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A corresponding states-based method for the estimation of natural gas compressibility factors

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ABSTRACT

In this communication, a corresponding states-based model for the calculation/estimation of the gas compressibility factor (*z*-factor) of natural gasses is proposed. The method applies the gene expression programming (GEP) algorithm. The parameters of the new model comprise the pseudo-reduced pressure and pseudo-reduced temperature. For assessing the performance and accuracy of the developed model, several statistical and graphical error analyses have been applied simultaneously. Additionally, comparisons have been made between this method and the most widely-used correlations and equations of state (EoS) available in the literature. Various statistical parameters are also used to evaluate the validity and the predictive capability of the newly developed method. Furthermore, the Leverage approach (Williams plot) is used to determine the realm of prediction capability of the new z-factor model and to detect any probable erroneous data points. The results obtained demonstrate that the newly proposed model is more reliable and more effective than the empirical models and EoS methods for prediction of *z*-factors of natural gasses.

1. Introduction

Natural gas is a multi-component mixture composed broadly of different components, comprising methane as the key component and more fundamental and important components like carbon dioxide (CO_2), nitrogen (N_2), ethane (C_2H_6), propane (C_3H_8), and heavier hydrocarbon components [1]. Natural gas is one of the cleaner and cheaper energy sources, compared with other hydrocarbon-based materials like oil and coal. It also has a longer predicted future availability compared to crude oil and coal [2]. Furthermore, there has been growing importance in natural gas being used in meeting the world energy demand due to its versatility and abundance compared to the other fuels, as well as its clean burning [3] characteristics. Therefore, it is important to develop reliable predictive methods for the physical properties related to natural gas, like gas compressibility factor (*z*-factor), for enable optimal exploitation and usage. The gas compressibility factor is a key thermodynamic parameter in the chemical and petroleum engineering disciplines such as phase equilibria of various hydrocarbon and non-hydrocarbon mixtures, analyzing *PVT* behavior, upstream and downstream calculations of petroleum industries, material balances, assessment of underground gas reserves, gas reservoir simulations, well-testing analysis and calculations associated with processing of gasses [4,5]. Moreover, the importance and role of *z*-factor cannot be overemphasized in process engineering calculations and in lower complexity simulations within a thermodynamics context.

Generally, the volumetric properties of the petroleum fluids are predicted from laboratory tests, empirically derived models, or thermodynamic models [6]. Normally, high-temperature and high-pressure apparatuses are utilized for the experimental measurements in order to investigate the volumetric properties of natural gasses [7]. Moreover, these measurements are expensive and time-consuming and it is impossible to measure properties for all possible compositions of natural gasses [8]. In addition to laboratory tests, equations of state (EoS) and empirically derived models can predict the properties related to petroleum fluids. To determine the natural gas *z*-factor, empirical correlations are more rapid and simpler than equations of state (involving a large number of parameters) which require longer computations and are more complicated [9]. Furthermore, with regard to the gas compressibility factor, all EoS models are implicit and consequently are the mathematical roots of the EoS [10]. It is worth noting that in spite of the above-mentioned drawback, EoS has some advantages; for instance

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they sacrifice a bit of precision in exchange for a smooth mathematical function for the model developed and reliable mathematical behavior in terms of the derivatives of the mathematical function. The partial derivatives of compressibility lead to various expressions, including the entropy, enthalpy, and Gibbs free energy residuals, which are in turn utilized to estimate fugacity coefficients and then used to describe phase equilibria [11].

As a result, accurate and fast calculation/estimation of the *z*-factor is of great importance and is one of the main challenges in most of the commercial process simulators utilized in chemical and petroleum engineering.

Among the intelligent techniques, genetic algorithm (GA) is a reliable population-based progressive optimization method based on the concept of evolution and genetic principles proposed by John Holland [12]. The genetic programming (GP) proposed by John Koza [13] may be considered as the next generation of GAs. GP is a novel evolutionary system which overcomes some restrictions associated with GAs. A variant and reformulation of this new mathematical approach (gene expression programming (GEP)) were proposed by Ferreira [14].

