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A New Correlation Based on Multi-Gene Genetic Programming for Predicting the Sweet Natural Gas Compressibility Factor

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Abstract: Gas compressibility factor (z-factor) is an important parameter widely applied in petroleum and chemical engineering. Experimental measurements, equations of state (EOSs) and empirical correlations are the most common sources in z-factor calculations. However, these methods have serious limitations such as being time-consuming as well as those from a computational point of view, like instability, convergence and accuracy. Accurate and fast estimation of this parameter is of interest and a challenging factor in the numerous calculations related to oil and gas processing plants. In this study, a meta-learning algorithm named multi-gene genetic algorithm (MGGP) was applied to predict the sweet gas compressibility factor. To assess the effectiveness of the MGGP model statistical criteria, is applied. The validity of this proposed model was compared with the experimental data. The results showed that the model has successfully predicted the sweet natural gas z-factor, especially at the midrange of operating conditions. However, the MGGP model seems to be inefficient in boundary values of Tpr (i.e. around 1 and 2). In addition, the MGGP model is compared with other z-factor correlations and it is revealed that the implementation of MGGP model lead to a more accurate and reliable estimation of the natural gas compressibility factor.

Keywords: Natural Gas, Compressibility Factor, Multi-Gene Genetic Programming, Correlations.

1. Introduction

Natural gas is one of the most significant energy sources with enormous global demand for petroleum combustions. This gas is a multi-component mixture of varying compositions, with methane as the main constituent and other non-hydrocarbon and heavier components. The precise knowledge of thermodynamic properties of natural gas is of vital importance for petroleum and chemical engineering calculations (Elsharkawy, 2004; Shokir, El-Awad, Al-Quraishi, & Al-Mahdy, 2012). The ratio of real volume to ideal volume, which indicates deviation behaviour of a gas with respect to an ideal in terms of gas volume, is named the gas deviation factor (T. H. Ahmed, 1989).

In most petroleum and natural gas engineering calculations, the compressibility factor is necessary in gas metering, compression, design of pipelines and surface facilities (Azizi, Behbahani, & Isazadeh, 2010; Elsharkawy, 2004).

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The most reliable and accurate manner to obtain physical properties of natural gas is resorting to accurate experimental measurements. These experiments are expensive and time-consuming, and it impossible to measure all compositions inside natural gases (T. Ahmed, 2006). On the other hand, when laboratory analysis is not available, empirical correlations and equations of state (EOSs) can estimate the petroleum fluid properties (T. H. Ahmed, 1989).

According to the available literature, there exist more than 20 correlations for calculating the z-factor, which are defined for special conditions (Azizi et al., 2010; Beggs & Brill, 1973; Heidaryan, Moghadasi, & Rahimi, 2010; Kumar, 2004; Sanjari & Lay, 2012). Moreover, most of these correlations require iterative procedures in obtaining the corresponding z-factor and may even present different results depending on the initial values for the iterative solutions (Chamkalani, Mae'soumi, & Sameni, 2013).

EOSs as another deterministic tool usually experience computational errors due to inadequate knowledge on the mixing rules and the important involved parameters in the equations. In addition, EOSs are more complex than the empirical correlations and involves a great number of parameters, which require more complicated and longer computations (Chamkalani, Zendehboudi, et al., 2013; Fayazi, Arabloo, & Mohammadi, 2014).

The artificial intelligence is introduced as an applied engineering tool in order to overcome challenging engineering problems. The implementation of such a promising tool has become the center of attention for researchers involved in studied on upstream and downstream petroleum and gas industry (Fayazi et al., 2014; Shateri, Ghorbani, Hemmati-Sarapardeh, & Mohammadi, 2015; Shokir et al., 2012). The artificial neural network (Baniasadi, Mohebbi, & Baniasadi, 2012; Kamyab, Sampaio, Qanbari, & Eustes, 2010), support vector machine (Kamari, Hemmati-Sarapardeh, Mirabbasi, Nikookar, & Mohammadi, 2013), particle swarm optimisation and genetic algorithm (Chamkalani, Mae'soumi, et al., 2013) have been extensively utilized in estimating the compressibility factor for different natural gas compositions. In this study, a new compositional model is proposed for estimating z-factor of sweet gases through a multi-gene genetic programming (MGGP) approach. MGGP is a modified version for the model structure selection, which is combined with the least square technique (LST) for parameter estimations. In order to achieve the objective of such model, a total of 540 data points for the variation of sweet natural gas compositions are collected from the related literature (Čapla, Buryan, Jedelský, Rottner, & Linek, 2002; Duschek, Kleinrahm, Wagner, & Jaeschke, 1989; Eubank, Scheloske, Hall, & Holste, 1987; Hall, Patil, Atilhan, & Ejaz, 2006; Magee, Haynes, & Hiza, 1997). The results of this proposed model are compared with other commonly used empirical correlations and several statistical criteria are used to evaluate the efficiency of this newly developed model.

