

# A Novel Simplification for the Prediction of Natural Gas Compressibility Factor

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## Authors' contributions

This work was carried out in collaboration among all authors. Author OOC designed the study, performed the statistical analysis and wrote the first draft of the manuscript. Author AOO managed the literature searches, analyzed of the study and supervised the findings. Author AN wrote the protocol and codes. All authors read and approved the final manuscript.

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## ABSTRACT

The need for a simpler, effective and less expensive predictive tool for the estimation of natural gas compressibility factor cannot be exaggerated. An accurate prediction of gas compressibility factor is essential because it plays a definitive role in evaluating gas reservoir properties used in the estimation of gas reserves, custody transfer and design of surface equipment. In this present work, a novel explicit correlation and a highly sophisticated computer program were developed to accurately predict natural gas deviation factor. The research also aims to effectively capture the relationship between Pseudo-reduced temperature and pressure in relations to the Z-factor. In this study, 3972 digitized data points extracted from Standing and Katz's Chart were regressed and analyzed using Microsoft Excel Spreadsheet, the extraction of this data was done using WebPlotDigitizer developed by Ankit Rohatgi of GitHub, Pacifica, CA, USA. The correlation was developed as a function of Pseudo-reduced temperature and pressure with tuned parameters distributed across  $1.05 \leq T_{pr} \leq 3.0$  and  $0 < P_{pr} \leq 8.0$ . Subsequently, the input ( $T_{pr}$  and  $P_{pr}$  values) of the feed data was used to validate the correlation and compare it with other known and published correlations. Statistical analysis of the results showed that a 99.8% agreement exists between the predicted and actual compressibility factors for the various test scenarios and case studies

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involving both sweet and sour gases. Also, the correlation was observed to outperform other models. Finally, the results were observed to perfectly mimic the Standing and Katz charts with an overall correlation coefficient of 99.76% and an adjusted  $R^2$  of 99.75%. The proposed correlation was subsequently used to develop a software using JavaScript. Undoubtedly, the proposed correlation and software are suitable for rapid and accurate simplification and prediction of natural gas compressibility factor.

*Keywords: Novel correlation; natural gas compressibility software; natural gas deviation predictive tool; gas compressibility factor; natural gas; z-factor.*

## 1. INTRODUCTION

The need for a simpler, effective and less expensive predictive tool for the estimation of natural gas compressibility factor cannot be exaggerated. Natural gas is recently considered as a viable alternative energy source because of its availability, environmental friendliness and higher calorific value [1]. This growing significance has prompted the need for more efficient and accurate characterization of its properties [2]. Natural gas compressibility factor (Z) also known as gas deviation factor or simply 'Z-factor' is an important thermodynamic property of natural gas [3]. Accurate prediction of this thermodynamics property is a prerequisite in the evaluation of gas formation volume factor, density, compressibility and viscosity; which are essential requirement for the evaluation of gas reserves, custody transfer and design of surface equipment [4,5].

Z-factor is generally used to account for the deviation of gases from ideal behaviors at higher operation conditions [6]. At lower, near atmospheric conditions, most gases behave like an ideal gas, however, as the operating conditions changes as encounter in field situations, the gases become more erratic and deviates greatly from the ideal gas conditions [7]. Modeling such gas properties with the ideal gas law could results into errors as great as 500% as opposed to 2-3% error observed at atmospheric conditions [8]. Real gas, as opposed to ideal gas, have significant volume, attractive and repulsive forces between their molecules and associated internal energy loss upon collision, thereby making them supercompressible [7,8]. To accommodate these changes in behavior, an empirical factor 'Z', called gas compressibility factor, gas deviation factor or Z-factor is introduced into the ideal gas equation to correct for the various deviations [9]. Equation 1 and 2 below defines the ideal and real gas equations respectively.

$$PV = nRT$$

1

$$PV = ZnRT$$

2

Where,

P = Pressure

V = Volume

n = No of mole

R = Gas constant

T = Temperature

Z = Gas deviation factor

Various attempts have been made to accurately predict the gas deviation factor. These efforts have been geared towards the various traditional evaluation methods which includes the experimental methods, mathematical methods (the use of equation of State, corresponding states method and correlations) and the artificial intelligence methods (the use of artificial neural network, fuzzy inference system, group method of data handling, adaptive neuro-fuzzy interference system and generic algorithm) [10,11]. One common objective of these various evaluation methods is the production of a simpler, effective and less expensive predictive tool.

This research aims to provide a simplified correlation and software that accurately represents the Standing and Katz Z-factor chart. Also, the paper seeks to efficiently capture the relationship between the pseudo-reduced temperature and pressure in relationship to the Z-factor. The subsequent sections give a background of the data acquisition, model development, validation and comparison with existing models, software development and analysis with case studies.

