Effects of natural gas compositions on CNG (compressed natural gas) reciprocating compressors performance

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A B S T R A C T
The aim of the current work is to investigate the effects of natural gas compositions on reciprocating compressor performance numerically. A numerical model has been built based on first law of thermodynamics, mass balance, AGA8 EOS (Equation of State) and thermodynamics relationships. The model could predict compressor parameters (pressure, temperature, mass flow rate, mass and valves motions) at various crank angles and cylinder volume. For validation, the numerical results are compared with previous experimental values and good agreement is encountered. The impact of key parameters such as: clearance, angular speed and molecular weight of natural gas have been investigated on the compressor performance. The results show that, for natural gas with higher molecular weight, suction valve opening time is less than natural gas with lower molecular weight. Also, the consuming indicated work per cycle for natural gas with lower molar weight (Khangiran composition with 98% methane) is approximately 50 kJ/kg more than higher molar weight (Ghasoo gas with 79% methane).

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1. Introduction
Reciprocating compressors are utilized extensively in various industries such as: power plants and refineries, refrigeration systems and CNG stations (Compressed Natural Gas stations). The key feature of these compressors is high pressure ratio achievement.

A reciprocating compressor is the heart of any CNG station. In CNG station, natural gas must be compressed from the distribution pipeline pressure (about 0.5 MPa) to a much higher value (20 MPa–25 MPa) [1,2]. This pressure rise is done by employing a multi-stage compressor (three or four stages). A major part of the initial and current costs of CNG stations are dependent on reciprocating compressor. Also, one of the greatest difficulties in CNG stations is high work required for compressing natural gas [2]. Accurate modeling of CNG compressors could improve design parameters that lead to efficiency enhancement and required work reduction.

There are two main methods for simulating reciprocating compressor. These are global and differential methods, which in both methods; the variables depend on crank angle [3]. Stouffs et al. [3] presented a global method for studying reciprocating compressors performance. They calculated the effective parameters such as: the indicated work per unit mass and volumetric effectiveness. In another work, Armaghani et al. [4] developed a simple global method to investigate the effect of engine speed on thermodynamics properties of an air reciprocating compressor. Their method was able to predict the volumetric effectiveness, the specific work and the indicated efficiency of the air typical compressor at different operating pressure ratios. Farzaneh-Gord et al. [5,6] have also developed a thermodynamic model for analyzing reciprocating compressors. In the study, they presented a method for determining optimized design parameters of an air compressor.

Casting et al. [7] presented a dynamic simulation and experimental validation of reciprocating compressors. Their research showed that the dead volumetric ratio and a friction factor have influences on volumetric efficiency and effective efficiencies respectively. Porkhial et al. [8] have developed a numerical program for compressors and compared the results with numerical studies by applying mass and energy balances. Pe’rez-Segarra et al. [9] did a detailed thermodynamic analysis of reciprocating compressors.
They focused on the volumetric efficiency, the isentropic efficiency, and the combined mechanical—electrical efficiency.

Elhaj et al. [10] have presented a numerical analysis for predictive behavior of two-stage reciprocating compressor. Winandy et al. [11] presented a simple model for investigating reciprocating compressor performance. In their study, the main objective was the calculating the required work and discharge temperature. Also Ndiaye et al. [12] presented a dynamic model of a hermetic reciprocating compressor in on-off cycling operation. Enrico Da Riva et al. [13] calculated the performance of a semi-hermetic reciprocating compressor that has been installed in a heat pump for generating 100 kW heating capacity. Damle et al. [14] presented a numerical model to foretell the thermodynamic parameters and power consumption of the compressor during compression process. Also Negrao et al. [15] studied the behavior of reciprocating compressor based on a semi-empirical numerical simulation. In the study, they calculated the variation of power consuming based on producer details. Yuan Ma et al. [16] presented a numerical program for analyzing the valves movement of CO₂ compressor. They compared the numerical result with the experimental values.

Natural gas is a mixture of various hydrocarbon molecules such as methane (CH₄), ethane (C₂H₆), propane (C₃H₈), butane (C₄H₁₀) and inert diluents such as molecular nitrogen (N₂) and carbon dioxide (CO₂). Several parameters affect the natural gas composition variations which is including geographical source, time of year, and treatments applied during production or transportation [17,18]. Therefore, natural gas does not describe a single type of fuel or a narrow range of characteristics [19,20]. For accurate studying natural gas process, it is essential to know thermodynamic properties of natural gas. To achieve this goal, AGA8 equation of state (EOS) could be employed [21,22]. American Gas Association has provided the AGA8 equation of state [21,23]. It incorporates both theoretical and empirical elements. This has provided the correlation with the degree of numerical flexiblity needed to achieve high accuracy for the compressibility factor and density of natural gas for custody transfer.