2. Background

The compressibility factor of a natural gas at a given condition can be obtained from the experimental chart as a function of the pseudo-reduced pressure and temperature. As for natural hydrocarbon gases, the Standing & Katz (1942) and Katz (1959) charts are the fundamental standards in oil and gas industry, although these charts are prepared for the binary mixtures of low molecular weight gases.

Several EOSs are developed and applied in calculating pressure-volume-temperature (PVT) properties of natural gas and crude oil systems and are usually expressed in the following format:

$$Z^3+a\times Z^2+b\times Z+C=0 \quad (1)$$

where constants a, b and c are the functions of pressure, temperature and phase composition, respectively. The EOSs introduced by Soave-Redlich-Kwong (Soave, 1972) and Peng & Rabinson (1976) are often used in the gas industry as predictive tools.

In addition to the complexity of calculations in some particular EOSs, the interactions between gas molecules and consequently gas PVT behaviour are not well simulated in most EOSs. These deficiencies cause significant errors in the predicted value of the compressibility factor, as addressed by Elsharkawy (2004).

The underlying principle in developing all correlations for gas compressibility factor is the law of corresponding states, indicating that all gases will exhibit the same behaviour, i.e. in terms of reduced pressure and temperature (Prausnitz, Lichtenthaler, & de Azevedo, 1998). Variation of the experimental compressibility factor with the pressure together with different fluids isotherms indicate that the compressibility factor varies with respect to pressure, temperature and a type of substance (Mohammadikhah, Abolghasemi, & Mohebbi, 2010). Moreover, for mixtures, the compressibility factor has a surplus

dependency on composition mole fraction. That is the functional relation between the compressibility factor and the mentioned parameters is complicated. For an n-species mixture, the compressibility factor functionality is (Prausnitz et al., 1998).

$$Z = Z\,(T_{rm}, P_{rm}, \omega_m, X_i, X_{i+1}, \ldots, X_{n-1}) \quad (2)$$

where ω is the acentric factor, P_r is the reduced pressure, T_r is the reduced temperature and x_i is mole fraction of ith-species. In some assessments the objective was to estimate the compressibility factor through fitting operation on the experimental data where these parameters are involved (Baniasadi et al., 2012; Mohammadikhah et al., 2010).

A new EOS based on the virial equation including M-factor is introduced lately. The M-factor theory explains that the compressibility factor of each substance depends on M-factor and reduced pressure and temperature (Baniasadi et al., 2012; Mohammadikhah et al., 2010; Mohebbi & Mohammadikhah, 2007; Nejad, Mohammadikhah, Abolghasemi, Moosavian, & Maragheh, 2009). Though M-factor is a combined parameter, it can be assumed as a new parameter with different properties than that of T_r or P_r which compose it. More details on calculation of M-factor (BP/RT) and M-factor theory, are available in the literature (Baniasadi et al., 2012; Mohammadikhah et al., 2010; Nejad et al., 2009). In the defining M-factor, B is second virial coefficient. Thus, the compressibility factor can be written as follows:

$$Z = Z\,(T_r, P_r, M) \quad (3)$$

Accordingly, by introducing the MGGP together with this theory, a new correlation is obtained for predicting the compressibility factor.

3. Multi-Gene Genetic Programming

MGGP is of the symbolic regression class, with the objective to find an explicit relation between one or more inputs and an output by applying mathematical symbols' functions and variables. Symbolic regression differs from conventional regression, where the coefficients/ functions are not calculated. Finding equations in symbolic regression is based on an extensive and continuously improving guided search in an evolving space (Kaydani, Mohebbi, & Eftekhari, 2014).

