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A calculation model of natural gas compression factor

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Abstract

"GBT/17747.2 Natural gas-Calculation of compression factor- Part 2 " refers to the calculation method of "*AGA8-92DC*" equation, which is very accurate for the calculation of conventional natural gas compressibility factor, but in the calculation process, a large number of intermediate variables, positioning parameters and interactive parameters are introduced, which makes the calculation process more complicated. Based on the critical state of mixed gas, a new fitting formula is proposed to replace the binary interaction parameters used in "*PR*" equation, so as to simplify the calculation process. Compared with the original "*PR*" equation and "*AGA8-92DC*" equation, the calculation results of conventional natural gas compressibility factor and acid natural gas compressibility factor are more close to the laboratory measured compressibility factor.

Keywords: compression factor, "*PR*" equation, critical states

1. Introduction

The method of calculating the compression factor using the equation of state is widely used because the calculation process is independent of the standard state. At present, there are about 50 to 60 using the traditional calculation method AGA8-92DC equation of state [1] to calculate the compression factor of conventional natural gas, it is necessary to use 8 characteristic parameters, 4 binary interaction parameters, 14 related equations, and the calculation process is complicated; In particular, sour natural gas refers to natural gas with a high content of acidic gases such as H_2S and CO_2 [2], and in case of calculating the compression factor of sour natural gas containing significant amounts of hydrogen sulphide, since hydrogen sulfide is a strongly polar molecule, it increases the intermolecular gravitational and repulsive forces and affects the intermolecular association parameters, thus causing large deviations in the calculation of acid gases in the AGA8-92DC equation of state. In 1972, Wichert and Aziz derived the correction rules for the critical parameters of non-hydrocarbon components from the mixing rule [3], and in 1981, Standing proposed a formula for calculating the density of the system derived from low relative molecular masses by the nature of the mixture [4], and in 1985, Sutton further proposed a density calibration rule for high molecular mass systems [5], these formulae played a further role in correcting the correlation parameters of acid gases, and there are three main methods for calculating the compression factor of acid gases in China [6]: the equation of state method, the empirical equation method, and the graphical plate method.

In this paper, the PR equation based on the empirical formula is used to calculate the conventional natural gas compression factor, which only requires the use of three critical parameters and two binary interaction coefficients. In the calculation of the conventional natural gas compression factor, the calculation process is relatively simple and can meet the needs of engineering calculations; in the calculation of the sour gas compression factor, due to the use of fewer correlation parameters, compared with the traditional AGA8-92DC calculation The optimised PR equation of state is closer to the "real" compression factor of sour gas than the traditional AGA8-92DC Equation.

2. Association formulation

In general the binary parameter k_{ij} is obtained by a joint calculation of several binary interaction parameters. The association formula is a replacement for the binary parameter k_{ij} , which is obtained by a data correction based on a least squares fitting formula of the form

$$s = 1 - \frac{8 \times \left(v_i v_j\right)^{0.5}}{\left(v_i^{\frac{1}{3}} + v_j^{\frac{1}{3}}\right)^3} \qquad (1)$$

v_i , v_j is the critical molar volume of a component natural gas, m3/mol; s is a substitution factor for the binary parameter of the gas and has no physical significance.

3. Calculate the natural gas compression factor using the PR equation [7]

3.1 Input of parameters

The known parameters are the molar fraction of the natural gas, the absolute pressure and the temperature of the gas; the output parameters are the compression factor of the natural gas

3.2 PR equation of state

The PR Equation of state is a semi-empirical three-phase polynomial and is used as a recommended calculation tool in ISO gas-liquid phase balance calculations in the form of

$$p=\frac{RT}{V-b}-\frac{a}{V^2+2Vb-b^2}$$

It consists of a gravitational and a repulsive term, and by substituting the Equation of state $PV=nZRT$, its deformation Equation can be obtained as follows

$$Z^3-(1-B)Z^2+\left(A-2B-3B^2\right)Z-\left(AB-B^2-B^3\right)=0 \quad (2)$$

With:

$$A=\frac{aP}{R^2T^2} \quad (3)$$

$$B=\frac{bP}{RT} \quad (4)$$

Solving Cubic *Equation (1)*, for one-component or single-phase gas mixtures, the Equation has only one real root, which is the compression factor of the phase; when the mixed components are in the two-phase region, the Equation has three real roots, the maximum value is the compression factor of the gas phase, the minimum value is the compression factor of the liquid phase, and the middle root is meaningless.

3.3 Determination of one-component parameters a, b

Parameters a and B are quantities related to natural gas pressure and temperature, For one-component gas, the critical temperature [8] and critical pressure can be used to calculate:

$$a=\frac{0.45724R^2T_c^2}{P_c}\times\alpha \quad (5)$$

$$b=\frac{0.0778RT_c}{P_c} \quad (6)$$

In the formula R is the gas constant, taken as 0.00831451MJ/kmolK; Tc , Pc are the critical temperature and critical pressure of the gas, the critical constants required for the calculation of the one-component of natural gas are listed in Table 1 as below.

