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# Accurate Compressibility Estimates for Natural Gas

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### Abstract

This document describes methods to calculate estimated gas compressibility without having the full gas composition. The purpose of these methods is for use cases where reasonable accuracy is required but not critical and the methods must be computationally efficient such that they can be used in programmable logic controllers, remote terminal units, and supervisory control and data acquisition systems; akin to the functionality of the NX-19 or AGA-8 Gross methods but with higher accuracy.

Multiple simplified calculation methods were evaluated with one method performing significantly better than the other methods. The best performing method was then tuned to better fit the reference data. The equations and associated source code for that method are contained as appendices in this report.

The methods discussed here were analyzed only with respect to the application to gas phase (including some supercritical conditions) natural gas with minimal helium, hydrogen, or hydrogen sulfide.

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# List of Acronyms

PAC	Programmable automation controller
PLC	Programmable logic controller
RTU	Remote terminal unit
SCADA	Supervisory control and data acquisition

# List of Nomenclature

A - G	Intermediate variables
cwa	Critical temperature composition adjustment factor
CO2	Mole fraction of carbon dioxide in the gas
N2	Mole fraction of nitrogen in the gas
Р	Static gas pressure in psia
Pc	Critical pressure in psia
Pic	Intermediate critical pressure
Pr	Reduced pressure
P <sub>rc</sub>	Reduced pseudo critical pressure
p1 – p5	Critical pressure coefficients
Sg	Specific gravity of the gas relative to air at base conditions
Sg <sub>HC</sub>	Specific gravity of the hydrocarbon portion of the gas
T	Static gas temperature in °F
T <sub>c</sub>	Critical temperature in °R

T <sub>ic</sub>	Intermediate critical temperature
Tr	Reduced temperature
T <sub>rc</sub>	Reduced pseudo critical temperature
t1 – t6	Critical temperature coefficients
У	An intermediate variable
Z	Calculated gas compressibility

# **1** Executive Summary

Gas compressibility calculations is an important parameter in the transportation of natural gas via pipelines. Its uses include measurement accounting, compressor performance evaluations, pipeline inventory calculations, and pipeline hydraulic design.

Equations of state are used to estimate the compressibility of a gas which changes with gas composition, pressure, and temperature. The most accurate calculation methods are very complicated and require more computational power and memory than is available (or needed) for many applications including programmable logic controllers (AKA PLC), programmable automation controllers (PAC), and remote terminal units (RTU). As such, there is a need for simplified equations of state that are faster to calculate yet provide reasonable accuracy.

While there are many simplified methods for calculating gas compressibility, most of them were developed through regressions of the Standing and Katz Diagram that was first published in 1941. (1) As a result, most of the available simplified gas compressibility methods are not tuned to the most current models/data and therefore suffer in accuracy. Many of the developed methods were produced for reservoir modeling and, as such, were tuned for much higher pressures than norm

For custody transfer gas measurement applications, it is recommended that the use rigorous methods, such as AGA-8 with full gas composition analysis continue to be used. For other applications, considerations should be given to adopt the recommendations as outlined in this report.

The target audience for this report include:

- Information technology support for supervisory control and data acquisition (SCADA) for pipeline inventory (AKA pack) calculations,
- Control system developers,
- Gas measurement specialists,
- Hydraulic system engineers, and
- Compression performance engineers.

# 2 Introduction

Efficient and accurate equations of state are required for many aspects natural gas engineering and operations. The accurate estimate of gas compressibility is important to the determination of gas density in gas measurement accounting. As such the most reliable and reliable equations of state should be used for that application. Those methods often require full gas composition and utilize large multi-parameter algorithms that utilize iterative calculations to estimate gas density until convergence is achieved. The calculated density is then compared to the density using the ideal gas law to calculate the gas compressibility. Therefore, any error in the calculated gas compressibility is directly proportional to errors in the gas density which will result in a corresponding error in the accounted standard volume accumulated through a gas meter.

But there are many other applications where the requirement for precise gas compressibility is less

important than necessary for custody transfer applications. These applications typically require more frequent compressibility calculations and therefore computational efficiency is more important than absolute accuracy.

- Applications
  - Compression performance,
  - Like pack calculations, and
  - Pipeline hydraulic simulations.