## 2. MATERIALS AND METHODS

### 2.1 Materials

The materials used in this project are:

- i. WebPlotDigitizer (Rohatgi, 2020)
- ii. Microsoft Excel spreadsheet

iii. Z-Factor (Designed software)

## 2.2 Methods

### 2.2.1 Data acquisition and analysis

3972 digitized data points were extracted directly from the Standing and Katz's chart using WebPlotDigitizer developed by Ankit Rohatgi of GitHub, Pacifica, CA, USA. The data points extracted were distributed across  $1.05 \leq T_{pr} \leq 3.0$  and  $0 < P_{pr} \leq 8.0$ . Subsequently, the extracted data were separated into six groups based on the data ranges for efficient data handling and analysis. Table 1 below shows the group distributions, the range of data within each group and the number of data points used for the analysis of each groups; while Figs. 1 and 2 below shows the digitization and data extraction for  $T_{pr} = 1.05$ .

### 2.2.2 Model development

The Data Analysis add-on on Microsoft Excel Spreadsheet was used to execute a multiple regression analysis on each group. Multiple regression analysis is generally used to examine the relationships between independent variables and a dependent variable [10]. In this case, the proposed correlation was developed as a function of Pseudo-reduced temperature and pressure; with the Pseudo-reduced temperature and pressure as the independent variables and the Z-factor as the dependent variable as shown in equation 3.

$$Z = f\{T_{pr}, P_{pr}\} \quad 3$$

The separated data points predefined in Table 1 for each group was used to regress for the groups; tuned coefficients were then generated for the various data ranges. The developed correlation and the associated tuned coefficients are presented in the result and discussion section.

### 2.2.3 Correlation validation and comparison

To validate the developed correlation, the input ( $T_{pr}$  and  $P_{pr}$  values) of the extracted data was used on the proposed correlation to predict the corresponding Z-factor. The input values were then used on selected well known and published explicit correlations. To compare the performance and accuracy of the new model, statistical error analysis was used. A combination of Mean Absolute Error (MAE), Mean Square Error (MSE), Root Mean Square Error (RMSE), Standard Deviation (SD) and Coefficient of

Determination ( $R^2$ ) was used to compare and ascertain the viability of the model. Also, the predicted values were related to the actual values with line charts for visualization. The results obtained from the analysis are presented in the result and discussion section of the paper. The selected correlations and their corresponding equations are presented in Table 2 below for brevity, the reader is encouraged to consult the various reference for more details about the correlations.

### 2.2.4 Software development

After the correlation has been validated and confirmed suitable and accurate for gas compressibility factor prediction. A highly sophisticated computer program was developed using JavaScript, the software was designed to use the proposed correlation to evaluate Z-factor. It was also designed to work as a simple-to-use, free and more accurate predictive tool for rapid analysis and evaluation. The software works by accepting the  $T_{pr}$  and  $P_{pr}$  values for datas within the correlation validity; performs an inbuilt selection to place the input value against a group to enhance coefficient selection then swiftly displays the results within seconds of data input. Fig. 3 shows the software interface while Fig. 4 (a) shows a quick analysis of  $T_{pr} = 1.67$  and  $P_{pr} = 4.50$  with the software. The procedure for the use of the software is described by the flowchart below.

## 3. RESULT AND DISCUSSION

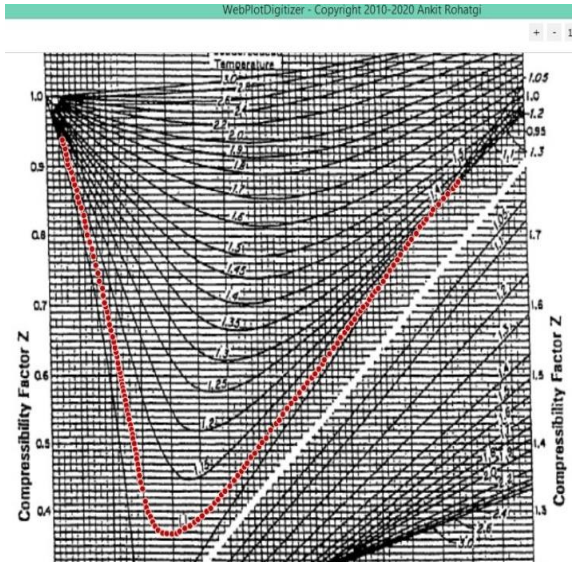
The correlation developed in this research is defined by equation 4 below, while Table 3 presents the tuned coefficients according to predefined groups. The correlation is valid for  $1.05 \leq T_{pr} \leq 3.0$  and  $0 < P_{pr} \leq 8.0$ .

$$\text{Proposed Correlation: } Z = \beta_0 + P_{pr}(\beta_1 + \beta_3 P_{pr}) + T_{pr}(\beta_2 + \beta_4 T_{pr}) + \beta_5 P_{pr} T_{pr} \quad 4$$