Table 1 :Critical constants for natural gas Component

Components	**ω**	**Critical Temp./K**	**Critical pressure/MPa**	**Critical density/g/cm^3**
H_2S	0.10000	373.15	8.936	0.346
N_2	0.03593	126.26	3.399	0.313
CO_2	0.22394	304.21	7.386	0.448
CH_4	0.01140	190.55	4.599	0.162
C_2H_6	0.09909	305.33	4.872	0.203
C_3H_8	0.15611	369.85	4.246	0.217
iC_4H_{10}	0.18465	407.85	3.640	0.221
nC_4H_{10}	0.19777	425.14	3.784	0.228
neoC_5H_{12}	0.19528	433.75	3.196	0.238
iC_5H_{12}	0.22606	460.39	3.370	0.221
nC_5H_{12}	0.24983	469.69	3.364	0.232
C_6H_{14}	0.29600	507.85	3.020	0.233

α is a factorless function of the comparison temperature T_r , which can be obtained from the following equation.

$$\alpha^{1/2}=1+K\left(1-T_r^{1/2}\right) \quad (7)$$

The coefficient K is a substance-specific constant, usually expressed as an eccentricity factor ω

$$K=0.37464+1.54226\omega-0.26992\omega^2 \quad (8)$$

Of which:

$$T_r=\frac{T}{T_c}$$

3.4 Determination of mixing component parameters **a, b**

For mixed gases, the coefficients a, b are further modified using the **van der Waals** Equation

$$a=\sum\sum x_ix_j\sqrt{a_ia_j}\left(1-k_{ij}\right) \quad (9)$$

$$b=\sum x_ib_i \quad (10)$$

x_i , x_j are the molar components of a gas and k_{ij} is a binary parameter, replaced by S in this paper.

3.5 Calculation steps

The steps to calculate the compression factor using the critical parameters of the natural gas fraction are

1) Input natural gas component x_i , absolute pressure P (MPa) and temperature of natural gas T (K).

2) Calculate the factorless function α for the comparison temperature T_r according to equations (7) and (8)

3) Substitute the critical temperature and critical pressure of the gas, T_c , P_c , into Equations(5) and (6) to obtain the one-component coefficients *a*, *b*.

4) Using the modified Equation (1) to obtain the parameter s , replace K_{ij} with the parameter s and calculate the coefficients *a*, *b* of the gas mixture by means of Equations (9) and (10).

5) Determine the PR Equation coefficients *A*, *B* by Equations (3) and (4) and substitute into Equation (2) to obtain the gas phase compression factor *Z* for natural gas.

4. Performance comparison

I. The ability to calculate the compression factor for conventional natural gas, using the results of Schedule C of: “GB/T17747.2 Calculation of the Compression Factor for Natural Gas Part II: Calculation with Molar Fractions” [9] as standard values, and to calculate its compression factor using the new PR correlation Equation and compare the deviation from the standard compression factor.

II. The ability to calculate the compression factor for sour gas, using the experimental values in Schedule 3 of SPE 74369 [10] as the calculation standard, comparing the deviation of the compression factor calculated by the AGA8-92DC calculation Equation with the standard compression factor calculated by the new PR correlation Equation [11]

4.1 Comparison of conventional natural gas compression factor calculation capabilities

Table 2: Gas sample composition (molar fraction)

Gas composition	**Gas sample 1**	**Gas sample 2**	**Gas sample 3**
CO2	0.006	0.005	0.076
N2	0.003	0.031	0.057
CH4	0.965	0.907	0.812
C2H6	0.018	0.045	0.043
C3H8	0.0045	0.0084	0.009
i-C4	0.001	0.001	0.0015
n-C4	0.001	0.0015	0.0015
i-C5	0.0005	0.0003	0
n-C5	0.0003	0.0004	0
C6	0.0007	0.0004	0

Table 3: Comparison of the results of the compression factor calculation

Distribution conditions		**1#gas sample**		**2# gas sample**		**3# gas sample**	
P/mPa	T/K	Int.Standard	This method	Int.Standard	This method	Int.Standard	This method
6	270	0.84053	0.82060	0.83348	0.82144	0.82609	0.80731
6	290	0.88006	0.86190	0.87484	0.86250	0.86944	0.852
6	330	0.93011	0.91546	0.92696	0.91572	0.92368	0.90929
12	270	0.72133	0.72063	0.71044	0.71652	0.6954	0.68881
12	290	0.79317	0.78512	0.78475	0.78237	0.77369	0.76174
12	330	0.88383	0.87101	0.87870	0.86939	0.87211	0.85699

In the three groups of conventional natural gas compared, the compression factor is calculated by using the correlation formula in this paper, and compared with the calculation results of AGA8-92DC equation, the maximum relative error is 2.3%, the minimum relative error is 0.097%, and the average relative error is 1.38% under the condition that the number of correlation parameters is reduced from 12 to 5, which meets the needs of engineering calculation.

