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Compressibility Factors for Naturally Occurring Petroleum Gases

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ABSTRACT

The Sutton gas specific gravity correlation gives values of pseudocritical properties which, when used with the Dranchuk and Abou-Kassem (DAK) representation of the Standing and Katz (SK) chart, currently provide the most accurate estimates of compressibility factors for naturally occurring petroleum gases. However, other correlations must be used to account for the presence of acid gases. A new gas specific gravity correlation is presented which takes into account the effects of the acid gases and nitrogen. The new correlation provides more accurate estimates of the compressibility factor than can be obtained by current methods and also eliminates the need for involving additional correlations to correct for the presence of acid gases and nitrogen. The new correlation was developed using a set of 1482 data points, ranging in composition from lean sweet to rich acid gases.

INTRODUCTION

Knowledge of the pressure-volume-temperature (PVT) behavior of natural gases is necessary to solve many petroleum engineering problems. Gas reserves, gas metering, gas pressure gradients, pipeline flow and compression of gases are some of the problems requiring the gas compressibility factor, or z factor. Typically, the z factor is determined by laboratory measurement. However, laboratory data is only applicable for the compositions and conditions investigated. When conditions of interest are different from those of the laboratory studies or data is not available, correlations must be used.

The basic methods for estimating the gas compressibility factor are relatively simple and well known.[1] The principle of corresponding states, Kay's pseudocritical point, and the SK chart are commonly used. If the composition of the gas is known, the pseudocritical temperature and pressure may be calculated using Kay's rules--molar averages of the critical properties of the mixture's components. Otherwise, the pseudocritical temperature and pressure may be estimated using correlations based on gas specific gravity. Then, the reduced temperature and pressure may be calculated and the SK chart or its representation by the DAK equation of state may be used to determine the z factor.

Sutton[2] presented more accurate methods for both cases. His method for calculating the pseudocritical temperature and pressure when the composition of the gas is known is based on the Stewart, Burkhardt, and Voo (SBV) equations given by:

$$T_{pc} = \frac{K^2}{J} \text{ and } p_{pc} = \frac{T_{pc}}{J}, \quad \ldots\ldots\ldots\ldots \text{(1a)}$$

where,

$$J = \frac{1}{3}\sum_j y_j\left(\frac{T_c}{p_c}\right)_j + \frac{2}{3}\left[\sum_j y_j\left(\frac{T_c}{p_c}\right)_j^{0.5}\right]^2$$

$$\text{and } K = \sum_j y_j\left(\frac{T_c}{\sqrt{p_c}}\right)_j. \quad \ldots\ldots \text{(1b)}$$

His gas specific gravity correlation for estimating the pseudocritical temperature and pressure when the composition of the gas is known, based on 634 compositions from 275 PVT reports, is given by:

$$T_{pc} = 169.2 + 349.5\gamma_g - 74.0\gamma_g^2,$$

and

$$p_{pc} = 756.8 - 131.0\gamma_g - 3.6\gamma_g^2. \quad \ldots\ldots \text{(2)}$$

References and illustrations at end of paper.

If the gas contains hydrogen sulfide or carbon dioxide, the Wichert and Aziz correlation:

$$T'_{pc} = T_{pc} - \varepsilon,$$

where,

$$\varepsilon = 120 \cdot \left[(y_{H_2S} + y_{CO_2})^{0.9} - (y_{H_2S} + y_{CO_2})^{1.6} \right] + 15 \cdot \left[(y_{H_2S})^{0.5} - (y_{H_2S})^{4} \right],$$

and,

$$p'_{pc} = \frac{p_{pc} T'_{pc}}{T_{pc} + y_{H_2S}(1 - y_{H_2S})\varepsilon}, \quad \ldots\ldots\ldots\ldots\ldots (3)$$

should be used to adjust the pseudocritical constants.[2-3] However, Ref. 2 is unclear on how Eqs. 3 should be applied to Eqs. 2.

In an earlier paper[4], we discussed Sutton's modification to the SBV rules in detail and presented a new modification which takes into account the effects of the heptane plus fraction, acid gases and nitrogen. This correlation, having a form similar to the SBV equations, was based on 896 data points from 134 PVT reports and is given by:

$$J = \alpha_0 + \sum_{i=1}^{3} \alpha_i y_i \left(\frac{T_c}{p_c}\right)_i + \alpha_4 \sum_j y_j \left(\frac{T_c}{p_c}\right)_j + \alpha_5 \left[\sum_j y_j \left(\frac{T_c}{p_c}\right)_j\right]^2 + \alpha_6 y_{C_{7+}} M_{C_{7+}} + \alpha_7 (y_{C_{7+}} M_{C_{7+}})^2,$$

and,

$$K = \beta_0 + \sum_{i=1}^{3} \beta_i y_i \left(\frac{T_c}{\sqrt{p_c}}\right)_i + \beta_4 \sum_j y_j \left(\frac{T_c}{\sqrt{p_c}}\right)_j + \beta_5 \left[\sum_j y_j \left(\frac{T_c}{\sqrt{p_c}}\right)_j\right]^2 + \beta_6 y_{C_{7+}} M_{C_{7+}} + \beta_7 (y_{C_{7+}} M_{C_{7+}})^2, \quad \ldots\ldots (4)$$

where $y_i \in \{y_{H_2S}, y_{CO_2}, y_{N_2}\}$, $y_j \in \{y_{C_1}, y_{C_2}, \cdots, y_{nC_6}\}$, and the α_i and β_i were shown in Table 3 of Ref. 4. Eqs. 4, used with Eqs. 1a and the DAK representation of the SK chart, provided more accurate estimates of the compressibility factor, simplified the prodedures, and included the effects of nitrogen.

