PROCEEDINGS OF 14th INTERNATIONAL EXERGY, ENERGY, AND ENVIRONMENT SYMPOSIUM

Editors
Professor İbrahim Dinçer
Professor M.Ziya Sogut

December 24-27, 2023

İstanbul/Türkive

14th INTERNATIONAL EXERGY, ENERGY, AND ENVIRONMENT SYMPOSIUM

December, 24-27, 2023

ORGANIZERS

SUPPORTERS

14th INTERNATIONAL EXERGY, ENERGY, AND ENVIRONMENT SYMPOSIUM

PROCEEDINGS BOOK

ORGANIZERS

December 24-27, 2023

İstanbul/Türkiye

Copyright

All rights reserved. No part of this publication may be reproduced, distributed, or transmitted in any form or by any means, including photocopying, recording, or other electronic or mechanical methods, without the prior written permission of the publisher, except in the case of brief quotations embodied in critical reviews and certain other non-commercial uses permitted by copyright law.

For permission requests, write to The Publisher, addressed to the Symposium Chair at the address below.

Piri Reis University, Istanbul, Turkey
Post Office District, Eflatun St. No:8, 34940 Tuzla/İSTANBUL

Copyright © 2024 by Piri Reis University

EDITED BY:
M.Ziya Sogut

E-ISBN : 978-625-98546-0-1
Published January, 2024
Not sold for money

IEEES-159

Prediction of Thermodynamic Properties for Compressed Natural Gas Mixtures

[1]Fatih Ozcan, [2]Muhsin Kiliç,
[1] Bursa Uludağ University, Orhangazi Yeniköy Asil Çelik Vocational School, Mechanical and Metal Technologies Department, Orhangazi/BURSA, 16810, Türkiye
[2] Bursa Uludağ University, Faculty of Engineering, Department of Mechanical Engineering, Nilüfer/BURSA, 16059, Türkiye

* E-mails: fatihozcan@uludag.edu.tr ; mkilic@uludag.edu.tr

Abstract
Pressures are changed during the transfer of compressed natural gas (CNG). In order to compute the thermodynamic properties of natural gas under these pressure changes, the compressibility factor (Z) must be found. AGA8 equation of state is one of the equations used to find the compressibility factor for different natural gas mixtures. In this study, this equation is scripted in MATLAB. The compressibility factor of the natural gas mixtures is calculated according to pressure and temperature. This calculation is used to compute the thermodynamic properties. To validate the procedure, the numerical values are compared with available measured values (%91 Methane) for density.

Keywords: Compressed Natural Gas, AGA8 Equation of State, Numerical Method, Matlab

I. Introduction

Compressed natural gas (CNG) is a clean-burning alternative to gasoline or diesel used in transportation. CNG contains methane and also other hydrocarbons such as butane, propane and ethane. Accurate prediction of thermodynamic properties for CNG is an essential requirement in optimum design and operation of most process equipment involved in storage and transportation. Accurate value of CNG compressibility factors is crucial in custody transfer operations.

An Equation of State (EOS) can describe the thermodynamic state of a fluid mixture. The AGA8-DC92 EOS and ISO-12213-2 is currently the industry standard to predict the density or compressibility factor of natural gas with an acceptable accuracy. The AGA8 EOS has been developed by American Gas Association. It contains both theoretical and empirical elements. It performs well and high accuracy for the temperature range between 143.15 K and 676.15 K, and pressure up to 280 MPa. The AGA8 has been also subject to various researches for thermodynamic property calculation. (AGA8-DC92 EoS, 1992). (Farzaneh-Gord et al., 2010) developed computer program to use The AGA8 EOS to find thermodynamic properties for natural gas such as internal energy and entalphy. (Farzaneh-Gord and Rahbari, 2012) used the AGA8 EOS to find thermodynamic properties for natural gas such as density, entalphy, speed of sound and Joule–Thomson coefficient. (Farzaneh-Gord et al., 2018) compare AGA8 and GERG2008 equation of state for flow meters in custody transfer.

II. The Numerical Method

The equation of state for the compressibility factor Z for the Detail Characterization Method is given in its condensed form by the following equations (Equations (1)-(14)) (AGA8-DC92 EoS, 1992):

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

where *D* is reduced density defined as follow:

$$D = K^3 d \quad (2)$$

where, *K* is the mixture size parameter calculated using the following equation

$$K^5 = \left[\sum_{i=1}^{N} x_i K_i^{\frac{5}{2}}\right]^2 + 2\sum_{i=1}^{N-1}\sum_{j=i+1}^{N} x_i x_j \left(K_{ij}^5 - 1\right)\left(K_i K_j\right)^{\frac{5}{2}} \quad (3)$$

In Eq. (3), x_i is the mole fraction of component i in the mixture, x_j is the mole fraction of component j in the mixture, K_i is the size parameter of component i, K_j is the size parameter of component j, K_{ij} is the binary interaction parameter for size, and N is the number of components in the gas mixture.