Computational efficiency is especially important for these applications because the calculations must be done more frequently (especially in the case of pipeline hydraulic modeling) and/or with limited hardware capability in both processor speed and memory.

There are already may equation of state methods that meet the computational efficiency requirements. The objective of this work is to identify the most accurate method(s) that will work across a wide range of gas compositions and operating pressures and temperatures. This is especially important with the increased transportation of natural pipelines carrying high ethane gas.

The methods discuss here are only applicable to pipelines transporting product as a single-phase gas that has minimal amounts of helium, hydrogen, or hydrogen sulfide.

# 3 Analysis

Screening of the various equations of state was performed and a subset was selected for evaluation for accuracy as compared to REFPROP (2). More details of the methods of comparison can be found in Appendix A, Evaluation and Selection of Simplified Methods.

# 3.1 Selected Equations of States Methods for Evaluation

The models selected for evaluation under this effort can be found in Table 1.

Model	Abbreviation	Calculation Type
AGA NX-19	ZNX-19	Direct solution
AGA-8 Gross, Method 1	Zaga-8Gross1	Iterative
AGA-8 Gross, Method 2	ZAga-8Gross2	Iterative
California Natural Gas Associa-	ZCnga	Direct solution
tion		
Kareem	ZKareem	Direct solution
Shell	ZShell	Direct solution
Tuned Kareem	ZKareemTuned	Direct solution
Trube	ZTrube	Iterative
Tuned Trube	ZTrubeTuned	Iterative

Table 1 – Selected	models	for	evaluation
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As a general rule, direct solution methods tend to be more processor efficient as they tend to have a lower number of total math operands executed than do iterative solutions. With that said, the algorithms used in the iterative solutions selected for evaluation tend to converge very quickly and are nearly as computationally efficient as the direct solution methods.

### 3.2 Relative model performance

The analysis was performed using a wide variety of (mostly) real natural gas compositions tested over a wide range of pressures and temperatures, a summary of the overall performance of the evaluated models is shown in Table 2.

Abbreviation	Sum of Error	Pearsons Correlation	Maximum Absolute	Average Absolute	Objective
	Squared		Error	Error	
ZNX-19	439.59	0.9311	187.8%	3.6%	275.90
Zaga-8Gross1	1469.48	0.6108	288.9%	6.6%	1024.64
ZAga-8Gross2	1454.55	0.6164	288.9%	6.6%	1004.41
ZCnga	351.95	0.9270	137.4%	4.6%	112.93
ZKareem	125.18	0.9891	108.6%	2.4%	127.13
ZKareemTuned	6.54	0.9972	30.5%	0.9%	2.30
ZShell	35.41	0.9920	141.6%	1.2%	12.48
ZTrube	35.25	0.9920	141.6%	1.2%	12.43
ZTrubeTuned	24.43	0.9941	127.9%	1.2%	8.68

The Objective being defined as a target used to identify the overall fit of a model. The objective is calculated by averaging the sum of the error squared, the maximum absolute error and the average absolute error and then dividing by the square of the Pearson correlation.

Of the models evaluated here, the tuned Kareem method performed well above the others in terms of accuracy.

# 4 Conclusions and Overall Recommendations

At the risk of introducing yet another equation of state, it is recommended that the tunned Kareem method is utilized for applications needing simplified methods for calculating gas compressibility. Details on the associated calculations can be found in Appendix B, Equations for the Recommended Method

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# Appendix A. Evaluation and Selection of Simplified Gas Compressibility Methods

# A.1. Equations of State

#### A.1.1 <u>Background</u>

Equations of state are models that predict the properties of various gases under varying pressure and temperature conditions. Currently, many different equations of state models exist because:

- Not all models are valid at modeling all substances under all conditions.
- Some models require full gas compositions while others only require inference information to composition such as the specific gravity relative to air or the caloric higher heating value.
- Some models require more computational power that others and therefore are not suitable for some hardware applications such as PAC/PLC and RTUs that have limited processor power and/or memory.