Reciprocating compressors is also employed in NG (Natural Gas) industry such as CNG stations. By modeling NG reciprocating compressors, it is possible to study effects of various parameters on their efficiency and to identify the optimum design parameters. The improvement of design parameters of these compressors leads to higher compressor performance. Also by modeling these compressors, it is possible to diagnosis possible defect which decrease compressor performance.

The objective of this work is to study effects of natural gas compositions on the reciprocating compressors performance thermodynamically. The thermodynamic simulation is based on first law of thermodynamics, conservation of mass and considering natural gas as a real gas mixture. In the current study, four typical natural gas compositions including: Khangiran, Kangan, Pars and Ghashoo has been selected for investigation. These gases have been selected due to highest different in their compositions among Iranian natural gases fields. Since it may be necessary to increase the pressure of sour natural gas, the Ghashoo gas composition (as sour gas with H₂S about 6.32 present) was also considered.

3. Methodology

Fig. 1 shows a schematic diagram of a typical NG reciprocating compressor with spring type suction and discharge valves. The connecting rod converted the reciprocating movement of piston to the rotary movement of crankshaft. NG within cylinder is assumed as a lump open thermodynamic system. It is also assumed that no leakage take place. The governing equation for thermodynamic modelling of reciprocating compressor is presented in the following sections.

3.1. First law equation

To develop a numerical model, the first law of thermodynamics, conservation of mass and AGA8 equation of state have been employed. As shown in Fig. 1, the interior of the cylinder is

<table>
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<th>Component</th>
<th>Mole fraction (%)</th>
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<td>C₆H₁₄</td>
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</table>
considered as a control volume. The boundaries of control volume consist of the cylinder wall, cylinder head and piston end face. The first thermodynamic law could be written as follow:

\[
Q_{cv} + \sum m_{i}\left(h_{i} + \frac{Ve^{2}}{2} + gz_{i}\right) = \sum m_{d}\left(h_{d} + \frac{Ve^{2}}{2} + gz_{d}\right)
\]

\[
+ \frac{d}{dt} \left[ m \left( u + \frac{Ve^{2}}{2} + gz \right) \right]_{cv}
\]

\[+ W_{cv}
\]

(1)

where \( W, h, u, Ve, m, z, g \) and \( Q \) are work rate, enthalpy, internal energy, velocity, mass flow rates, altitude, acceleration of gravity and heat transfer respectively. Also \( s, d \) and \( cv \) subscripts stand for suction, discharge and control volume conditions. By ignoring variations of kinetic and potential energies, the equation (1) could be simplified as follow:

\[
\frac{dQ_{cv}}{dt} = dm_{s}h_{s} = dm_{d}h_{d} + d\left( mu_{cv}\right) + dW_{cv}
\]

(2)

The variation in work can be calculated as follow:

\[
\frac{dW_{cv}}{dt} = P_{cv}dV_{cv}
\]

(3)

In equation (3) \( P \) and \( V \) are pressure and volume respectively. By replacing equation (3) in equation (2), the equation (4) can be acquired:

\[
\frac{dQ_{cv}}{dt} = dm_{s}h_{s} = dm_{d}h_{d} + d\left( mu_{cv}\right) + P_{cv}\frac{dV_{cv}}{dt}
\]

(4)

Also, differentiating respect to time could be converted to crank angle by considering the following equation:

\[
d = \frac{d}{d\theta} = \frac{d\theta}{dt} = \omega \frac{d}{d\theta}
\]

(5)

Where \( \theta \) and \( \omega \) are the crank angle and rotational speed of the crank shaft respectively. Finally, the first law of thermodynamic could be modified as below:

\[
\frac{dQ_{cv}}{d\theta} = dm_{s}h_{s} = dm_{d}h_{d} + d\left( mu_{cv}\right) + P_{cv}\frac{dV_{cv}}{d\theta}
\]

(6)

3.2. Piston motion equation

The accurate instantaneous piston displacement from top dead center in terms of the crank angle could be presented as [25]:

\[
x(\theta) = \frac{S}{2} \left[ 1 - \cos \theta + \frac{L}{a} \left( 1 - \sqrt{1 - \left( \frac{a}{L} \sin \theta \right)^{2}} \right) \right]
\]

(7)

where \( a, L \) and \( S \) are lengths of rod, crank and stroke respectively. The momentarily volume of cylinder is obtained as [25]:

\[
V_{cv}(\theta) = A_{cv} \times S(\theta) + V_{0}
\]

(8)

where \( V_{0} \) is the dead volume.