In order to understand the functionality notion of MGGP, at the first step, a brief discussion of Genetic programming (GP) is necessary. GP is an evolutionary computation technique that has been successfully applied in various kinds of engineering problems. Unlike the common optimisation methods such as genetic algorithm, where potential solutions are represented as numbers, genetic programming provides the potential solutions structurally based so-called tree representation. Each one of the genes in GP consists of functions (F) and terminals (T). The set of operator's F can contain the basic arithmetic operations, while the terminal's T contains input variables and constants of the problem. Potential solutions may be illustrated as a rooted, labelled tree with ordered branches, using operations from the function set and arguments from the terminal set (Koza, 1992). Genetic programming provides a platform with genetic operators (random generation, mutation, crossover and others) that produce, alter and select individuals in population.

MGGP (D. Searson, Willis, & Montague, 2007; D. P. Searson, Leahy, & Willis, 2010) is a vigorous alternative of the standard GP, which integrates a model structure selection ability of genetic programming (GP) with classical regression approach. MGGP provides structured, transparent and concise mathematical model of a set of data by linear combinations of low order non-linear transformations of the input-output variables. Unlike traditional GP, which is based on the evaluation of a single tree (model) expression, each symbolic model in MGGP is a weighted linear combination of the outputs from a number of GP trees. Each one of these trees may be considered as a gene, representing a traditional GP tree. Genes are acquired incrementally by individuals in order to improve fitness (e.g. to reduce the model's root mean squared errors in a data set). More explanation on MGGP is available in the related literature (D. Searson et al., 2007; D. P. Searson et al., 2010).

4. Implementation of Model

In this work, according to M-factor EOS, M-factor, P_r and T_r are selected as input variables of the model, whereas the sweet natural gas compressibility factor is set as the output. Here data on 540 different types of natural gas (Čapla et al., 2002; Duschek et al., 1989; Eubank et al., 1987; Hall et al., 2006; Magee et al., 1997) are applied in training and testing MGGP. Table 1 summarizes the ranges of the M-factor, reduced temperature and reduced pressure and z-factor of the experimental data used in this model.

In order to apply the MGGP predictive algorithm, various parameters must be adjusted, the selected values of which would

affect the model generalisation capability. These parameters are selected based on trial and error approach or some previously suggested values. Selecting proper number of population and generation depends on the number of variables and complexity of problems. A sizable number of population and generations are tested to find models with minimal error. Other parameters that must be adjusted are the maximum number of genes in an individual and the maximum tree depth, which directly influence the size and the number of solutions explored within the search space. Although, the greater numbers for these parameters increase the success of the MGGP by complex evolved solutions, the speed of the algorithm decreases. The allowable number of genes and tree depth must be set to optimal values as the trade-offs between the running time and complexity of the evolved solutions. During the identification process, the functions containing the basic arithmetic operators and mathematical functions are applied to accomplish the optimum MGGP models (Kaydani et al., 2014).

For supervised learning, the data are usually split into training and test sets; the training set consists of a set of data used only for learning (i.e. to fit the genetic model evolution) and the test set is a set of data used in assessing the generalized performance of a trained model (i.e. external evaluation). Usually, 90% of this data is used for training process and the remaining 10% is categorized as the testing data. The parameter settings applied in MGGP implementation in this study are tabulated in Table 2. The criterion applied in stopping the training phase, is the minimum root mean squared error (RMSE) as defined by (D. P. Searson et al., 2010):

$$\mathrm{RMSE} = \sqrt{\frac{\sum(X^{cal} - X^{act})^2}{\mathrm{N}}} \qquad (4)$$

The fitness or quality of a candidate solution is determined by measuring this parameter between the actual and predicted outputs. The GPTIPS toolbox computer program (D. Searson, 2009), developed subject to MATLAB software, is applied in this work to generate the model.

Table 1. The Range of Experimental Data used in this Study.