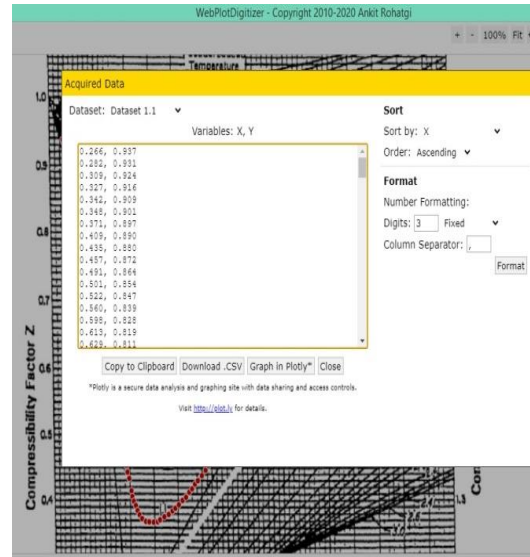
Fig. 5 below presents a graphical representation of the result obtained from the use of the input ( $T_{pr}$  and  $P_{pr}$  values) of the extracted data on the proposed correlation. The results obtained were compared with the actual values for all data range using a line graph for easy visualization, while Fig. 6 presents a cross plot of the predicted value against the actual value. From Fig. 5, it can be observed that the predicted values model the actual values across the data range while Fig. 6 shows a cluster of the values about the 45° line indicating an agreement between the predicted Z-factor value and the actual Z-factor value.

**Table 1. Group distribution**

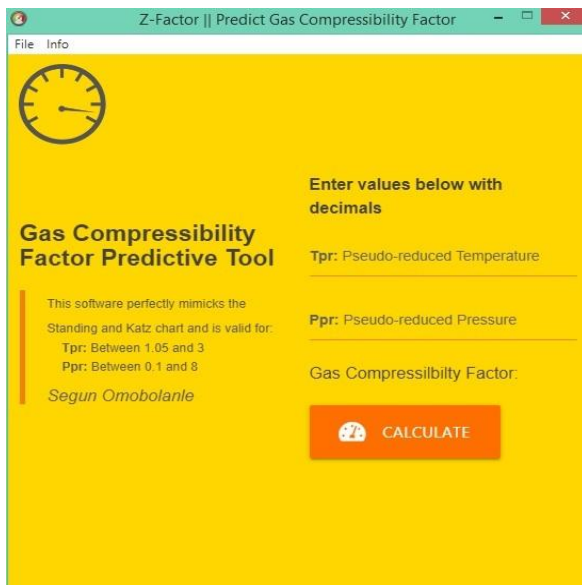
Group	Data Range	Separated Data Points
Group 1	$1.05 \leq T_{pr} \leq 1.2$ $0 < P_{pr} < 3.0$	521 Data Points
Group 2	$1.2 < T_{pr} \leq 2.0$ $0 < P_{pr} < 3.0$	1018 Data Points
Group 3	$2.0 < T_{pr} \leq 3.0$ $0 < P_{pr} < 3.0$	323 Data Points
Group 4	$1.05 \leq T_{pr} \leq 1.2$ $3.0 \leq P_{pr} < 8.0$	341 Data Points
Group 5	$1.2 < T_{pr} \leq 2.0$ $3.0 \leq P_{pr} < 8.0$	1121 Data Points
Group 6	$2.0 < T_{pr} \leq 3.0$ $3.0 \leq P_{pr} < 8.0$	648 Data Points