3.3. Conservation of mass

Considering the control volume of Fig. 1, the conservation of mass equation could be written as follows:

\[
\frac{dm_{cv}}{dt} = m_{s} - m_{d}
\]

(9)

By replacing equation (5) in equation (9), the conservation of mass equation could be rewritten as:

\[
\frac{dm_{cv}}{d\theta} = \frac{1}{\omega} \left[ m_{s} - m_{d} \right]
\]

(10)

where \( m_{s} \) and \( m_{d} \) are the mass flow rates through suction and discharge valves respectively, which are computing from following equations [26,27]:

\[
m_{s} = \begin{cases} 
C_{ds}P_{s}A_{s}\sqrt{\frac{2(P_{s} - P_{cv})}{P_{s}}} & \text{for } P_{s} > P_{cv} \text{ and } x_{s} > 0 \\
-C_{ds}P_{cv}A_{s}\sqrt{\frac{2(P_{cv} - P_{s})}{P_{cv}}} & \text{for } P_{cv} > P_{s} \text{ and } x_{s} > 0 
\end{cases}
\]

(11)

\[
m_{d} = \begin{cases} 
C_{dd}P_{d}A_{d}\sqrt{\frac{2(P_{d} - P_{cv})}{P_{d}}} & \text{for } P_{d} > P_{cv} \text{ and } x_{d} > 0 \\
-C_{dd}P_{cv}A_{d}\sqrt{\frac{2(P_{cv} - P_{d})}{P_{d}}} & \text{for } P_{cv} > P_{d} \text{ and } x_{d} > 0 
\end{cases}
\]

(12)

where \( A_{s} \) and \( A_{d} \) are the flow areas through the suction and discharge valves. They are obtained by:

\[
A_{s} = 2\pi x_{s}r_{s} \quad A_{d} = 2\pi x_{d}r_{d}
\]

(13)

where \( x_{s} \) and \( x_{d} \) are the suction and discharge displacement from the closed valve position, and, \( r_{s} \) and \( r_{d} \) are radius of suction and discharge valves respectively.

Due to non-ideality of the valve, it does not shut down instantaneously as soon as a negative pressure difference is created from its reference motion, turn the direction and shut the opening. Coefficient of \( C_{ds} \) and \( C_{dd} \) account these non-ideality of valves.

3.4. Valve movement equation

The valve dynamic equations are derived based on the following assumption:

(i) The valve is considered as a single degree of freedom system.
(ii) The valve plate is rigid.
(iii) The valve displacement is restricted by a suspension device.

Reference point of motion is the closed position of the valve. The valves do not have any negative displacement. Considering the forces acting on the valve plates, the general equation of motion for a valve plate is then given by Ref. [28]:

\[
\frac{d^{2}x_{s}}{d\theta^{2}} = \frac{1}{m_{s}\omega^{2}} \left\{ -k_{s}x_{s} + C_{fs}A_{s}(P_{s} - P_{cv}) + F_{ps} \right\} \text{ for } x_{s} > 0 \text{ and } x_{s}^{max} > x_{s}
\]

(14)

\[
\frac{d^{2}x_{d}}{d\theta^{2}} = \frac{1}{m_{d}\omega^{2}} \left\{ -k_{d}x_{d} + C_{fd}A_{d}(P_{cv} - P_{d}) + F_{pd} \right\} \text{ for } x_{d} > 0 \text{ and } x_{d}^{max} > x_{d}
\]

(15)

where \( F_{ps} \) and \( F_{pd} \) are pre-load forces, that these forces are neglected respect to the other forces. Also \( m_{s} \) and \( m_{d} \) are masses
of suction and discharge, respectively. Coefficient of $C_f$ and $C_d$ account loss of the energy due to the orifice flow and these coefficients can be obtained from previous study [29].

### 3.5. Heat transfer equation

Heat transfer due to convection in compression chamber can be calculated for each crank angle from below equation [30–37]:

$$\frac{dQ}{d\theta} = \frac{\alpha A}{\omega} (T_{cv} - T_w)$$

(16)

where $\alpha$, $A$, $T_{cv}$ and $T_w$ are the heat transfer coefficient, surface area in contact with the gas, the in-cylinder gas temperature and the wall temperature respectively. Adair et al. [30] observed that the cylinder wall temperature varies less than $\pm 1$ °F, as a result the wall temperature is assumed constant.