4.2 Acid gas calculation capacity comparison.

Table 4: Gas sample composition (molar fraction)

Composition	**sample1**	**Sample2**	**Sample3**	**Sample4**	**Sample5**	**Sample6**	**Sample7**	**Sample8**	**Sample9**	**sample10**
H2S	0.0708	0.1693	0.0034	0.1826	0.0383	0.2816	0.1047	0.0680	0.2327	0.1078
CO2	0.0096	0.0576	0.6352	0.0866	0.0058	0.0608	0.0163	0.0209	0.0287	0.0616
N2	0.0064	0.0011	0.0386	0.0037	0.0020	0.0383	0.0244	0.1019	0.0304	0.0040
CH4	0.6771	0.6619	0.1937	0.5213	0.7564	0.4033	0.7352	0.6857	0.5601	0.7414
C2H6	0.0871	0.0412	0.0303	0.1165	0.0706	0.0448	0.0498	0.0590	0.0820	0.0327
C3H8	0.0384	0.0188	0.0174	0.0142	0.0336	0.0248	0.0181	0.0282	0.0345	0.0121
i-C4	0.005	0.0044	0.0033	0.0039	0.0104	0.0060	0.0059	0.0047	0.0085	0.0022
n-C4	0.0156	0.0076	0.0093	0.0083	0.0135	0.0132	0.0073	0.0116	0.0110	0.0061
i-C5	0.0056	0.0032	0.0039	0.0095	0.0072	0.0079	0.0040	0.0085	0.0000	0.0057
n-C5	0.0082	0.0036	0.0047	0.0000	0.0055	0.0081	0.0037	0.0000	0.0071	0.0000
C6	0.0083	0.0052	0.0051	0.0103	0.0077	0.0121	0.0053	0.0035	0.0028	0.0046
C7+	0.0656	0.0261	0.0551	0.0431	0.0490	0.0991	0.0253	0.0080	0.0022	0.0218

Table 5 :Comparison of results of sour gas compression factor calculations

sample	**P/psi**	**T/F**	**Z**			**Error %**	
			Z （SPE）	**Z （etc）**	**AGA8-92DC**	**Etc**	**AGA8-92DC**
1	4669	296	0.970	1.010	/	4.12	/
2	4050	255	0.914	0.909	0.892	-0.55	-2.41
3	4825	219	0.851	0.852	0.808	0.12	-5.05
4	5385	216	0.942	0.937	0.924	-0.53	-1.91
5	5095	325	1.011	1.050	1.031	3.86	1.98
6	4190	250	0.838	0.895	0.768	6.80	-8.35
7	4255	290	0.968	0.979	0.965	1.14	-0.31
8	2347	157	0.823	0.859	0.825	4.37	0.24
9	1000	120	0.802	0.798	0.785	-0.5	-2.12
10	5065	189	0.95	0.943	0.951	-0.74	0.11

In the appendix of SPE 74369, Predicting the Properties of Sour Gases and Condensates: Equations of State and Empirical Correlations, the component sum of gas sample one was 99.77%, which did not satisfy the requirement of AGA8- The sum of components in the 92DC was 99.77%, which did not meet the requirement of 100±0.01% in the AGA8-92DC, and the sum of components in the remaining nine groups was 100%. The calculation of the compression factor was carried out separately for these nine groups of sour gas using the algorithm of this paper and the AGA8-92DC equation. Using the SPE laboratory measurements as the standard, among the nine groups of sour natural gas compared, the average error of the compression factor calculated using the AGA8-92DC equation was -1.98%, with a maximum error of -8.35% and a minimum error of 0.11%; the average relative error of the compression factor calculated using the correlation equation in this paper was 1.55%, with a maximum error of 6.8% and a minimum error of 0.12%.

In addition, Mr Du Zhimin who is from The State Key Laboratory of Oil and Gas Reservoir Geology and Development Engineering [11] proposed 15 traditional algorithmic models for natural gas in sour gas reservoirs, also based on SPE 74369 test data, and the average relative error of the compression factor calculated using this paper's correlation formula was better than 12 of these models.

5. Conclusion

I. Using the correlation equation in this paper, the average relative error of 1.38%, compared with the calculation of the AGA8-92DC equation, meets the needs of engineering calculations , and the number of relevant parameters for the calculation is reduced from 12 to 5, which help to simplify the calculation process greatly

II. Based on the experimental results of SPE 74369 sour natural gas compression factor, the correlation equation proposed in this paper improves the accuracy of compression factor calculation by 22% compared with the AGA9-92DC equation, and is more applicable to the calculation of sour natural gas compression factor.

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