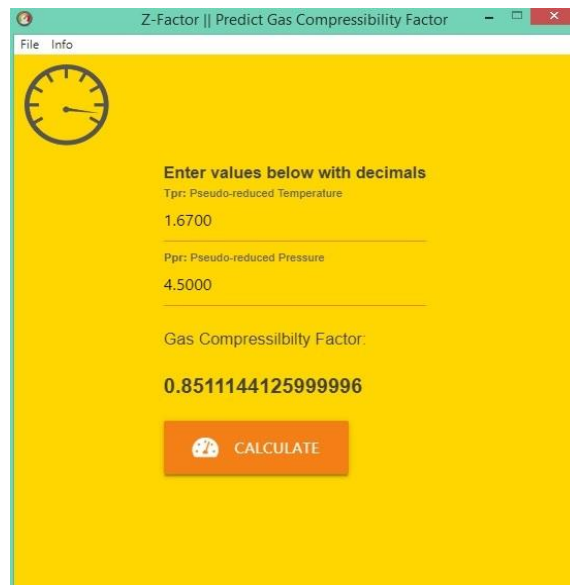
**Fig. 1. Digitization of Chart**



**Fig. 2. Extraction of data**



**Fig. 3. Software interface**



**Fig. 4 (a). Quick analysis with software**

**Table 2. Table of selected correlations**

Correlation Name	Model	Range of Validity
Azubuike et al. [12,12a]	$Z = 0.4326 + 0.2775T_{Pr} + \alpha P_{Pr}$	$1.02 \leq T_{Pr} \leq 2.2$
	$\alpha = 0.04984 - 0.0377T_{Pr} + 0.002971P_{Pr}$	$0.1 \leq P_{Pr} \leq 20$
Obuba et al. [1]	$Z = 6.41824 - 0.013363P_{Pr} - 3.351293T_{Pr}$	$1.26 \leq T_{Pr} \leq 1.7805$
Azizi et al. [9]	$Z = A + \frac{B + C}{D + E}$	$0.2 \leq P_{Pr} \leq 8$
	Where A, B, C, D and E are independent equations	$1.1 \leq T_{Pr} \leq 2.0$
Heidaryan et al. [10]	$Z = \frac{A_1 + A_2 \ln(P_{Pr}) + A_3 (\ln P_{Pr})^2 + A_4 (\ln P_{Pr})^3 + \frac{A_5}{T_{Pr}} + \frac{A_6}{T_{Pr}^2}}{1 + A_7 \ln(P_{Pr}) + A_8 (\ln P_{Pr})^2 + \frac{A_9}{T_{Pr}} + \frac{A_{10}}{T_{Pr}^2}}$	$1.2 \leq T_{Pr} \leq 3.0$
	Where A <sub>1</sub> to A <sub>10</sub> are tuned coefficients	$0.2 \leq P_{Pr} \leq 15$
Shell Oil Company	$Z = A + BP_{Pr} + (1 - A)\exp(-C) - D\left(\frac{P_{Pr}}{10}\right)^4$	Valid for all ranges under consideration.
	Where A, B, C and D are independent equations	

**Table 3. Table of tuned coefficients**

Group	Data Range	Tuned Coefficients
Group 1	$1.05 \leq T_{pr} \leq 1.2$ $0 < P_{pr} < 3.0$	$\beta_0 = -3.2219972; \beta_1 = -1.0436231; \beta_2 = 6.8875605; \beta_3 = 0.1303664;$ $\beta_4 = -2.6676404; \beta_5 = 0.3795069$
Group 2	$1.2 < T_{pr} \leq 2.0$ $0 < P_{pr} < 3.0$	$\beta_0 = -0.2172753; \beta_1 = -0.4121281; \beta_2 = 1.5323799; \beta_3 = 0.0147404;$ $\beta_4 = -0.4684477; \beta_5 = 0.1828234$
Group 3	$2.0 < T_{pr} \leq 3.0$ $0 < P_{pr} < 3.0$	$\beta_0 = 0.8214235; \beta_1 = -0.0714658; \beta_2 = 0.1275471; \beta_3 = 0.0018574;$ $\beta_4 = -0.0224132; \beta_5 = 0.0241995$
Group 4	$1.05 \leq T_{pr} \leq 1.2$ $3.0 \leq P_{pr} < 8.0$	$\beta_0 = -1.0494353; \beta_1 = 0.3694465; \beta_2 = 0.7124665; \beta_3 = 0.0016586;$ $\beta_4 = 0.3409197; \beta_5 = -0.2491262$
Group 5	$1.2 < T_{pr} \leq 2.0$ $3.0 \leq P_{pr} < 8.0$	$\beta_0 = -0.7952649; \beta_1 = 0.0838507; \beta_2 = 1.3059620; \beta_3 = 0.0061400;$ $\beta_4 = -0.1945660; \beta_5 = -0.0656840$
Group 6	$2.0 < T_{pr} \leq 3.0$ $3.0 \leq P_{pr} < 8.0$	$\beta_0 = 0.3478762; \beta_1 = 0.0207613; \beta_2 = 0.3691067; \beta_3 = 0.0022844;$ $\beta_4 = -0.0480460; \beta_5 = -0.0092499$