To calculate convective heat transfer coefficient, $\alpha$, the Woschni correlation has been employed [31]. This correlation is originally derived for internal combustion engine. The correlation could also predict the heat transfer rate during compression stage of engine motion. Consequently, it could be used to model heat transfer in a reciprocating compressor. According to the correlation, the heat transfer coefficient is given by:

$$\alpha = 3.26D^{-0.2}p^{0.8}T^{-0.55}V_p^{0.8}$$

(17)

where, $V_p$ and $D$ are the characteristic velocity of gas and diameter of the cylinder respectively. According to Woschni correlation, the correlation characteristic velocity for a compressor without swirl is given as [31]:

$$V_p = 2.28Ve\rho$$

(18)

where, $Ve\rho$ is average velocity of the piston.

### 3.6. Procedure for calculating thermodynamic properties

Clearly for obtaining in-control volume properties, in first step, the two independent thermodynamic properties should be calculated and then other thermodynamics properties could be computed. In this study, the two independent thermodynamic properties are density and internal energy. By using conservation of mass and first law of thermodynamic equations, density (or specific volume) and internal energy could be calculated firstly. Then, AGA8 EOS has been used for computing thermodynamic properties of natural gas mixture as real gas (See Appendix A). Farzaneh-Gord and Rahbari [23] have provided the detailed procedure of calculation natural gas thermodynamics properties.

### 4. Numerical procedure

As mentioned in the previous section, first law and conservation of mass equations are employed to calculate two independent thermodynamic properties. These equations are discretized as follow [25]:

$$\frac{\Delta m_{cv}}{\Delta \theta} = \frac{m_{cv} - m_d}{\omega} \Rightarrow m_{cv}^{i+1} - m_{cv}^i = \Delta \theta (\frac{m_{cv}^i - m_d}{\omega}) \Rightarrow m_{cv}^{i+1} = m_{cv}^i + \Delta \theta \left(\frac{m_{cv}^i - m_d}{\omega}\right)$$

(20)

By using Runge-kutta method, the specific internal energy and $m_{cv}$ are calculated from equations (19) and (20) for each crank angle. Finally by knowing in-cylinder volume, one could calculate density at each crank angle as:

$$\rho^{i+1} = \frac{m_{cv}^{i+1}}{V_{cv}^{i+1}}$$

(21)

These two thermodynamic properties (density and specific internal energy) are enough to identify other thermodynamic properties. For calculating pressure and temperature for each time step, thermodynamic table which formed based on AGA8 EOS, are used. The table is arranged according to internal energy ($u$) and density ($\rho$). Functions of pressure and temperature are prepared by Curve fitting method.

**Fig. 2.** Flowchart of extended AGA8 model. As illustrated in the figure, the input of the algorithm is internal energy, density and natural gas composition. These two thermodynamic properties (density and specific internal energy) are enough to identify the other thermodynamic properties (temperature, pressure).

The calculation continues until the crank angle is smaller than or equal to 360° (or $\theta < 360$).

The values of work and indicated work per in-control volume mass are also calculated as the following equations:

$$\Delta m_{cv} = \frac{m_{cv} - m_d}{\omega} \Rightarrow m_{cv}^{i+1} - m_{cv}^i = \Delta \theta \left(\frac{m_{cv}^i - m_d}{\omega}\right) \Rightarrow m_{cv}^{i+1}$$

$$= m_{cv}^i + \Delta \theta \left(\frac{m_{cv}^i - m_d}{\omega}\right)$$

Fig. 2. Flowchart of extended AGA8 model.
\[ W = \frac{F}{C_2} P dV = \frac{F}{C_2} \sum_{j=1}^{N} P_j dV_j \quad (22) \]

\[ W_{\text{Indicated}} = \frac{1}{m_{cv}} \int P_d V = \frac{1}{m_{cv}} \sum_{j=1}^{N} P_j dV \quad (23) \]

In which \( N \) and \( F \) are the number of steps and the frequency respectively. Frequency could be obtained as:

\[ F = 2\pi \times \omega \quad (24) \]

5. Results and discussion

Firstly, for validation the numerical method, the numerical results have been compared with available experimental values [38]. Venkatesan et al. [38] reported in-cylinder parameters variation for a reciprocating air compressor experimentally. Fig. 3 compares the in-cylinder pressure variation between numerical results and experimental values [38]. For experimental values, the volume displaced by the piston is larger than the amount of air entering into the cylinder during suction period. The suction and discharge pressures are assumed constant in the numerical study. As a result, a decrease in cylinder pressure is anticipated for the experimented case. This could be observed in the figure. Similarly, the volume displaced by the piston is greater than the volume of air discharged through discharge port for the experimented case during discharge period. Therefore, an increase in cylinder pressure is anticipated. Table 2 presents a comparison between numerical and experimental values of peak pressure and volume flow rate. Generally, there are a good agreement between the measured and numerical values.