This paper reports on further studies using a larger data base. We present an update for the coefficients of Eqs. 4, based on the expanded data base, and a new gas specific gravity correlation. Both Eqs. 4 and the new correlation eliminate the need for Eqs. 3 and include the effects of nitrogen; and can be used with Eqs. 1a to calculate more accurate estimates of the compressibility factor.

EXPANDED DATA BASE

Our previous work on gas compressibility correlations used a data base with a limited number of high specific gravity gases and gases with high impurities content. The data set has been expanded by about 60 %, with emphasis on adding gases to correct these deficiencies. For this study, we added 586 data points from 37 PVT reports from the literature[5-13] and other sources[14-15]. **Table 1** shows the range of composition, physical properties, and conditions of the resulting data base. Our expanded data base contains significantly more gases with specific gravities ranging from 1.3 to 1.8. Additionally, it contains significantly more gases with impurities than the data base used by Sutton. While the maximum concentrations of hydrogen sulfide and carbon dioxide are quite large, only ten percent of the samples had an acid gas concentration greater than twelve percent.

Updated Coefficients for Eqs. 4. Our previous analysis was repeated using the expanded data base to develop the new coefficients for Eqs. 4 shown in **Table 2.** We then evaluated the SBV rules, Sutton's modification to the SBV rules (SSBV) and Eqs. 1a and 4 using the expanded data base. The average absolute errors of the calculated compressibility factors were 2.23, 1.53, and 1.07 percent, respectively. These results were consistent with those in Ref. 4 and are shown in **Table 3**, for four different subsets of the data, ranging from lean sweet gases to rich acid gases, and **Figs. 1 through 4. Figs. 2** and **4** show the distribution of the errors with the experimental z factor. Higher errors occurred at lower z factors. Even though the gases in Sutton's data base contained no hydrogen sulfide and only limited amounts of carbon dioxide and nitrogen, the z factors calculated using his modification fitted the expanded data base very well. This fact gives a great deal of confidence in the theoretical basis of the form of the SBV equations.

EVALUATION OF SPECIFIC GRAVITY CORRELATIONS

To evaluate the current gas specific gravity correlations, we first assumed that the amount of impurites in the mixture was known. The technique given by Standing[3] for applying the Wichert and Aziz correlation, Eqs. 3, was used to correct for the presence of acid gases. We evaluated Standing's reservoir gas correlation and Sutton's correlation, Eqs. 2. The results of these calculations using our data base are shown in **Table 3** and **Fig. 5**. The average absolute error was 1.99 and 1.42 percent, respectively. We then assumed that the amount of impurites in the mixture was unknown. As may be seen in **Fig. 6**, the error was as large as 27 percent and the maximum error varied linearly with the amount of impurities in the mixture.

DEVELOPMENT OF THE NEW METHOD

Our objective was a method for estimating the pseudocritical constants when composition is not known which, if used with the DAK representation of the SK chart, more accurately reproduces the experimental compressibility factors. The data discussed above was used with the DAK equation of state and a minimization procedure to determine the inferred pseudocritical constants. This set of inferred pseudocritical values was then used with multiple regression analysis to develop a new correlation for J and K to be used with Eqs. 1a in calculating values for the pseudocritical point. We later refer to the new method as the proposed gas specific gravity correlation.

Procedure. A multidimensional conjugate gradient algorithm[16] was used to find the point on the z-p_{pr}-T_{pr} surface given by the

DAK representation of the SK chart which minimized the difference between experimental and calculated z factors. The experimental compressibility factor, pressure and temperature, and pseudocritical constants calculated using Sutton's modification to SBV rules were used as initial guesses. The algorithm converged for all the data points and returned values for the inferred pseudocritical temperature and pressure. Based on our previous finding, that much of the scatter in comparing calculated to inferred values of pseudocritical temperature and pressure, ocurred at the last steps of a depletion study–a difficult laboratory procedure, 121 data points were not used in our correlations. We attempted but were unable to correlate the inferred pseudocritical temperature and pressure with gas specific gravity because of the large amount of impurities in the gases of our data base.

Inferred Values of J and K. The 1482 remaining pairs of the inferred pseudocritical constants and Eqs. 1a were used to find the inferred values for the SBV parameters J and K, as shown below:

$$J_{(\text{inferred})} = \frac{T_{pc(\text{inferred})}}{p_{pc(\text{inferred})}}, \text{ and}$$

$$K_{(\text{inferred})} = \frac{T_{pc(\text{inferred})}}{\sqrt{p_{pc(\text{inferred})}}}. \qquad \ldots\ldots (5)$$

After finding that the inferred values of J and K were strongly related to the specific gravity of the gas mixture as can be observed in **Figs. 7** and **8**, we decided to use a regression model similar to Eqs. 4, which was originally developed by Corredor[17]. Notice the data points in the lower right half of both figures. These two samples, which contain very high concentrations of carbon dioxide, obviously are outliers with respect to the relationships between J and K and specific gravity. The correlations can be improved by omitting them; however, they were retained in the data base because they were correlatable by the model discussed below.