Parameter	*Min*	*Max*
T_r	1	2
P_r	0.02	8
M-factor	-0.2	0.15
Z-factor	0.385	1.012

Table 2. The MGGP Parameters for Training Z - Factor Model

Parameter	*Values*
Function set	×, ÷,+, -, power, ln
Fitness function	RMSE
Population size	200
Number of generations	300
Maximum tree depth	4
Maximum number of gens allowed as individual	3
Selection method	Tournament
Tournament size	4

5. Results and Discussion

The best approach based on MGGP in predicting the sweet natural gas z-factor, with minimum errors is solving the following equation:

$$Z = 7.185\times10^{-5} P_r (P_r - 7.679)(M - P_r + 1625) + M \times p_r^2 (0.001067 P_r - 0.007883) + 0.01435 T_r \times P_r (P_r - 7.622) \times (T_r - 6.045) + 1.032 \quad (5)$$

The comparison of statistical values of the experimental training, test data set and MGGP predicted values is given in Table 3 where the MGGP model provides a very accurate representation of the statistical data and indicates the accuracy of the MGGP algorithm in predicting the compressibility factor of sweet natural gas.

The results of the MGGP model are compared statistically with experimental data for predicting sweet natural gas compressibility factors at different values of T_{pr} and P_{pr} in Table 4. As observed here the model has successfully predicted the gas compressibility factor especially in pseudo-reduced pressure and pseudo-reduced temperature midrange. The MGGP model is not without its shortcomings in predicting the gas compressibility factor in boundary values of pseudo-reduced temperature (i.e. the values by about 1 and 2).

Table 3. Performance of MGGP Model in Training and Test Data Set

Parameter	*Training data set*	*Test data set*
AARE%	1.547	1.592
RMSE	0.0159	0.0163
APE	0.142	0.145
R-square	0.980	0.972

Table 4. Comparison of Experimental Data and those Predicted Values of Sweet Gas Compressibility Factor for Gas Mixtures for Different Values of Ppr and Tpr

Tpr=1.20			Tpr=1.27			Tpr=1.42			Tpr=1.78			Tpr=1.86		
Ppr	Z (MGGP)	Z (Exp)	Ppr	Z (MGGP)	Z (Exp)	Ppr	Z (MGGP)	Z (Exp)	Ppr	Z (MGGP)	Z (Exp)	Ppr	Z (MGGP)	Z (Exp)
0.415	0.931	0.916	0.424	0.939	0.929	0.483	0.952	0.946	0.499	1.001	0.972	0.637	1.005	0.978
0.760	0.856	0.840	1.106	0.814	0.809	0.918	0.890	0.898	1.206	0.965	0.948	1.241	0.985	0.959
1.048	0.800	0.774	1.386	0.772	0.759	1.309	0.843	0.856	1.766	0.944	0.929	1.874	0.969	0.944
1.294	0.758	0.715	1.867	0.714	0.679	3.006	0.733	0.736	2.321	0.930	0.915	2.430	0.960	0.934
3.316	0.586	0.564	2.294	0.676	0.628	3.747	0.732	0.735	3.443	0.919	0.902	3.645	0.955	0.929
3.667	0.588	0.585	4.211	0.660	0.662	4.682	0.764	0.766	4.612	0.930	0.912	4.923	0.964	0.945
5.083	0.668	0.709	5.598	0.767	0.771	5.983	0.848	0.841	6.014	0.956	0.949	6.401	0.978	0.987
RMSE	0.027		RMSE	0.023		RMSE	0.007		RMSE	0.018		RMSE	0.032	
R-square	0.961		R-square	0.968		R-square	0.992		R-square	0.952		R-square	0.632	

In order to evaluate the accuracy of MGGP model for sweet gas compressibility factor prediction against the existing correlations, namely Shell oil company (Kumar, 2004), Heidaryan-Moghadasi-Rahimi (Heidaryan et al., 2010), Azizi-Behbahani-Isazadeh (Azizi et al., 2010) and Sanjari & Lay (2012), two data sets (Table 5) are applied. Tables 6 and 7 contain statistical data on fit accuracy of the models with observed data. These tables show that there is a good agreement between the results of the MGGP model and the experimental data in comparison with other empirical correlations, which are especially of mid-range operation conditions. In order to show the accuracy of the MGGP model statistically especially in mid-range operation conditions (the range of experimental data in Table 1), results of z-factor prediction are exposed based on MGGP model formulation and some other correlations in Table 8. It is clear that this newly introduced model provides an accurate representation of the statistical values such as average absolute relative error (AARE), root mean squared error (RMSE) and R-square (R^2) over the full range of operating conditions in predicting z-factor.