The remaining results are for a specific compressor with NG as working fluid. The basic specifications required for modeling the reciprocating NG compressor are listed in Table 3. This information includes the geometric properties and thermodynamic conditions. The effects of various parameters are also investigated in separate sections.

Fig. 4 shows the variation of in-cylinder pressure for various natural gas compositions versus a) cylinder volume and b) crank angle. The modeling starts from TDC (Top Dead Center) where cylinder volume is same as clearance volume. By piston movement from TDC towards BDC (Bottom Dead Center), the cylinder volume is increasing and consequently pressure is reducing. For all natural gas compositions, graphs are coincidence until suction valve is opened. For all figures in this section (Figs. 5–9), once suction valve is opened suction process starts. The figure clearly shows the significantly of natural gas compositions on the pressure profiles.

Variation of in-cylinder temperature for various natural gas compositions versus a) cylinder volume and b) crank angle has been presented in Fig. 5. At the beginning of suction process,

Table 2

<table>
<thead>
<tr>
<th>Peak pressure (bar)</th>
<th>Free air delivered (liter/min)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Experimental [39]</td>
<td>11.58</td>
</tr>
<tr>
<td>Predicted</td>
<td>11.51</td>
</tr>
<tr>
<td>Error (%)</td>
<td>0.6</td>
</tr>
</tbody>
</table>

Fig. 4. Variation of in-cylinder pressure for various natural gas compositions versus a) cylinder volume and b) crank angle.
temperature decreases by suddenly entering high pressure NG into the cylinder. Then an increasing trend starts till half of the cycle. Temperature drop in suction process is mainly due to the specific volume decrement and Joule-Thomson effect. NG is a real gas with positive Joule–Thomson coefficient so temperature drop due to pressure drop is expected. As shown this figure, the final in-cylinder temperature is highest for the Kangiran gas composition with lowest molar weight (highest methane percentage).

Fig. 6 shows the variations of a) suction and b) discharge valves motion for various natural gas compositions versus crank angle. The figure illustrates that valves vibration happens during opening and closing time. As showed in this figure, with increasing the molecular weight of natural gas, the valves opening time increases.

Fig. 7 illustrates a) suction and b) discharge mass flow rates for various natural gas compositions versus crank angle. It could be realized that there is backward flow for suction valve. Note from the figure, the suction and discharge mass flow rates is highest for the Ghashoo gas composition with highest molar weight (lowest methane percentage). This is mainly due to higher density for such gas. The figure shows the significantly of natural gas compositions on the mass flow rate profiles.

Fig. 8 shows the variation of a) in-cylinder mass and b) density for various natural gas compositions as a function of crank angle. The mass of NG within cylinder are raised while the suction port is open. Then, it stays on a specific value for each natural gas composition during the compression process. By opening the
discharge port, a sudden discharge happens at the beginning but it continues with a more balanced procedure afterwards. Also as expected (due to higher density), the in-cylinder mass of Ghasoo composition is higher comparing to other natural gas compositions. This again shows the significance of natural gas compositions on the process. More explanation could be argued that the density of the NG is higher for low methane percentage comparing to the high methane composition. For this reason, the mass flow rate that entering control volume is higher for composition with low methane percentage and consequently, in-cylinder mass is higher for these compositions (for example Ghashoo).

5.1. Effect of angular speed on compressor performance for various natural gas compositions

In this section, the effects of angular speed on compressor performance for various natural gas compositions are presented. The investigated angular speeds are between 500 rad/s to 2100 rad/s.

The variation of mass flow rate against various molar weights of natural gas is shown in Fig. 9. It should be noted, as molecular weight increases, the natural gas density increases too. It consequently increases the mass flow rate. It is evident that as the angular speed increases, the mass flow rate also increases. This can be explained by the relationship between angular speed and the number of cycle in same time. Increasing the angular speed increases the frequency and consequently the mass flow rate.