Proposed Specific Gravity Correlation. Multiple regression techniques were used with the 1482 pairs of inferred J and K as dependent variables to empirically find a correlation incorporating the first four terms of Eqs. 4 and the gas specific gravity. The new correlations are given by Eqs. 6.

$$J = \alpha_0 + \sum_{i=1}^{3} \alpha_i y_i \left(\frac{T_c}{p_c}\right)_i + \alpha_4 \gamma_g + \alpha_5 \gamma_g^2,$$

and,

$$K = \beta_0 + \sum_{i=1}^{3} \beta_i y_i \left(\frac{T_c}{\sqrt{p_c}}\right)_i + \beta_4 \gamma_g + \beta_5 \gamma_g^2, \quad \cdots\cdots (6)$$

where $y_i \in \{y_{H_2S}, y_{CO_2}, y_{N_2}\}$, and the α_i and β_i are shown in **Table 4**. Eqs. 6 directly account for the effects of hydrogen sulfide, carbon dioxide, and nitrogen, eliminating the need for Eqs. 3. The new method for calculating the z factor uses only Eqs. 1a and 6 and the DAK representation of the SK chart. Note that the new method is simplier than current methods. While Eqs. 6 contains terms similar to those in Eqs. 1b, the introduction of terms for nonhydrocarbon gases is a departure from the current method.

Results. To evaluate Eqs. 1a and 6, we again assumed that the amount of impurities in the mixture was known. **Figs. 9** and **10** compare values of the pseudocritical constants calculated using Eqs. 1a and 6 with the inferred values. The results of z factor calculations are shown in **Table 3** and **Fig. 11**. The average absolute error of the calculated z factor was 1.30 percent using the proposed correlation. We then assumed that the amount of impurities in the mixture was unknown. As indicated in **Fig. 12**, the error was again as large as 27 percent and the maximum error varied linearly with the amount of impurities in the mixture. **Table 5** shows a comparison of errors made in using the gas specific gravity correlations when the amount of impurities are unknown. Notice that the errors are relatively small if the gas is lean and sweet. However, the errors can be large if the gas contains more than five percent acid gas and is at a high pressure. The right half of **Fig. 12** shows results from several samples containing a large amount of impurities. The large errors are attributable to high concentrations of acid gas alone. The large range in error at a constant composition is attributable to variation in pressure. Generally, the larger errors occurred at the higher pressures.

CONCLUSIONS

1. A set of z factors, temperatures, pressures, and gas compositions covering a very wide range of naturally occurring petroleum gases and nonhydrocarbon impurities has been used to develop two new pseudocritical property correlations for use in calculating z factors. These correlations may be used with confidence for any naturally occurring petroleum gas with an acid gas content as high as 50 percent and nitrogen content as high as ten percent.

2. One proposed correlation, based on gas composition, is a modification of the SBV mixing rules, which does not require the use of other correlations for the properties of the heptanes plus fraction or the effect of acid gas and nitrogen. This correlation resulted in z factors which fitted the data base with an average absolute error of 1.1 percent and a maximum error of 5.8 percent.

3. The other proposed correlation, based on gas specific gravity and the amounts of nonhydrocarbon impurities in the gas, also does not require the use of other correlations for the effect of acid gas and nitrogen. This correlation resulted in z factors which fitted the data base with an average absolute error of 1.3 percent and a maximum error of 7.3 percent.

4. The presence of nonhydrocarbon impurities in a gas must be accounted for when using a gas specific gravity correlation. Errors in z factors as high as 27 percent occurred when high concentrations of acid gas were ignored.

NOMENCLATURE

J = SBV parameter, °R/psia
K = SBV parameter, °R/psia$^{0.5}$
M = molar mass, lb-mole
$M_{C_{7+}}$ = molar mass of heptane plus fraction, lb-mole
p = pressure, psia
p_c = critical pressure, psia

p_{pc} = pseudocritical pressure, psia
p_{pr} = pseudoreduced pressure
r = correlation coefficient
T = temperature, °R
T_c = critical temperature, °R
T_{pc} = pseudocritical temperature, °R
T_{pr} = pseudoreduced temperature
$y_{C_{7+}}$ = mole fraction of heptane plus fraction
y_i = mole fraction of the i-th component
z = gas compressibility factor
α_i = coefficients of the correlations for J
β_i = coefficients of the correlations for K
γ_g = specific gravity of the gas mixture
ε = Wichert and Aziz pseudocritical temperature adjustment parameter, °R

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TABLE 1--RANGE OF DATA

Variable	Mean	Minimum	Maximum
Hydrogen Sulfide	2.45	0.00	51.37
Carbon Dioxide	3.38	0.00	67.16
Nitrogen	1.87	0.00	15.68
Methane	71.15	19.37	94.73
Ethane	8.21	2.30	18.40
Propane	4.04	0.06	12.74
iso-Butane	0.90	0.00	2.60
n-Butane	1.55	0.00	6.04
iso-Pentane	0.64	0.00	2.24
n-Pentane	0.88	0.00	3.92
Hexane	0.65	0.00	4.78
Heptane Plus	4.28	0.00	14.94
$M_{C_{7+}}$	135.2	98.0	295.0
$\gamma_{C_{7+}}$	0.779	0.710	0.884
z	0.989	0.698	2.099
T, °F	243.8	78.0	326.0
p, psia	3758.6	514.0	12814.0
γ_g (air = 1)	0.972	0.613	1.821