Mathematical methods for solving equations of state include:

- Direct regressions.
- Multi-range regressions
- Iterative solutions
- Cubic

Equation of state methods include (but is certainly not limited to): (3)

- Van der Waals
- Peng-Robinson (AKA PR)
- Redlich-Kwong (AKA RK)
- Soave-Redlich-Kwong (AKA SRK and RKS)
- Benedict-Webb-Rubin (AKA BWR)
- Benedict-Webb-Rubin-Starling (AKA BWRS)
- GERG-2008 (4)
- AGA-8/AGA-10 (5)
- REFPROP (2)
- Pitzer
- Trube (6)
- NX-19
- Kareem
- Shell Oil (AKA Kumar)
- Sutton
- Riazi-Daubert
- Corredor
- Piper
- Whichert-Aziz

- Casey (3)
- Sutton
- Kareem
- Beggs-Brill
- TEQP
- Papay
- California Natural Gas Association CNGA
- Heidaryan
- Gopal
- Whitson
- Kesler-Lee
- Bahadori
- Al-Anazi and Al-Quraishi

It should be noted that this is a very incomplete list. An indication of both the importance of equations of state and the challenges to generate them simply and accurately.

### A.1.2 Criteria for Evaluation

The objective of this effort is to narrow the list of equations of state to find models that meet the following criteria:

- Suitable for simplified gas compositions (specific gravity and composition of nitrogen and carbon dioxide).
- Minimal code intensity such that:
  - They can be deployed in remote terminal units, programmable logic controllers, and SCADA.
- Does not utilize the solving of roots or has piecewise regressions where discontinuities can exist. This typically produces more reliable calculations and allows the estimation of partial derivatives such that extended gas properties can be estimated.
- Must be suitable for a wide range of 'real' natural gas compositions.
- Must accommodate a wide range of pressure and temperature conditions.

# A.2. Gas composition

To assess the capabilities of the equation of state models, 80 natural gas compositions were selected, the majority of which were garnered from the informational postings of interstate natural gas companies in the United States. The compositions were wide ranging as indicated in Table 2.

Parameter	Maximum	Minimum	Average
Carbon Dioxide	15.00%	0.00%	0.76%
Nitrogen	16.81%	0.00%	3.26%
Methane	100.00%	68.54%	86.11%
Ethane	24.76%	0.00%	7.59%

Propane	6.32%	0.00%	1.46%
Normal Butane	2.87%	0.00%	0.36%
Iso Butane	1.67%	0.00%	0.17%
Normal Pentane	1.30%	0.00%	0.11%
Iso Pentane	0.81%	0.00%	0.08%
Hexane	0.87%	0.00%	0.06%
Heptane	0.87%	0.00%	0.05%
Total Inerts	17.35%	0.00%	4.02%
Specific Gravity	0.7793	0.5539	0.6398
Higher Heating Value	1297.3	900.3	1075.5

It should be noted that some of these parameters are outside the stated ranges of some of the equations of state. For example, NX-19 has a limit of 15% of total inerts.

# A.3. **REFPROP Reference**

REFPROP was selected as the reference to compare compressibility calculations against the other equations of state models. It was selected as being one of the most accurate models available for pure fluids and mixtures, is actively being supported, and is widely available.

Calculations were performed using REFPROP with full detailed composition analysis to calculate the gas compressibility, density, speed of sound, and phase. Pressures for the calculations ranged from 14.73 to 2350 psia (0.1016 to 16.202 MPa) and temperatures from -220 to 300 °F (-140 to 149 °C). Conditions where liquid drop-out was indicated were excluded from the dataset (single phase gas conditions only). In total, more than 20,000 state points were calculated.

This set of data was then used to compare how other equations of state calculated gas compressibility for the same pressure and temperature conditions for each gas composition. These comparisons are reviewed in section 3.5.

# A.4. Evaluation of Simplified Equations of state

#### A.4.1 <u>California Natural Gas Association</u>

A simplified method that is commonly used is the California Natural Gas Association (CNGA) method. (7) This method is very lightweight computationally at the expense of accuracy as shown in Figure 1. The accuracy deviates the most at relatively low compressibility, typically at low temperatures and moderate to high pressures.



Figure 1 – Gas compressibility unity comparison, CNGA method

While relatively simple to implement, the accuracy of this model would not be sufficient for many applications. Largest errors were for cold gas (<0 °F) and high temperatures (>100 °F) with high specific gravities (>0.7).