Fig. 10 shows the variation of mean discharge temperature against various molar weights of natural gas. Based on the figure, it is evident that with increasing the angular speed, the mean discharge temperature increases. This can be explained by the relation between angular speed and in-cylinder mass. With increasing angular speed, the in-cylinder mass in one cycle is reduced considerably. The more in-cylinder mass cause in-cylinder gas to cool less and consequently, the discharge temperature stays low for lower angular speeds. In other hand, with increasing molecular weight, the mean discharge temperature deceases. It is due to the higher density for natural gas with higher molecular weight. Considering on equation of state for a gas, for a constant pressure process, as density increases, the temperature will decrease.

Figs. 11 and 12 show the effects of angular speed on work and input indicated work per cycle for various natural gas compositions respectively. It could be realized, the consuming indicated work per cycle for NG with highest methane percentage is significantly higher than NG with lowest methane percentage. For example the consuming indicated work per cycle for Khangiran composition with 98% methane is about 50 kJ/kg higher than Ghasoo gas with 79% methane. With increasing molar mass, in-cylinder mass increases, however the in-cylinder pressure does not vary noticeably. This is reason for decreasing the indicated work per mass. As the indicated work is obtained by dividing work to one cycle mass flow, the indicated work in natural gas compositions with high methane percentage is higher than the low methane percentage compositions.
5.2. Effect of clearance value on compressor performance for various natural gas compositions

Due to various reasons such as the heat expansion of compressor pieces, exist of clearance in reciprocating compressor is unavoidable. To study effects of clearance value on compressor performance, clearances percent are varied among 7, 9, 11, 13 and 15 in this section. Fig. 13 shows the variation of mass flow rate against natural gas molecular weight for various clearance percentages. Fig. 14 presents the variation of mean discharge temperature against natural gas molecular weight for various clearance percentages. As it is shown, the effect of clearance value on discharge temperature isn’t much. For example, discharge gas temperature difference for clearances 7% and 15% is about 0.5 K. As molecular weight decreases, the discharge temperature of compressed gas is increased. As an example, temperature difference of expanded gas between clearances 7% and 15% just before suction process is 2.5 K.

Fig. 15 presents the influence of variation of clearance on work for various natural gas compositions. It could be realized, in similar angular speed, the consuming indicated work per cycle for NG with highest methane percentage is significantly higher than NG with the lowest methane percentage. For example, in similar clearance, the consuming work for Khangiran composition with 98% methane is about 5 kW higher than Ghasoo gas with 79% methane.

Fig. 16 shows the indicated work in various clearances for various natural gas compositions. The results show that change in clearance doesn’t have significant effects on the indicated work. In other hand, as it was evident in the previous figures, as the gas density increases, in-cylinder mass also increases. Therefore, based on Equation (23), in the same pressure and volume, increasing in-cylinder mass could be reduced indicated work.
6. Conclusion

Natural gas compression processes are sometimes carried out by the reciprocating compressors in natural gas industries when high pressure ratio is required. Comprehension the demeanor of these compressors and inspecting effects of various parameters on their performance are attractive subject. Because of the diversity of NG compositions, the effect of the natural gas composition variation on the compressor performance is an important subject. Hence, in this study, the effects of natural gas composition variation on the compressor performance were evaluated.

The first laws of thermodynamics, mass conservation equation and AGA8 EOS have been employed as tools to investigate the effects of natural gas composition variation on performance of one stage CNG reciprocating compressors.

The effects of natural gas compositions variation on thermodynamic parameters such as: pressure, temperature, in-cylinder mass and mass flow rates were studied. The effects of various parameters such as: angular speed, clearance and natural gas compositions on required work per unit mass of gas are also investigated. The main results could be summarized as follows:

- For all natural gas compositions, as the angular speed increases, the required indicated work per cycle increases too.
- For various natural gas compositions, as the molecular weight increases, the valves opening time increases too.
- The mean discharge temperature for NG with lower molecular weight (higher present of methane) is more than NG with higher molecular weight (lower present of methane).
- The consuming work per cycle for Khangiran gas (with 98% methane) is significantly higher than the Ghasoo gas (with 79% methane).

Considering the above comments, one could conclude that the natural gas composition has significant effects on compressor performance and should be considered as an important parameter.