TABLE 2--UPDATED COEFFICIENTS FOR EQS. 4

	J		K	
i	α_i	Standard Error	β_i	Standard Error
0	5.2073E-02	8.8370E-03	-3.9741E-01	2.2271E-01
1	1.0160E+00	2.3018E-02	1.0503E+00	1.5428E-02
2	8.6961E-01	2.1985E-02	9.6592E-01	1.6132E-02
3	7.2646E-01	4.1292E-02	7.8569E-01	4.2227E-02
4	8.5101E-01	1.5402E-02	9.8211E-01	1.5134E-02
5	0.0	0.0	0.0	0.0
6	2.0818E-02	2.10E-04	4.5536E-01	4.546E-03
7	-1.506E-04	7.0E-06	-3.7684E-03	1.73E-04
r^2	0.981		0.979	

TABLE 3--ACCURACY OF COMPRESSIBILITY FACTOR CALCULATIONS

	Pseudocritical Property Correlation					
	Composition Known			Gravity and Impurities Known		
	SBV	SSBV	Eqs. 4	Standing	Sutton	Eqs. 6
Lean Sweet Gases ($0.61 < \gamma_g < 0.99$) - 628 data points						
($y_{C_{7+}} < 4\%$ & $y_{H_2S} + y_{CO_2} < 5\%$)						
Average Error	-0.023	-0.014	0.001	-0.004	0.001	0.003
Maximum Absolute Error	0.065	0.067	0.054	0.089	0.079	0.076
Average Absolute Error, %	2.508	1.577	1.040	1.293	1.304	1.361
Maximum Absolute Error, %	6.668	4.582	5.831	5.882	6.371	7.280
Lean Acid Gases ($0.63 < \gamma_g < 1.42$) - 369 data points						
($y_{C_{7+}} < 4\%$ & $y_{H_2S} + y_{CO_2} \geq 5\%$)						
Average Error	-0.010	-0.002	-0.001	-0.006	-0.002	-0.003
Maximum Absolute Error	0.046	0.046	0.030	0.063	0.053	0.035
Average Absolute Error, %	1.627	1.267	1.015	1.295	1.163	1.176
Maximum Absolute Error, %	6.467	6.518	3.647	6.356	6.450	4.386
Rich Sweet Gases ($0.84 < \gamma_g < 1.82$) - 439 data points						
($y_{C_{7+}} \geq 4\%$ & $y_{H_2S} + y_{CO_2} < 5\%$)						
Average Error	-0.014	0.008	0.003	-0.034	0.009	0.001
Maximum Absolute Error	0.148	0.056	0.053	0.162	0.075	0.061
Average Absolute Error, %	2.556	1.608	1.173	3.070	1.681	1.356
Maximum Absolute Error, %	7.571	5.816	4.410	9.795	7.856	4.709
Rich Acid Gases ($0.84 < \gamma_g < 1.82$) - 167 data points						
($y_{C_{7+}} \geq 4\%$ & $y_{H_2S} + y_{CO_2} \geq 5\%$)						
Average Error	-0.012	0.011	0.001	-0.032	-0.004	-0.002
Maximum Absolute Error	0.063	0.057	0.048	0.143	0.059	0.043
Average Absolute Error, %	1.656	1.689	1.069	3.307	1.715	1.235
Maximum Absolute Error, %	5.789	7.719	3.674	9.829	6.786	5.350
Total - 1603 data points						
Average Error	-0.016	-0.003	0.001	-0.016	0.002	0.001
Maximum Absolute Error	0.148	0.067	0.054	0.162	0.079	0.076
Average Absolute Error, %	2.230	1.526	1.073	1.990	1.418	1.304
Maximum Absolute Error, %	7.5[illegible]	7.719	5.831	9.829	7.856	7.280

TABLE 4--PROPOSED GAS SPECIFIC GRAVITY CORRELATION

	J		K	
i	α_i	Standard Error	β_i	Standard Error
0	1.1582E-01	7.450E-03	3.8216E+00	1.7133E-01
1	-4.5820E-01	1.3616E-02	-6.5340E-02	8.684E-03
2	-9.0348E-01	1.5387E-02	-4.2113E-01	1.0812E-02
3	-6.6026E-01	3.9664E-02	-9.1249E-01	4.1073E-02
4	7.0729E-01	1.3878E-02	1.7438E+01	3.1914E-01
5	-9.9397E-02	6.055E-03	-3.2191E+00	1.3925E-01
r^2	0.979		0.975	

TABLE 5--ACCURACY OF GAS SPECIFIC GRAVITY CORRELATIONS WHEN IMPURITIES ARE UNKNOWN

		$y_{H_2S} + y_{CO_2} < 5\ \%$		$y_{H_2S} + y_{CO_2} \geq 5\ \%$	
		Sutton	Eqs. 6	Sutton	Eqs. 6
$y_{C_{7+}} < 4\ \%$	Avg. Abs. Error, %	1.273	1.224	4.133	3.994
	Max. Abs. Error, %	5.359	5.699	27.22	27.03
$y_{C_{7+}} \geq 4\ \%$	Avg. Abs. Error, %	1.909	1.408	4.012	3.347
	Max. Abs. Error, %	8.048	4.859	24.64	21.99