### A.4.2 <u>NX-19</u>

NX-19 is a method developed by PRCI in the 1960's for the purpose of calculating gas compressibility for the use in custody transfer gas measurement. (8) The method is stated to be applicable to natural gases that have a specific gravity less than 0.75 total diluents (nitrogen and carbon dioxide) of less than 0.15 on a mole fraction basis. Comparison against the REFPROP methods is shown in Figure 2.



Figure 2 – Gas compressibility unity comparison, NX-19 method

While the method is more accurate than the CGNA method, there are specific gas compositions where the model's is not suitable. The largest deviations were at cold temperatures (< 0 °F) and high specific gravities (> 0.7).

#### A.4.3 <u>AGA8 Gross</u>

The American Gas Association first published in 1992 and includes two simplified methods for calculating gas compressibility known respectively as method 1 and method 2. (5) (9) (10) (11) At the time this standard was first published, these methods were intended to supersede NX-19 as the predominant method of calculating gas compressibility for custody transfer measurement.

The performance of the two methods produce almost identical results for the gas compositions and operating conditions evaluated as shown in Figure 3.



Figure 3 – Gas compressibility unity comparison, AGA-8 Gross Methods 1 and 2

Of note are the cases where the gas compressibility is calculated by the AGA-8 methods as 1.0. In most of these cases, the compositions or operating conditions were outside the bounds of the model and a calculated compressibility of 1.0 was returned with a corresponding error message. The other conditions where the compressibility is constant across the range (e.g., the horizontal trends just below the out of bound points) are unexplained.

#### A.4.4 <u>Kareem</u>

The Kareem (et. Al) model (12) is a direct solution method built upon the Standing and Katz correlations. The performance of the model is shown in Figure 4.



Figure 4 – Gas compressibility unity comparison, Kareem method

The overall performance of the model is very good with the largest deviations at areas where a low compressibility is calculated. The model can be trusted to have reasonable accuracy when the calculated compressibility is between 0.7 and 1.

#### A.4.5 <u>Shell</u>

The Shell method (3) was analyzed and the unity comparison to REFPROP is shown in Figure 5.



Figure 5 – Gas compressibility unity comparison, Shell method

Overall, the Shell method performed reasonably well. However, there were conditions where the model could not calculate a result. Those points were at temperatures that approached the critical temperature.

#### A.4.6 <u>Trube</u>

The Trube method (6) is an iterative method that solves for real density using equations of state. When the density calculation converges, gas compressibility is calculated by comparing the calculated density to the density using the ideal gas law thus allowing for solving gas compressibility. The performance of the Trube model is shown in Figure 6.



Figure 6 – Gas compressibility unity comparison, Trube method

The overall performance is good but there are some outlier points noted. The outliers are attributed to errors in the estimation of the critical pressures and temperatures using this method.

### A.4.7 <u>Tuned Trube</u>

Based on the reasonable performance of the Trube method, an effort was made to tune the coefficients used in the Trube model in an attempt to produce better accuracy. Marginal improvements were made as can be seen in Figure 7.



Figure 7 - Gas compressibility unity comparison, tuned Trube method

Although the performance is better than the base Trube model, the overall performance improvement isn't significant and still has outliers.

### A.4.8 <u>Tuned Karem</u>

Similar to the tuned Trube method, the coefficients used in the Karem model were tuned to enhance the accuracy of the model, the results are shown in Figure 8.



Figure 8 - Gas compressibility unity comparison, tuned Kareem method

The tuned mode significantly improved the overall performance as compared to the Kareem method. The tuning reliably extended the model for the full range of gas compositions and pressures/temperatures evaluated in this analysis.

#### Appendix B. Equations for the Tuned Karem method

The methods identified here are based on US customary units (e.g., psia and °F). Conversion from other units is easily accomplished and won't be detailed here.

The process of calculating gas compressibility using the Karem method first involves calculating the reduced pressures and temperatures as compared to the critical pressures and temperatures. The critical pressures and temperatures are a function of the gas composition. As we don't have a full gas composition, the critical values are estimated based on the specific gravity (Sg) adjusted to exclude the inerts (Sg<sub>HC</sub>):

$$Sg_{HC} = (Sg - 0.9672 N2 - 1.5195 CO2) / (1 - N2 - CO2)$$
 [1]

Where:

CO2 is the mole fraction of carbon dioxide in the gas, and N2 is the mole fraction of nitrogen in the gas.