Table 5. Compositions of Two Sweet Natural Gas Mixtures Used to Evaluate the Accuracy of the MGGP Model

Component	mole (%)	
	No. 1	No. 2
C_1	0.9658	0.9064
C_2	0.0182	0.0455
C_3	0.0041	0.0083
i-C_4	0.0010	0.0010
n-C_4	0.0010	0.0016
i-C_5	0.0005	0.0003
n-C_5	0.0003	0.0004
C_6	0.0006	0.0004
N_2	0.0027	0.0313
CO_2	0.0059	0.0047

Table 6. Comparison of Experimental Data and those Predicted Values of Sweet Gas Compressibility Factor for Gas Mixture No.1 (See Table 5) at Tpr=1.41

P_{pr}	Z (Experimental)	Z (MGGP model)	Z (Kumar, 2004)	Z (Sanjari & Lay, 2012)	Z (Heidaryan et al., 2010)
0.47	0.9457	0.9520	0.9360	0.9449	0.9331
0.89	0.8975	0.8904	0.8718	0.8956	0.8550
1.28	0.8546	0.8424	0.8145	0.8529	0.7922
1.62	0.8185	0.8066	0.7691	0.8184	0.7515
2.27	0.7619	0.7579	0.7073	0.7679	0.7088
2.90	0.7300	0.7336	0.6807	0.7438	0.6984
3.27	0.7228	0.7292	0.6788	0.7437	0.7022
4.44	0.7490	0.7573	0.7206	0.7735	0.7465
5.57	0.8110	0.8273	0.7956	0.8220	0.8164
7.43	0.9404	0.9464	0.9365	0.9320	0.9565
0.47	0.9457	0.9520	0.9360	0.9449	0.9331
0.89	0.8975	0.8904	0.8718	0.8956	0.8550
RMSE		0.008	0.034	0.011	0.037
R-square		0.990	0.987	0.993	0.921

Table 7. Comparison of Experimental Data and those Predicted Values of Sweet Gas Compressibility Factor for Gas Mixture No.2 (See Table 5) at Tpr=1.34

Ppr	Z (Experimental)	Z (MGGP model)	Z (Kumar, 2004)	Z (Sanjari & Lay, 2012)	Z (Heidaryan et al., 2010)
0.45	0.9372	0.9441	0.9261	0.9343	0.9220
0.85	0.8805	0.8764	0.8505	0.8757	0.8397
1.2	0.8310	0.8250	0.7856	0.8270	0.7721
1.51	0.7875	0.7849	0.7331	0.7869	0.7248
2.08	0.7195	0.7294	0.6637	0.7301	0.6712
2.61	0.6787	0.6963	0.6315	0.7012	0.6497
3.2	0.6649	0.6796	0.6283	0.7060	0.6490
3.93	0.6839	0.6869	0.6576	0.7209	0.6718
4.99	0.7456	0.7415	0.7316	0.7632	0.7335
6.62	0.8677	0.8795	0.8645	0.8630	0.8630
0.45	0.9372	0.9441	0.9261	0.9343	0.9220
0.85	0.8805	0.8764	0.8505	0.8757	0.8397
RMSE		0.009	0.034	0.018	0.035
R-square		0.993	0.981	0.990	0.965

Table 8. Accuracy of the Various Methods for Predicting Z-Factor of Natural Gas Samples

Parameter	**MGGP model**	**Sanjari & Lay (2012)**	**Heidaryan et al. (2010)**	**Shell oil company (Kumar, 2004)**
AARE	0.010389	0.016126	0.038519	0.042001
RMSE	0.002071	0.003714	0.008355	0.008191
R-square	0.991485	0.991003	0.933504	0.979353

6. Conclusions

In this study, a new equation is introduced based on a multi-gene genetic programming for predicting compressibility factor of sweet natural gas has. For obtaining this equation, according to M-factor EOS, the M-factor, T_r and P_r are selected as the input variables. The capability of this equation in predicting of the compressibility factor is implemented the findings are compared with experimental data. Moreover, the comparison of the prediction accuracies of the MGGP model with other empirical correlations indicates that this newly introduced equation is more efficient in predicting the compressibility factor. Therefore, this new equation can be applied in chemical and petroleum engineering software packages in predicting the real gas behaviour, which significantly affects the design aspects of equipment involved in gas processing plants.

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