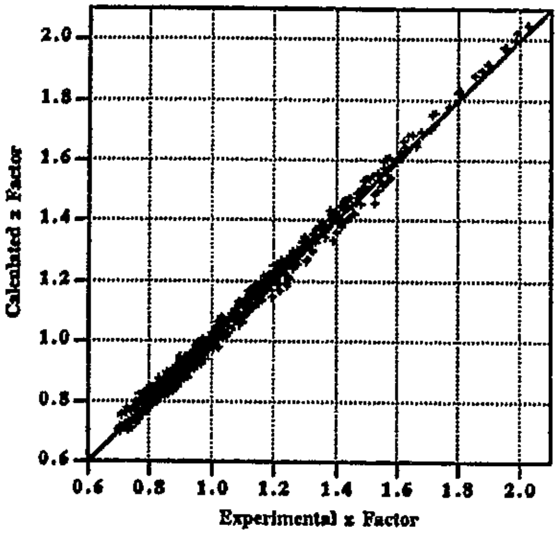

Fig. 1--Calculated z Factor using Sutton's Modification to SBV Rules

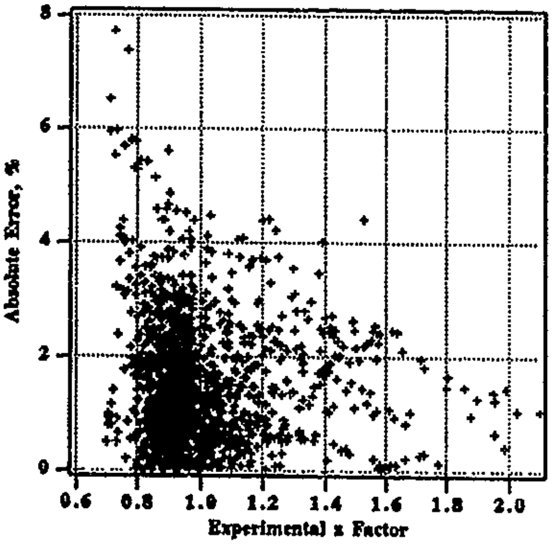

Fig. 2--Error in Calculated z Factor using Sutton's Modification to SBV Rules

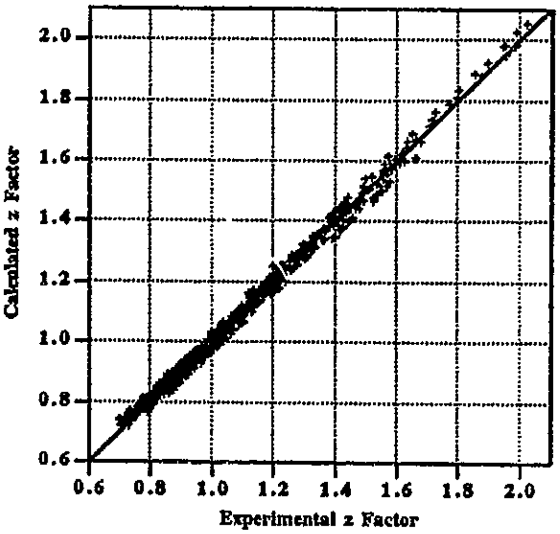

Fig. 3--Calculated z Factor using Proposed Modification to SBV Rules

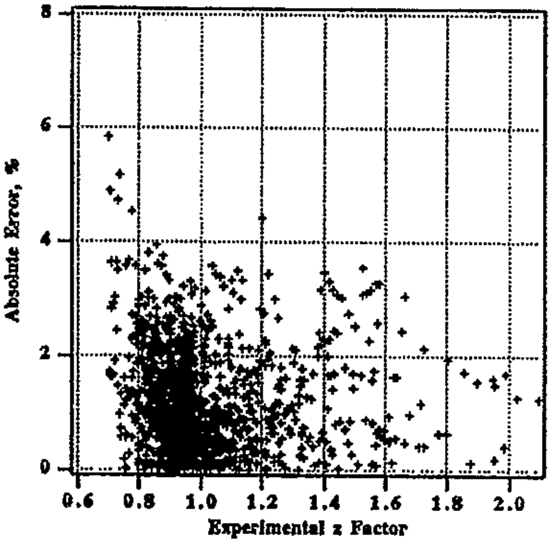

Fig. 4--Error in Calculated z Factor using Proposed Modification to SBV Rules

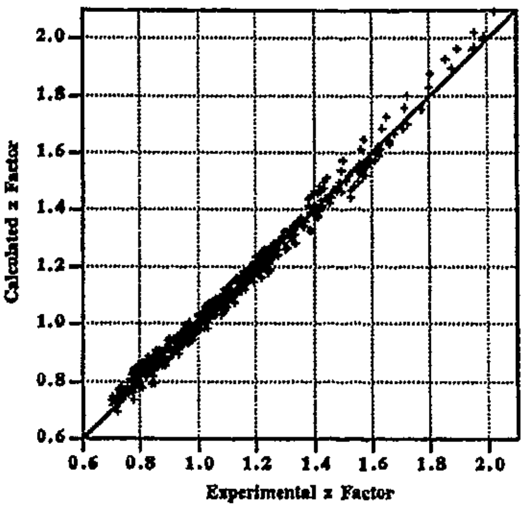

Fig. 5--Calculated z Factor using Sutton's Specific Gravity Correlation with Impurities Known