In this article, the GEP [14] mathematical approach is applied to develop an accurate and reliable method for the determination of the gas compressibility of around 900 data points at different temperature and pressure conditions. Subsequently, the results obtained for the newly proposed GEP model are compared against literature-reported data and previously published correlations and EoS calculations. In assessing the validity of the GEP model, several statistical parameters are considered. Moreover, the Leverage approach (Williams plot) is utilized to determine the prediction capability of the new z-factor model and also to identify probable erroneous data points.

2. Gas compressibility factor

2.1. Ideal gas behavior

The gas compressibility factor is defined as the ratio of the molar volume actually occupied by a gas to the molar volume related to an ideal gas at a given/same temperature and pressure [15]. In other words, compressibility factor of gasses is a dimensionless quantity which is a function of pressure and temperature. According to the kinetic theory related to gasses [8], the volume of a molecule is insignificant and/or unimportant compared to the total bulk volume. Also, it is assumed that there are neither attractive forces nor repulsive forces among the gas molecules [8]. A mathematical equation called an equation of state (EoS) is a relationship among pressure (P), volume (V), and temperature (T) for a given quantity of moles of gas (n). Consequently, the abovementioned relationship is mathematically expressed by the following equation:

$$PV = n'RT \tag{1}$$

where P represents pressure, V denotes the volume, n' is the number of moles, R is the Universal Gas Constant, and T is the temperature.

2.2. Real gas behavior

Gasses that deviate from ideal behavior are known as real gasses. The ideal gas EoS shows low deviations from experimental data at atmospheric pressure (2–3% of average absolute relative deviation) whereas, its application at high pressures is not recommended due to the high deviations from real gas behavior [8]. The deviation dramatically increases with an increase in temperature and pressure and is dependent on the gas composition as well.

To correlate the pressure, volume and temperature (*PVT*) parameters, various EoSs have been reported for real gasses. In order to present the relationship among the parameters above (*PVT* variables), an equation is formulated as follows:

$$PV = Zn'RT \tag{2}$$

where P is the pressure, V denotes the volume, Z represents the gas compressibility factor, n' is the number of moles, R is the Universal Gas Constant, and T stands for temperature.

Investigation of the compressibility factor for natural gasses of different compositions has shown that *z*-factor can be used in generalized form with adequate accuracy for most engineering calculation purposes when it is expressed in terms of two dimensionless properties [8], which are as follows:

$$P_{pr} = \frac{P}{P_{pc}} \tag{3}$$

$$T_{pr} = \frac{T}{T_{pc}} \tag{4}$$

where P_{pr} denotes the pseudo-reduced pressure, T_{pr} is the pseudo-reduced temperature, T_{pc} is the pseudo-critical temperature and P_{pc} is the pseudo-critical pressure. The pseudo-critical properties are given by the following equations:

$$P_{pc} = \sum_{i=1}^{n} y_i P_{ci} \tag{5}$$

$$T_{pc} = \sum_{i=1}^{n} y_i T_{ci} \tag{6}$$

where P_{ci} denotes the critical pressure, T_{ci} is the critical temperature and y_i is the mole fraction of component *i*. The values of critical pressure and temperature (P_c and T_c) for the components of natural gasses [16] are presented in the supplementary material.

2.3. Determination of the critical properties of plus fraction components

There are many empirically derived correlations that can be used for the determination of plus properties of natural gas components. A review was undertaken by the late Ali Danesh [16]. As recommended, one of the most reliable methods for this purpose is the correlation proposed by Twu [17] as follows:
critical temperature:

$$T_c = T_c{}^o[(1 + 2f_T)/(1-2f_T)]^2 \tag{7}$$

where

$$f_T = \Delta SG_T\left[-0.362456/T_b^{\frac{1}{2}} + \left(0.0398285-0.948125/T_b^{\frac{1}{2}}\right)\Delta SG_T\right] \tag{8}$$

where

$$\Delta SG_T = exp[5(SG^o-SG)]-1 \tag{9}$$

critical volume:

$$V_c = V_c{}^o[(1 + 2f_V)/(1-2f_V)]^2 \tag{10}$$

where

$$f_V = \Delta SG_V\left[0.466590/T_b^{\frac{1}{2}} + \left(-0.182421 + 3.01721/T_b^{\frac{1}{2}}\right)\Delta SG_V\right] \tag{11}$$