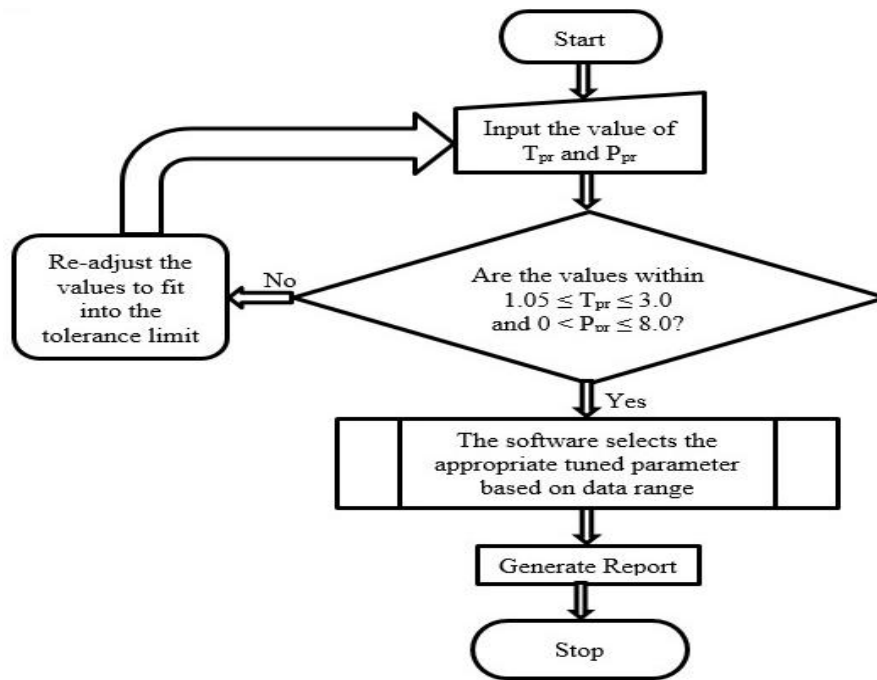


Fig. 4(b). Flowchart for the software path

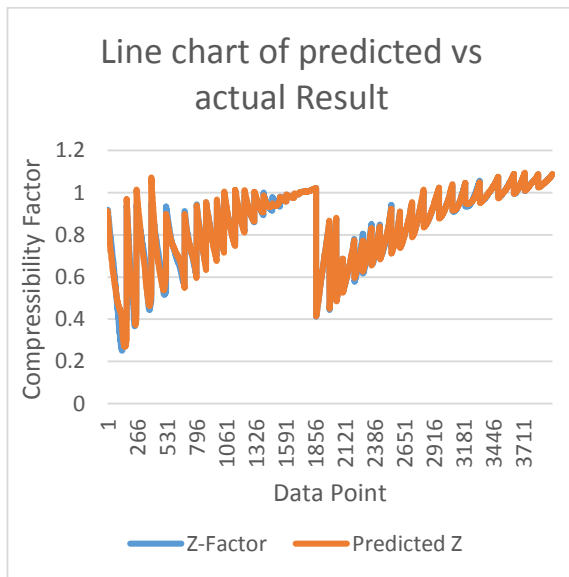


Fig. 5. Line chart of results

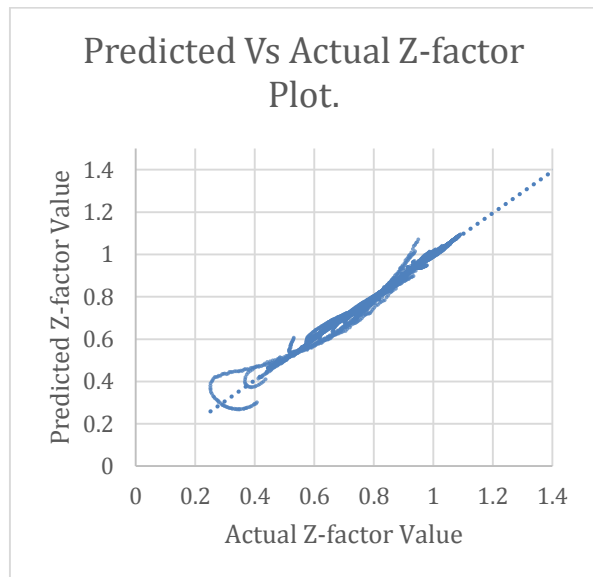


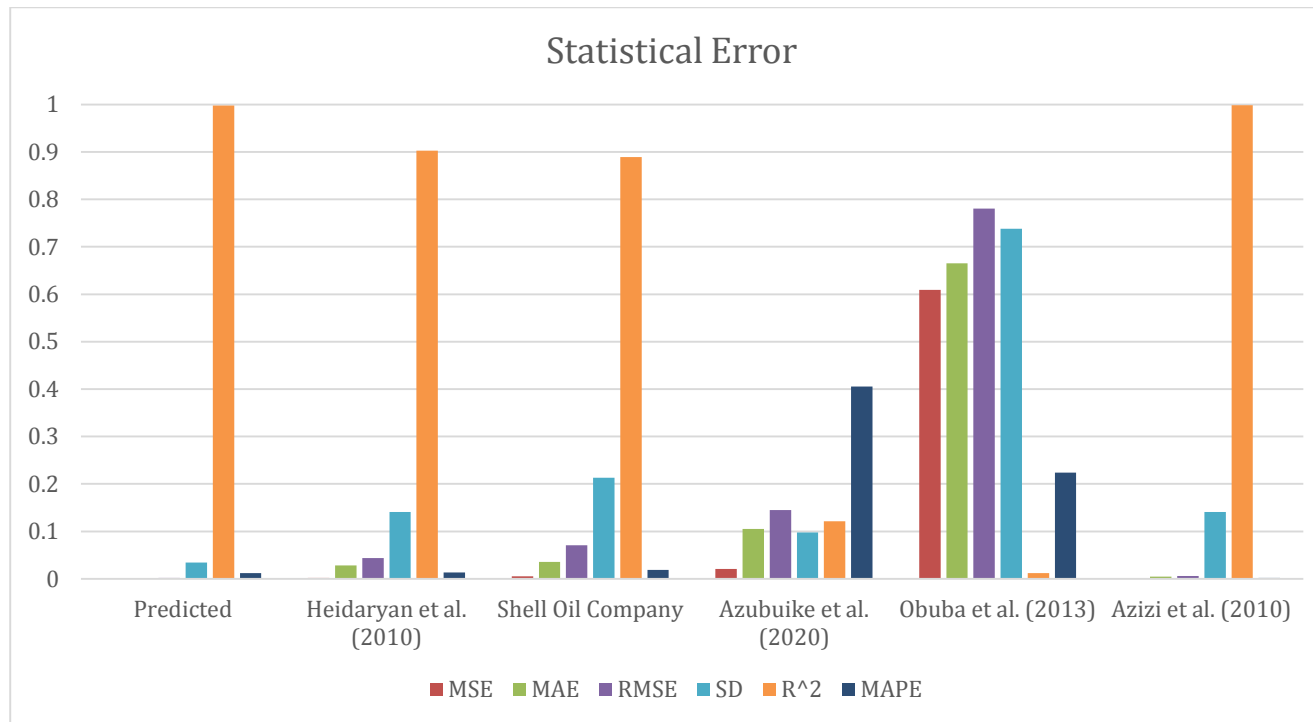
Fig. 6. Cross plot of results

Table 4 below presents the statistical error analysis and the various statistical parameters that were used to compare the performance and accuracy of the new model against other existing models. The proposed correlation compared accurately with a coefficient of determination of 0.9976 and an adjusted  $R^2$  of 0.99759; other parameter used are the Mean Absolute Error (MAE), Mean Square Error (MSE), Root Mean Square Error (RMSE), Mean Absolute Percentage

Error (MAPE) and Standard Deviation (SD), also presented in Table 4. From Table 4, it can be observed that Azizi et al. [9] compared accurately with the proposed model; however, the proposed model surpasses Azizi et