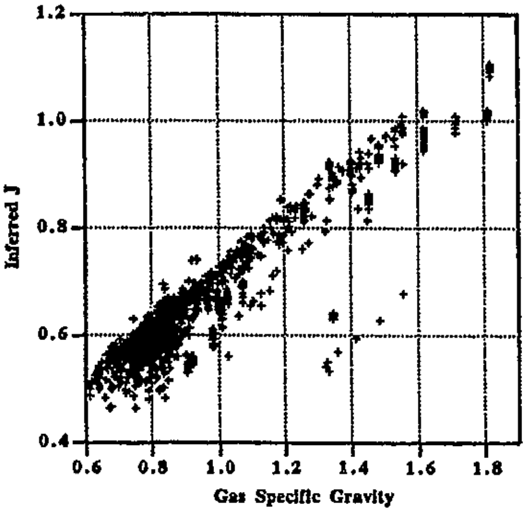

Fig. 7--Variation of the Inferred Value of J with the Specific Gravity of the Gas Mixture

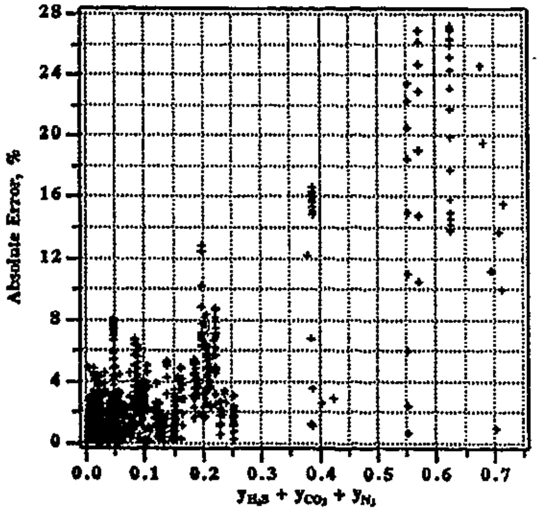

Fig. 6--Error in Calculated z Factor using Sutton's Specific Gravity Correlation with Impurities Unknown

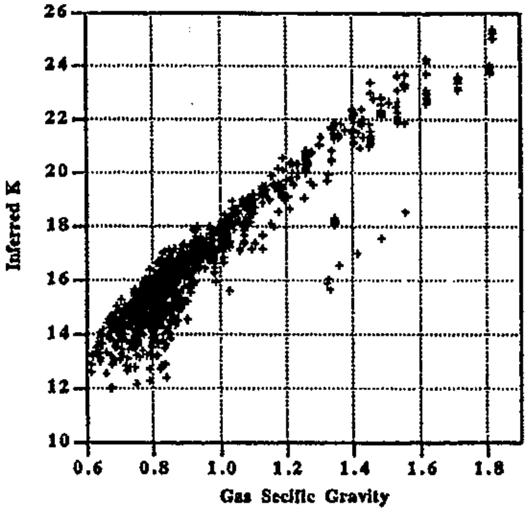

Fig. 8--Variation of the Inferred Value of K with the Specific Gravity of the Gas Mixture

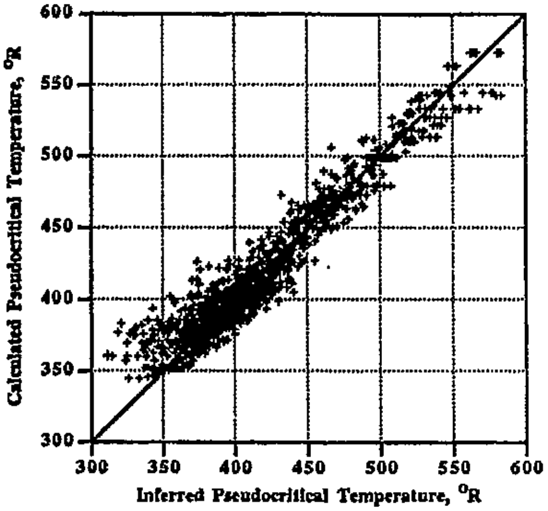

Fig. 9--Calculated Pseudocritical Temperature using Proposed Specific Gravity Correlation

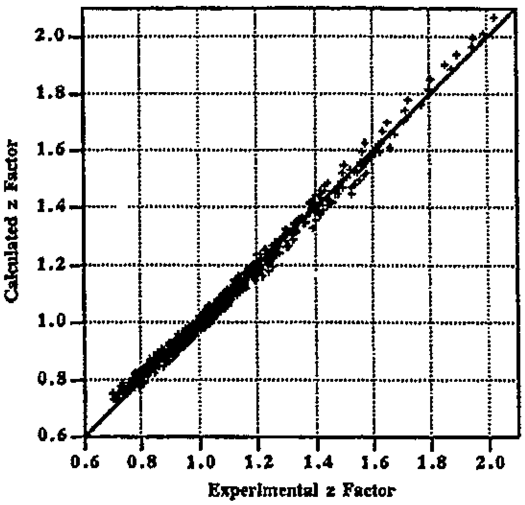

Fig. 11--Calculated z Factor using Proposed Specific Gravity Correlation with Impurities Known