Acknowledgment

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Appendix A. Real gas effect

To study the effect of real gas in simulations, AGA8 equation of state (EOS) has been used. It incorporates both theoretical and empirical elements. This has provided the correlation with the degree of numerical flexibility needed to achieve high accuracy for the compressibility factor and density of natural gas for custody transfer. It shows good performance and high accuracy for the temperature range between 143.15 K and 676.15 K, and pressure up to 280 MPa. The general form of AGA8 EOS is defined as follows [25]:

$$P = Z \rho_m RT$$  \hspace{1cm} (A1)

where $Z$, $\rho_m$ and $R$ are compressibility factor, molar density and universal gas constant respectively.

In AGA8 method, the compressibility factor should be calculated by employing the following equation [25]:

$$Z = 1 + B \rho_m - \rho_r \sum_{n=1}^{18} C_n + \sum_{n=1}^{18} D_n^*$$  \hspace{1cm} (A2)

Where, $\rho_r$ is reduced density and defined as follows:

$$\rho_r = K^3 \rho_m$$  \hspace{1cm} (A3)

where in equation (A3), $K$ is mixture size parameter and calculated following equation [25]:

$$K^5 = \left( \sum_{i=1}^{N} x_i K_i^5 \right)^2 + 2 \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} x_i x_j (K_i^5 - 1) (K_j^5)$$  \hspace{1cm} (A4)

In equation (A4), $x_i$ is mole fraction of component $i$ in mixture, $x_i$ is mole fraction of component $j$ in mixture, $K_i$ is size parameter of component $i$, $K_j$ is size parameter of component $j$, $B_{ij}$ is binary interaction parameter for size and $N$ is number of component in gas mixture.

In equation (A2), $B$ is second virial coefficient and given by the following equation [25]:

$$B = \sum_{n=1}^{18} a_n T^{-u_n} \sum_{i=1}^{N} x_i B_{nj}^{*} E_{nj}^{*} (K_i K_j)^{5/2}$$  \hspace{1cm} (A5)

where, $B_{nj}^{*}$ and $E_{nj}$ are defined by the following equations [25]:

$$B_{nj}^{*} = (G_{ij} + 1 - g_{nj})^{8} (Q_{i} Q_{j} + 1 - q_{nj})^{Q_{nj} (F_{j}^{1/2} F_{j}^{1/2} + 1 - f_{nj})^{f_{nj}} \times (S_{i} S_{j} + 1 - s_{nj})^{S_{nj} (W_{i} W_{j} + 1 - w_{nj})^{W_{nj}}$$  \hspace{1cm} (A6)

$$E_{nj} = E_{ij} (E_{ij})^{1/2}$$  \hspace{1cm} (A7)

In equation (A7), $G_{ij}$ is defined by the following equation [25]:

$$G_{ij} = \frac{G_{ij} (G_{i} + G_{j})}{2}$$  \hspace{1cm} (A8)

In equations (A4) to (A8), $a_n, f_{nj}, g_{nj}, q_{nj}, s_{nj}, u_n, w_n$ are the equation of state parameters, $E_{i}, E_{j}, G_{i}, K_{i}, Q_{i}, S_{i}, W_{i}$ are the corresponding characterization parameters and $E_{ij}^{*}, G_{ij}^{*}$ are corresponding binary interaction parameters.

In equation (A2), $C_n, n = 1, ..., 58$ are temperature dependent coefficients and defined by the following equation [25]:

$$C_{n} = a_n (G + 1 - g_{nj})^{8} (Q^{2} + 1 - q_{nj})^{Q_{nj} (F + 1 - f_{nj})^{f_{nj} U_{nj}^{5} T^{-u_n}}$$  \hspace{1cm} (A9)
In equation (A9), $G, F, Q, U$ are the mixture parameters and defined by the following equations [25]:

$$U^S = \left( \sum_{i=1}^{N} x_i E^S_i \right)^2 + 2 \sum_{i=1}^{N} \sum_{j=i+1}^{N} x_i x_j \left( U^S_{ij} - 1 \right) (E^S_i E^S_j)$$

(A10)

$$G = \sum_{i=1}^{N} x_i G_i + 2 \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} x_i x_j \left( G^*_{ij} - 1 \right) (G_i + G_j)$$

(A11)

$$Q = \sum_{i=1}^{N} x_i Q_i$$

(A12)

$$F = \sum_{i=1}^{N} x_i^2 F_i$$

(A13)

where in equation (A10), $U_{ij}$ is the binary interaction parameter for mixture energy.

In equation (A2), $D^*_n$ is defined by the following equation:

$$D^*_n = \left( b_n - c_n h_n^{b_n} \right) \rho_n^e \exp \left( - c_n \rho_n^{b_n} \right)$$

(A14)

Coefficients of equation (35) are introduced in Ref. [25].