al [9] in range of validity and applicability, making it more preferred for wider range of  $T_{pr}$  beyond the scope of Azizi et al [9]. Also, Fig. 7 presents a graphical representation of Table 4.

**Table 4. Statistical error analysis**

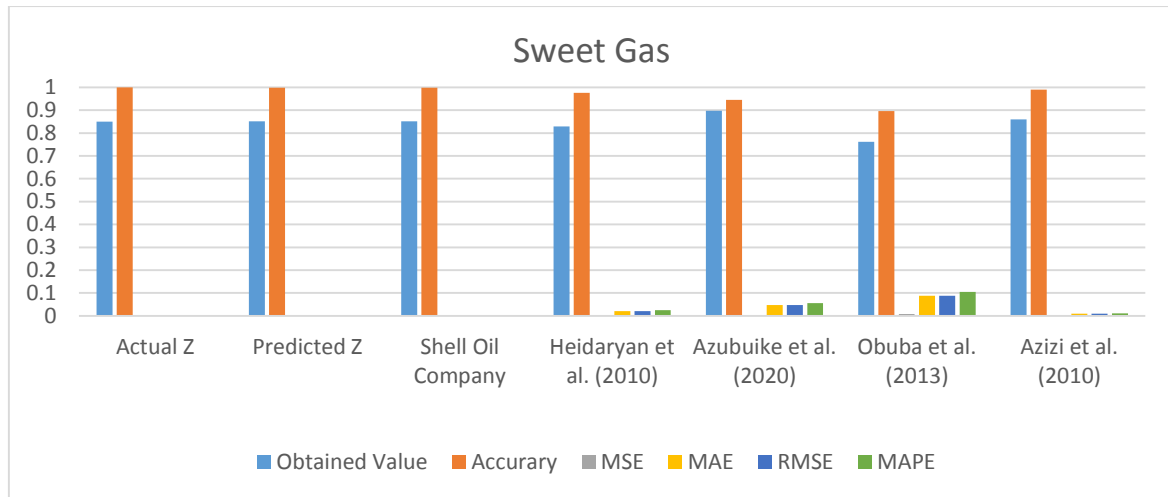
Correlations	MSE	MAE	RMSE	SD	R <sup>2</sup>	MAPE
Predicted	2.76003E-06	0.001264015	0.001661334	0.03401491	0.997616531	0.012266
Heidaryan et al. [10]	0.001934514	0.027989445	0.043983108	0.14091319	0.902547189	0.013596
Shell Oil Company	0.005021933	0.035720902	0.070865597	0.21285195	0.889127208	0.01902
Azubuiké et al. [12,12a]	0.021111358	0.104877575	0.145297482	0.09760843	0.121659469	0.40572
Obuba et al. [1]	0.608940905	0.664940719	0.780346657	0.73801845	0.011885652	0.22401
Azizi et al. [9]	3.56759E-05	0.004601185	0.005972933	0.14091403	0.998202674	0.0019332



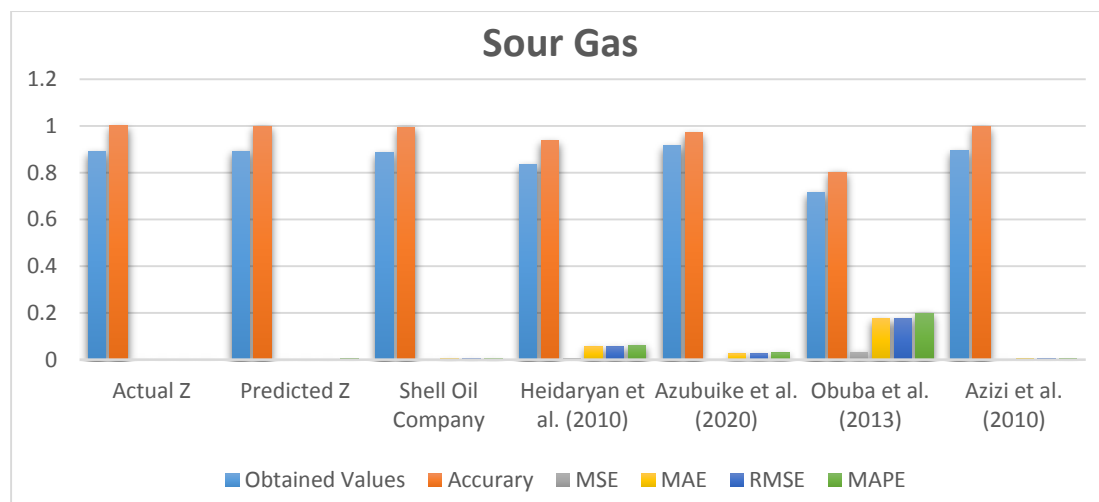
**Fig. 7. Graphical comparison of statistical parameters**