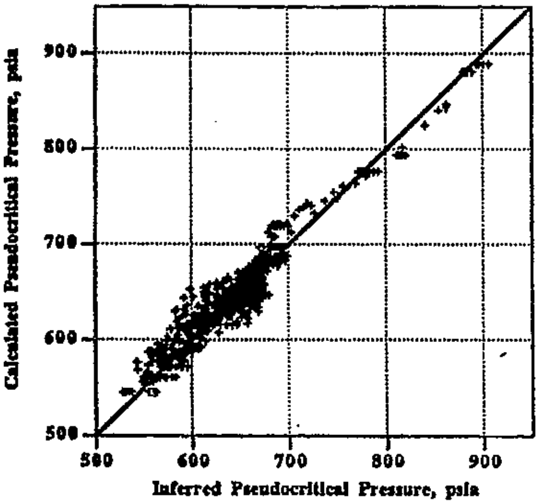

Fig. 10--Calculated Pseudocritical Pressure using Proposed Specific Gravity Correlation

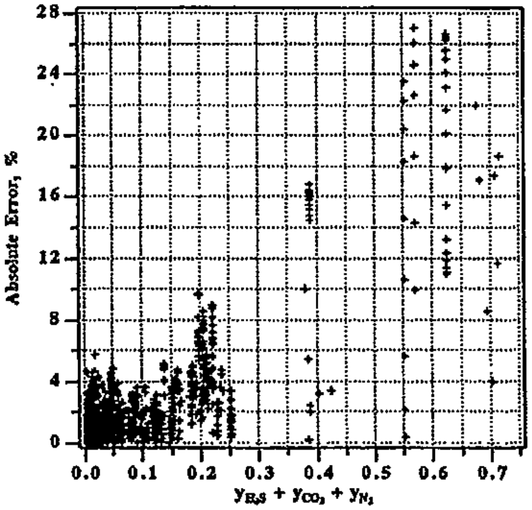

Fig. 12--Error in Calculated z Factor using Proposed Specific Gravity Correlation with Impurities Unknown

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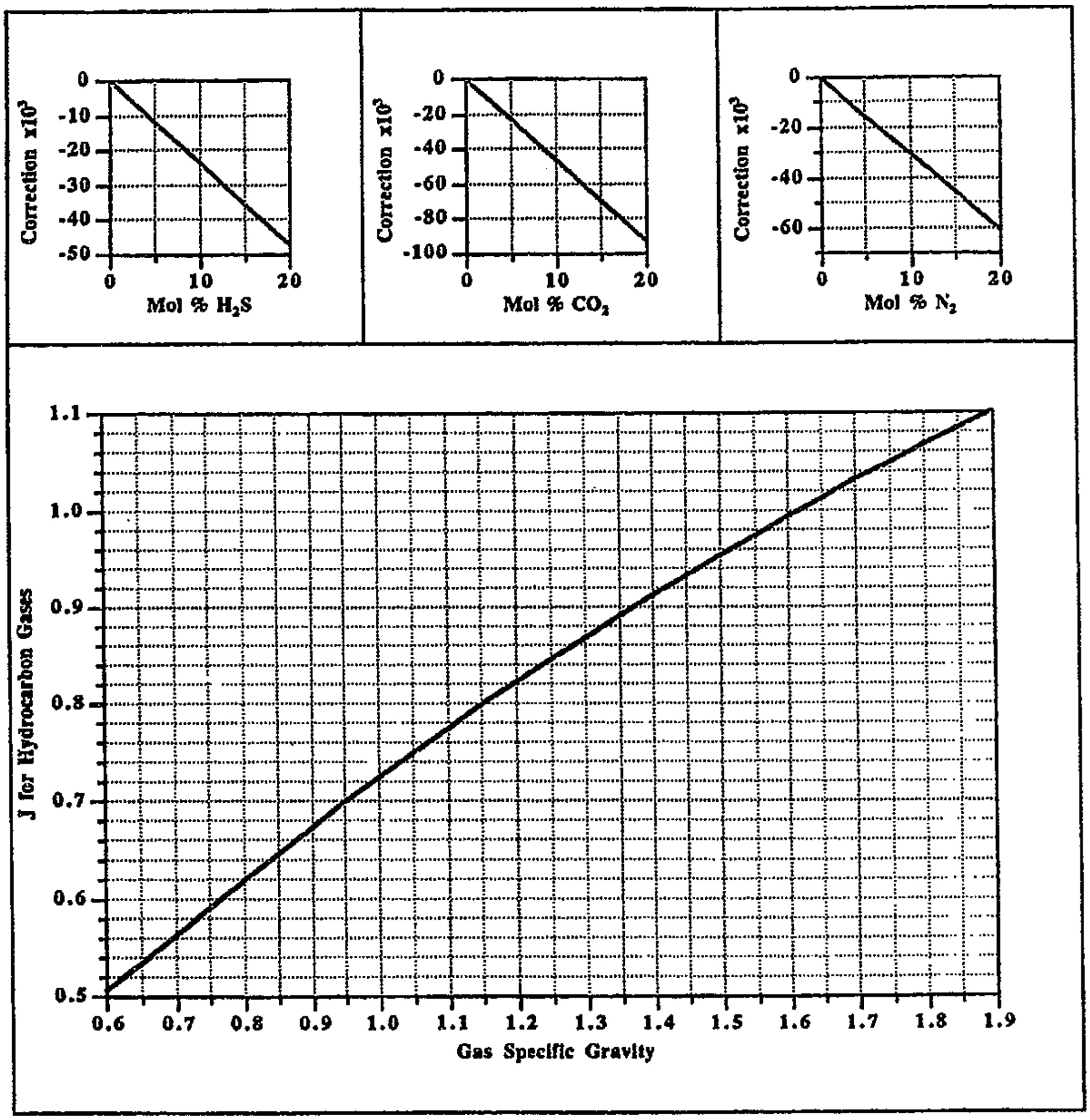
J as a Function of Gas Specific Gravity and Amount of Impurities