Calculating the reduced critical temperature  $(T_{rc})$  is done by:

$$T_{RC} = t1 + t2 Sg_{HC} - t3 Sg_{HC}^{2}$$
[2]

Where coefficients t1 through t3 are defined in Table 3.

The intermediate critical temperature () is calculated by:

$$T_{iC} = (1 - N2 - CO2) T_{RC} - t4 N2 + t5 CO2$$
[3]

Where coefficients t4 and t5 are also defined in Table 3.

The critical temperature composition adjustment factor (cwa) is:

$$cwa = t6 (CO2^{0.9} - CO2^{1.6})$$
 [4]

Where coefficient t6 is found in Table 3.

The critical temperature (T<sub>c</sub>) is:

$$T_c = T_{ic} - cwa$$
<sup>[5]</sup>

Calculate the reduced critical pressure (P<sub>r</sub>) as:

$$P_{RC} = p1 + p2 Sg_{HC} + p3 Sg_{HC}^{2}$$
[6]

Where coefficients p1 through p3 are found in Table 3.

Calculate the intermediate critical pressure (Pic) as:

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$$P_{ic} = (1 - N2 - CO2) P_{ic} + p4N2 + p5CO2$$
[7]

Where coefficients p4 and p5 are found in Table 3.

The critical pressure (P<sub>c</sub>) is estimated by:

$$P_c = \frac{P_{ic}(T_{ic} - cwa)}{T_{ic}}$$
<sup>[8]</sup>

The reduced pressure  $(P_r)$  and temperature  $(T_r)$  are then calculated by:

$$P_r = \frac{P}{P_r}$$
[9]

$$T_r = \frac{\frac{T_c}{(T + 459.67)}}{T_c}$$
[10]

 $I_c$  The intermediate values for A-G and y are then calculated:

$$A = \frac{a1 P_r e^{(a2 \left(1 - \frac{1}{T_r}\right)^2)}}{T}$$
[11]

$$B = \frac{a_3}{T_r} + \frac{a_4}{T_r^2} + \frac{a_8 P_r^6}{T_r^6}$$
[12]

$$C = a9 + \frac{a8 P_r}{T_r} + \frac{a7 P_r^2}{T_r^2} + \frac{a6 p_r^3}{T_r^3}$$
[13]

$$D = \frac{a10 e^{(a11\left(1 - \frac{1}{T_r}\right)^2)}}{a10 e^{(a11\left(1 - \frac{1}{T_r}\right)^2)}}$$
[14]

$$E = \frac{a12}{T} + \frac{a13}{T^2} + \frac{a14}{T^3}$$
[15]

$$F = \frac{a_{15}}{T} + \frac{a_{16}}{T^2} + \frac{a_{17}}{T^3}$$
[16]

$$G = a18 + \frac{a19}{T_{r}}$$
[17]

$$y = \frac{D'P_r}{(\frac{(1+A^2)}{C} - \frac{A^2B}{C^3})}$$
[18]

Gas compressibility (Z) is then calculated as:

$$Z = \frac{(D P_r (1 + y + y^2 + y^3))}{((D P_r + E y^2 - F y^G)(1 - y)^3)}$$
[19]

Parameter	Original Value	Tuned Value
t1	168	160.8645
t2	325	344.9765
t3	12.5	9.635898
t4	227.3	178.7269
t5	547.6	573.4464
t6	120	111.3906
p1	677	606.5302
p2	15	-17.1152
р3	-37.5	-64.2998
p4	493	352.3388
р5	1071	918.9365
a1	0.317842	0.373852
a2	0.382216	-0.26743
a3	-7.76836	-8.49935
a4	14.29053	14.304
a5	0.000002	0.000369
а6	-0.00469	0.001819
а7	0.096254	0.100306
a8	0.16672	0.092584
a9	0.96691	1.02959
a10	0.063069	0.054126
a11	-1.96685	-1.07476
a12	21.0581	21.40866
a13	-27.0246	-27.8239
a14	16.23	13.42556
a15	207.783	202.2976
a16	-488.161	-488.924
a17	176.29	157.0994
a18	1.88453	1.75652
a19	3.05921	2.474073

#### Table 3 - Karem method parameters