**Table 5. Case 1 reservoir composition**

Components	$y_i$
CO <sub>2</sub>	0.02
N <sub>2</sub>	0.01
C <sub>1</sub>	0.85
C <sub>2</sub>	0.04
C <sub>3</sub>	0.03
i-C <sub>4</sub>	0.03
n-C <sub>4</sub>	0.02



**Fig. 8. Analysis of case 1**



**Fig. 9. Analysis of case 2**

### 3.1 Case Study

#### 3.1.1 Case 1: sweet gas reservoir

Table 5 below gives the composition of a reservoir with an initial reservoir pressure and temperature of 3000 psia and 180° F, respectively. Calculate the gas reservoir

compressibility under initial reservoir conditions [6].

The reported result is 0.85 [6] solving the same problem with the earlier defined accepted models gives the results presented in Table 6 and Fig. 8. The procedure of the proposed model is presented in the appendix.



**Table 6. Result analysis for case 1**

<b>Tpr</b>	<b>Ppr</b>		<b>Actual Z</b>	<b>Predicted Z</b>	<b>Shell Oil Company</b>	<b>Heidaryan et al. [10]</b>	<b>Azubuiké et al. [12,12a]</b>	<b>Obuba et al. [1]</b>	<b>Azizi et al. [9]</b>
1.67	4.5	Obtained Value	0.85	0.85111	0.85104	0.82889	0.89715	0.76145	0.859004
		Accuracy	1	0.998694118	0.998776	0.975165	0.944529	0.895824	0.989407
		MSE	0	1.2321E-06	1.08E-06	0.000446	0.002223	0.007841	8.11E-05
		MAE	0	0.00111	0.00104	0.02111	0.04715	0.08855	0.009004
		RMSE	0	0.00111	0.00104	0.02111	0.04715	0.08855	0.009004
		MAPE	0	0.0013059	0.0012235	0.024835	0.055471	0.10418	0.010593

**Table 7. Result analysis for case 2**

<b>Tpr</b>	<b>Ppr</b>		<b>Actual Z</b>	<b>Predicted Z</b>	<b>Shell Oil Company</b>	<b>Heidaryan et al. [10]</b>	<b>Azubuiké et al. [12,12a]</b>	<b>Obuba et al. [1]</b>	<b>Azizi et al. [9]</b>
1.68	5.55	Obtained Values	0.89	0.8917	0.8854	0.8348	0.9154	0.7139	0.893629
		Accuracy	1	0.998089888	0.994831	0.937978	0.971461	0.802135	0.995922
		MSE	0	2.89E-06	2.12E-05	0.003047	0.000645	0.031011	1.32E-05
		MAE	0	0.0017	0.0046	0.0552	0.0254	0.1761	0.003629
		RMSE	0	0.0017	0.0046	0.0552	0.0254	0.1761	0.003629
		MAPE	0	0.0019101	0.0051685	0.062022	0.028539	0.19786	0.0040778

### 3.1.2 Case 2: Sour gas reservoir

Calculate the deviation factor of a sour natural gas at 3500 psia and 160°F. The compositional analysis of the gas shows that it contains 5% CO<sub>2</sub>, 10% H<sub>2</sub>S and has a specific gravity of 0.7 [8].

The reported result is 0.89 [8]. Solving the same problem with the various models gives the results presented in Table 7 and Fig.9. The procedure of the proposed model is presented in the appendix.

From the analysis of the various case studies [13-50] considered, it can be observed that the proposed model gave the most accurate results with an outstanding accuracy above 99.8% in both scenarios. It should also be noted that Fig. 4 in the software development section solves the first case study with an equivalent performance.

## 4. CONCLUSION

In this research, a novel explicit correlation and a software application for rapid and accurate simplification and prediction of natural gas compressibility factor were developed. 3972 digitized data points was extracted from the Standing and Katz's chart for the development of the model. Upon evaluation and comparison with other existing models for different case studies, the proposed correlation and software were observed to outperformed other models and perfectly mimic the Standing and Katz charts with a 99.8% accuracy, an overall correlation coefficient of 99.76% and an adjusted R<sup>2</sup> of 99.75%.

## COMPETING INTERESTS

Authors have declared that no competing interests exist.