NOTE: Use this chart for J, the companion chart for K, and the Stewart, Burkhardt and Voo equations,

$$T_{pc} = \frac{K^2}{J} \; \& \; p_{pc} = \frac{T_{pc}}{J} \text{ to estimate } T_{pc} \; \& \; p_{pc}.$$

See Piper, McCain, & Corredor, "Compressibility Factors for Naturally Occurring Petroleum Gases", SPE 26668, presented at the 1993 SPE Annual Technical Conference and Exhibition in Houston, Texas, October 3-6, 1993.

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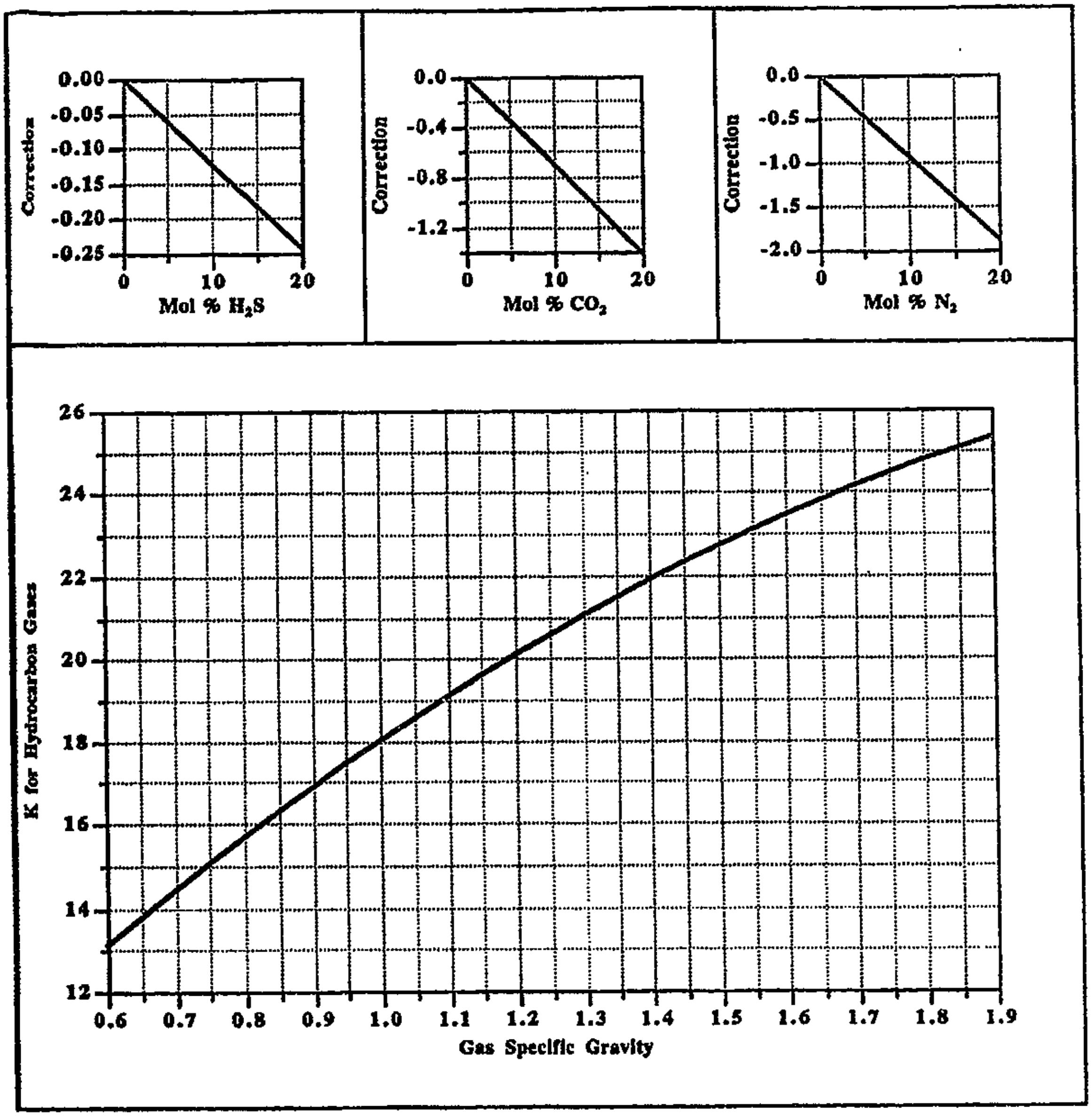
K as a Function of Gas Specific Gravity and Amount of Impurities



NOTE: Use this chart for K, the companion chart for J, and the Stewart, Burkhardt and Voo equations,

$$T_{pc} = \frac{K^2}{J} \ \& \ p_{pc} = \frac{T_{pc}}{J} \text{ to estimate } T_{pc} \ \& \ p_{pc}.$$

See Piper, McCain, & Corredor, "Compressibility Factors for Naturally Occurring Petroleum Gases", SPE 26668, presented at the 1993 SPE Annual Technical Conference and Exhibition in Houston, Texas, October 3-6, 1993.