Therefore, accumulated mass in the NGV tank and consequently, the fill ratio decrease with increasing temperature. As the pressure within the NGV tank reaches more rapidly to the desired value (20.5 MPa), refueling time becomes shorter with increasing ambient temperature. According to abovementioned explanations, the optimal condition occurs at 273.15 K ambient temperature. Comparing the best final results of three and four CSTs, it can be derived that despite more energy in three CST, no significant change appears in the cylinder stored mass. Thus, the four CST is optimal.

4. CONCLUSION

In this research, thermodynamic simulations of the compression and fast filling processes have been performed based on AGA-8 equation of state. These simulations are used to estimate the consumed work and energy in CNG compressors and coolers and to analyze FFP. Therefore, the compressor work, lost heat in the coolers and also the final condition of the cylinder have been calculated at different pressure arrangements of the three and four CSTs for five different ambient temperatures. In the following, optimization is performed for three and four CSTs based on PSO algorithm. The optimum condition is considered as a point in which the least consumed work and energy in compressor

Table 2. The optimum results for four CSTs

$T_{amb}(k)$	273.15	288.15	298.15	313.15	318.15
$P_{s_1}(MPa)$	4.0	4.0	4.0	4.0	4.0
$P_{s_2}(MPa)$	8.1	8.1	8.1	8.1	8.1
$P_{s_3}(MPa)$	16.0	16.0	16.0	16.0	16.0
$P_{s_4}(MPa)$	20.5	20.5	20.5	20.5	20.5
$t_m(s)$	75.0	71.1	68.8	66.2	65.3
$T_r(k)$	327.982	347.591	360.406	379.12	385.241
$M_r(Kg)$	3.1057	2.8185	2.6623	2.4683	2.4108
FR	0.7818	0.7094	0.6701	0.6213	0.6068
$Rwork(kJ/Kg)$	285.936	305.258	317.69	335.891	341.812
$Tecooling(kJ/Kg)$	380.809	386.817	391.872	400.767	403.948

and coolers and the most accumulated CNG in NGV tank are obtained simultaneously. Comparing the optimum results of three and four CSTs with each other, the best results can be achieved through four CSTs (4-8.1-16-20.5) at 273.15 K ambient temperature. The results of FFP show that the temperature increment inside the cylinder is the main reason of NGV tank under-filling. As the temperature increases during FFP, the gas pressure inside the NGV fuel tank increases rapidly to its desirable pressure, resulting in NGV tank under-filling.

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