The second virial coefficient B is given by the following equations, where N is the number of components in the gas mixture and the values of i and j both range from 1 to N:

$$B = \sum_{n=1}^{18} a_n T^{-u_n} \sum_{i=1}^{N} \sum_{j=1}^{N} x_i x_j E_{ij}{}^{u_n} \left(K_i K_j\right)^{\frac{3}{2}} B_{nij}^{*} \quad (4)$$

In Equation (4), B_{nij}^{*} and $E_{ij}{}^{u_n}$ are defined by the following equations:

$$B_{nij}^{*} = \left(G_{ij} + 1\text{-}g_n\right)^{g_n} \left(Q_i Q_j + 1\text{-}q_n\right)^{q_n} \left(F_i^{\frac{1}{2}} F_j^{\frac{1}{2}} + 1\text{-}f_n\right)^{f_n} \left(S_i S_j + 1\text{-}s_n\right)^{s_n} \left(W_i W_j + 1\text{-}w_n\right)^{w_n} \quad (5)$$

The binary parameters E_{ij}, and G_{ij}, are calculated using the following equations:

$$E_{ij} = E_{ij}^{*} \left(E_i E_j\right)^{\frac{1}{2}} \quad (6)$$

$$G_{ij} = \frac{G_{ij}^{*}\left(G_i + G_j\right)}{2} \quad (7)$$

In Equations (4) – (7), T is the temperature, N is the number of components in gas mixture, a_n, f_n, g_n, q_n, s_n, u_n, and w_n are the equation of state parameters, E_i, F_i, G_i, K_i, Q_i, S_i, and W_i are the corresponding characterization parameters.

In Equation (1), C_n^{*}, n = 13, . . ., 58, are temperature-dependent coefficients defined by the following equation:

$$C_n^{*} = a_n (G + 1\text{-}g_n)^{g_n} (Q^2 + 1\text{-}q_n)^{q_n} (F + 1\text{-}f_n)^{f_n} U^{u_n} \quad (8)$$

The mixture parameters U, G, Q, and F are calculated using the following equations, where in the double sums, i ranges from 1 to N-1 and, for each value of i, j ranges from i+1 to N:

$$U^5 = \left[\sum_{i=1}^{N} x_i E_i^{\frac{5}{2}}\right]^2 + 2 \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} x_i x_j \left(U_{ij}{}^5\text{-}1\right) \left(E_i E_j\right)^{\frac{5}{2}}$$

$$G = \sum_{i=1}^{N} x_i G_i + \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} x_i x_j \left(G_{ij}^{*}\text{-}1\right)\left(G_i + G_j\right) \quad (10)$$

$$Q = \sum_{i=1}^{N} x_i Q_i \quad (11)$$

$$F = \sum_{i=1}^{N} x_i{}^2 F_i \quad (12)$$

In the computation of the compressibility factor Z using the Detail Characterization Method, the composition of the gas and the absolute temperature T of the gas are known, and the absolute pressure P is known. The problem then is to compute the molar density d using the equation of state expression for the pressure P. For this purpose, Equation (1) is substituted into Equation (13) to obtain an equation for the pressure:

$$P = ZdRT \quad (13)$$

In Equation (13), P is pressure (kPa), Z is compressibility factor, d is molar density (kmol/m^3), R is universal gas constant (J/mol-K), and T is temperature (K). The molar density is calculated using Newton–Raphson iterative method in Matlab.

The density of natural gas (kg/m^3) is calculated by using the following equation:

$$\rho = M_w d \quad (14)$$

where M_w and d are molecular weight (kg/kmol) and molar density (kmol/m^3), respectively. The AGA8 model is intended for a specific range of the gas components. It is not recommended for
the gases with mole percentages outside of the value given (AGA8-DC92 EoS, 1992).

III. Composition of Natural Gas

Natural gas may contain up to 21 components. (ISO-12213-2, 2006) The primary component is Methane (CH_4) in the mixture. It also contains heavier hydrocarbons such as Ethane (C_2H_6), Propane (C_3H_8) and Butane (C_4H_{10}). Table 1 shows an experimental analysis of natural gas composition of %91 Methane (Patil,2007).

Table 1. Mole percent of natural gas component used in density calculation

Component	NG Experimental (%)
Methane (CH_4)	*90.991*
Nitrogen (N_2)	*2.031*
Carbon Dioxide (CO2)	*0.403*
Ethane (C_2H_6)	*2.949*
Propane (C_3H_8)	*1.513*
i-Butane (i-C_4H_{10})	*0.755*
n-Butane (n-C_4H_{10})	*0.755*
i-Pentane (i-C_5H_{12})	*0.299*
n-Pentane (n-C_5H_{12})	*0.304*

IV. Results and discussions

Figure 1 and figure 2 show effects of pressure and temperature on natural gas compressibility factor for experimental natural gas. The compressibility factor decreases as pressure increases and increases as temperature increases. The value of compressibility factor approaches to 1 as pressure decreases for all temperatures.