Substituting equation (A2) in equation (A1), the temperature, pressure and composition of natural gas are known. The only unknown parameter is molar density. The molar density is calculated using Newton–Raphson iterative method.

The density of natural gas is then calculated by the following equation:

$$\rho = M_w \rho_m$$

(A15)

where, $M_w$ is molecular weight of mixture and $\rho_m$ is molar density. With being known molar density, compressibility factor is calculated using equation (A2).

AGA8 model is indented for specific range of the gas components. Table A.1 shows range of gas characteristics to which AGA8 EOS model could be employed [25].

### A.1. Computing enthalpy ($h$)

Assuming enthalpy is functions of temperature and molar specific volume, the enthalpy residual function is defined as follows [39]:

$$h_m - h_{m, I} = \int_{\nu_m \rightarrow -\infty}^{\nu_m} \left[ T \left( \frac{\partial P}{\partial T} \right)_{\nu_m} - P \right] d\nu_m + \int_{\nu_m \rightarrow -\infty}^{\nu_m} RT \left( \frac{\partial Z}{\partial \rho_{m, I}} \right)_T d\nu_m$$

(A16)

In equation (A16), $h_m$ is molar enthalpy for real gas, $h_{m, I}$ molar enthalpy for ideal gas and $\nu_{m, I}$ is molar specific volume for ideal gas. By changing the variable of $\nu_m$ to $\rho_m$ and calculation of partial differential values in equation (A16), enthalpy residual function becomes as follows:

$$h_m - h_{m, I} = -RT^2 \int_{0}^{\rho_m} \left( \frac{\partial Z}{\partial \rho_m} \right) \frac{d\rho_m}{\rho_m} + RT (Z - 1)$$

(A17)

Molar enthalpy for ideal gas $h_{m, I}$ could be calculated as follow [39]:

$$h_{m, I} = \sum_{j=1}^{N} x_j h_{m, I}$$

(A18)

Where in equation (A18), $x$ is mole fraction of component $j$ in mixture and $h_{m, I}$ is molar enthalpy for ideal gas and for component $j$ in mixture. Coefficients in equation (A18) are given in Ref. [34].

### A.2. Computing internal energy ($u$)

Assuming internal energy is functions of temperature and molar specific volume, the internal energy residual function could be calculated as [39]:

$$u_m - u_{m, I} = -RT^2 \int_{0}^{\rho_m} \left( \frac{\partial Z}{\partial \rho_m} \right) \frac{d\rho_m}{\rho_m}$$

(A19)

Where, $u_m$ is molar internal energy for real gas and $u_{m, I}$ is molar internal energy for ideal gas. Molar internal energy for ideal gas could be calculated using the following equation [40]:

$$u_{m, I} = h_{m, I} - \int_{0}^{\rho_m} RT d\rho_m$$

(A20)

In equation (A20), $h_{m, I}$ is molar enthalpy for ideal gas, $T$ is temperature and $R$ is universal gas constant.

### References


Nomenclature

\( a \): lengths of rod m
\( A \): area \((\text{m}^2)\)
\( C_d \): orifice discharge coefficient
\( C_p \): constant pressure specific heats \((\text{kJ/kg K})\)
\( g \): gravitational acceleration \((\text{m/s}^2)\)
\( h \): specific enthalpy \((\text{kJ/kg})\)
\( L \): crank m
\( m \): mass \((\text{kg})\)
\( M \): molecular weight \((\text{kg/kmol})\)
\( n \): angular Speed \((\text{rad/s})\)
\( P \): pressure \((\text{bar or Pa})\)
\( Q \): heat transfer rate \((\text{kW})\)
\( S \): stroke m
\( T \): temperature \((\text{K or °C})\)
\( u \): internal energy \((\text{kJ/kg})\)
\( v \): specific volume \((\text{m}^3/\text{kg})\)
\( V \): volume \((\text{m}^3)\)
\( V_d \): dead volume \((\text{m}^3)\)
\( W \): work \((\text{kJ/kg})\)
\( \psi \): angular Speed \((\text{rad/s})\)
\( \theta \): degree (degree)

Subscript

\( d \): discharge condition
\( cv \): control volume condition
\( s \): suction condition
\( p \): piston

Greek Letters

\( \rho_m \): molar density
\( \rho_r \): reduce density
\( \gamma \): gas gravity
\( \rho_{m:s} \): molar specific volume