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## APPENDIX

### Analysis of Solutions to Case Study

#### Case Study 1

**Question:** Table 5 gives the composition of a reservoir with an initial reservoir pressure and temperature of 3000 psia and 180° F, respectively. Calculate the gas reservoir compressibility under initial reservoir conditions [6].

#### Analysis of Solution

The reported result is 0.85 [6]

Components	y <sub>i</sub>	T <sub>ci</sub> , °R	T <sub>pc</sub> = y <sub>i</sub> T <sub>ci</sub>	P <sub>ci</sub>	P <sub>pc</sub> = y <sub>i</sub> P <sub>ci</sub>
CO <sub>2</sub>	0.02	547.91	10.96	1071	21.42
N <sub>2</sub>	0.01	227.49	2.27	493.1	4.93
C <sub>1</sub>	0.85	343.33	291.83	666.4	566.44
C <sub>2</sub>	0.04	549.92	22.00	706.50	28.26
C <sub>3</sub>	0.03	666.06	19.98	616.40	18.48
i-C <sub>4</sub>	0.03	734.46	22.03	527.9	15.84
n-C <sub>4</sub>	0.02	765.62	15.31	550.6	11.01
			T <sub>pc</sub> = 383.38	P <sub>pc</sub> = 666.38	

From the above, T<sub>pc</sub> = 383.38 while P<sub>pc</sub> = 666.38

$$P_{pr} = \frac{P}{P_{pc}} = \frac{3000}{666.38} = 4.50; \quad T_{pr} = \frac{T}{T_{pc}} = \frac{180+460}{383.38} = 1.67$$

From the values of the P<sub>pr</sub> and T<sub>pr</sub>; it can be observed that the values fall into group 5 (Check Table 3), thus the tuned coefficients for group 5 are used for the analysis.

$$\text{Recall that } Z = \beta_0 + P_{pr}(\beta_1 + \beta_3 P_{pr}) + T_{pr}(\beta_2 + \beta_4 T_{pr}) + \beta_5 P_{pr} T_{pr}$$

And the tuned coefficient for group 5 are;  $\beta_0 = -0.7952649$ ;  $\beta_1 = 0.0838507$ ;  $\beta_2 = 1.3059620$ ;

$$\beta_3 = 0.0061400; \beta_4 = -0.1945660; \beta_5 = -0.0656840$$

Inserting the P<sub>pr</sub>, T<sub>pr</sub> and the tuned coefficients into the proposed equation; we have  
 $Z = -0.7952649 + (4.5*(0.0838507+(0.0061400*4.5))) + (1.67*(1.3059620 + (-0.1945660*1.67))) + (-0.0656840*4.50*1.67) = 0.851111$

The predicted natural gas compressibility from the proposed correlation is 0.851111

#### Case Study 2

**Question:** Calculate the deviation factor of a sour natural gas at 3500 psia and 160°F. The compositional analysis of the gas shows that it contains 5% CO<sub>2</sub>, 10% H<sub>2</sub>S and has a specific gravity of 0.7 (Tarek, 2001).

#### Analysis of Solution

Calculating the uncorrected Pseudo-critical properties of the gas from Brown et al. (1948) as presented by Standing (1922) in the form of a correlation; the uncorrected Pseudo-critical properties are:

$$T_{pc} = 168 + 325Y_g - 12.5Y_g^2; \quad T_{pc} = 168 + 325(0.7) - 12.5(0.7)^2 = 389.38^\circ\text{R}$$

$$P_{pc} = 677 + 15Y_g - 37.5Y_g^2;$$

$$P_{pc} = 677 + 15 (0.7) - 37.5 (0.7)^2 = 669.1 \text{ psia}$$

Correcting the pseudo-critical properties

$$A = y_{H_2S} + y_{CO_2}$$

$$A = 0.1 + 0.05 = 0.15$$

$$B = y_{H_2S}$$

$$B = 0.10$$

$$\varepsilon = 120 [A^{0.9} - A^{1.6}] + 15 (B^{0.5} - B^{4.0});$$

$$\varepsilon = 120 [0.15^{0.9} - 0.15^{1.6}] + 15 (0.10^{0.5} - 0.10^{4.0}) = 20.735$$

$$T'_{pc} = 389.38 - 20.735 = 368.64^\circ R$$

$$P'_{pc} = \frac{P_{pc} T'_{pc}}{T_{pc} + B(1-B)\varepsilon}$$

$$P'_{pc} = \frac{669.1 * 368.64}{389.38 + (0.1(1-0.1)(20.635))} = 630.44$$

$$T_{pr} = \frac{160 + 460}{368.64} = 1.68$$

$$P_{pr} = \frac{3500}{630.44} = 5.55$$

This values also fall within group 5, therefore;

Inserting the  $P_{pr}$ ,  $T_{pr}$  and the tuned coefficients into the proposed equation; we have

$$Z = -0.7952649 + (5.55 * (0.0838507 + (0.0061400 * 5.55))) + (1.68 * (1.3059620 + (-0.1945660 * 1.68))) + (-0.0656840 * 5.55 * 1.68) = 0.8517$$

The predicted natural gas compressibility from the proposed correlation is 0.8517

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