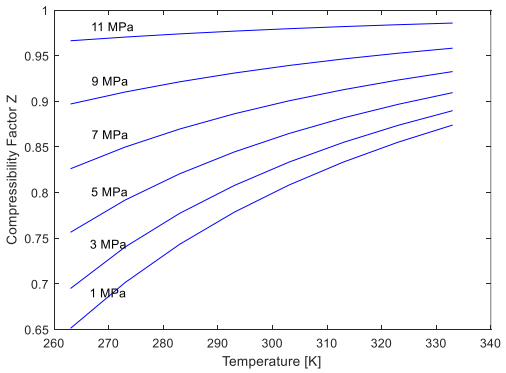


Fig. 1. Effects temperature on compressibility factor

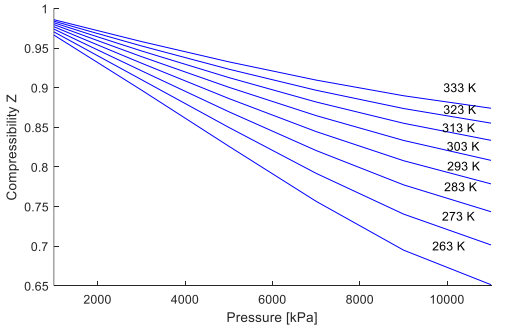


Fig. 2. Effects pressure on compressibility factor

Numerical method predicts the natural gas density in addition of compressibility factor. To validate the results, the numerical and available experimental values (Patil,2007) have been compared. The percent error and average absolute percent deviation (AAPD) have been employed as comparisons tools:

$$\% \text{ Error } = \frac{\text{Property}_{\text{Cal}} - \text{Property}_{\text{Exp}}}{\text{Property}_{\text{Exp}}} * 100 \quad (15)$$

$$\% \text{ AAPD } = \frac{1}{n} \sum \left| \frac{\text{Property}_{\text{Cal}} - \text{Property}_{\text{Exp}}}{\text{Property}_{\text{Exp}}} * 100 \right| \quad (16)$$

Density is calculated by utilizing Eq. (14). Table 1 shows mole percent of natural gas used in density calculation. Considering the experimental values, one could conclude that the density calculation has high accuracy with AAPD of 0.1787%.

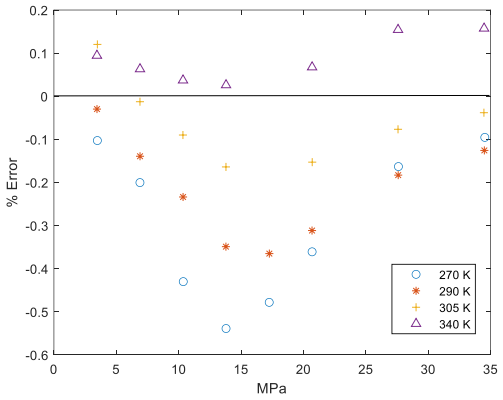


Fig. 3. Error percent in density calculation

Figure 3 illustrates error percent for density calculations. According to Figure 3, as temperature increases or pressure decreases, error percent decreases. This shows that as the natural gas behavior approaches closer to an ideal gas, accuracy of the AGA8 EOS for prediction density.

V. Conclusion

Accurate prediction of thermodynamic properties for CNG is an essential requirement in optimum design and operation of most process equipment involved in compressed, storage and transfer. In current study, Matlab program has been developed to calculate the property of natural gas mixture such as density in addition of the compressibility factor. To validate the numerical procedures, the numerical values have been compared with natural gas composition of %91 Methane mixture density values. The validations show that the average absolute percent deviation (AAPD) for density calculation is 0.1787%.

References

AGA8-DC92 EoS, 1992. Compressibility and Super Compressibility for Natural Gas and Other Hydrocarbon Gases, Transmission Measurement Committee Report, no. 8, AGA Catalog no. XQ 1285, Arlington, VA.

Farzaneh-Gord, M., Khamforoush, A., Hashemi, S., Pourkhadem, H., 2010. Computing thermal properties of natural gas by utilizing AGA8 equation of state. Int. J. Chem. Eng. Appl. 1, 20.

Farzaneh-Gord M., Rahbari HR., 2012. Numerical procedures for natural gas accurate thermodynamic properties calculation. Journal of Engineering Thermophysics; 21(4). https://doi.org/10.1134/S1810232812040017

Farzaneh-Gord M., Mohseni-Gharyehsafaa B., Toikkab A., Zverevab I., 2018. Sensitivity of natural gas flow measurement to AGA8 or GERG2008 equation of state utilization. Journal of Natural Gas Science and Engineering 57 305–321. https://doi.org/10.1016/j.jngse.2018.07.014

ISO-12213-2, 2006. Natural Gas-Calculation of Compression Factor, pt. 2: Calculation Using Molar Composition Analysis, ISO, Ref. no. ISO-12213-2:1997(E).

Patil, P., Ejaz, S., Atilhan, M., Cristancho, D., Holste, J.C., Hall, K.R., 2007. Accurate density measurements for a 91% methane natural gas-like mixture. J. Chem. Thermodyn. 39, 1157–1163.