

Sour Natural Gas and Liquid Equation of State

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Abstract

The major gaseous impurities in the subquality natural gas sources are acidic components, such as hydrogen sulfide and carbon dioxide. Considering that H_2S easily dissociates into hydrogen and elemental sulfur, thermodynamic properties and specially phase equilibria of liquid and gaseous systems containing hydrogen, hydrogen sulfide, carbon dioxide, other acidic components, and light hydrocarbons are of much interest to the natural gas and gas condensate production industries.

In this paper we report the development of a simple and accurate cubic equation of state for prediction of thermodynamic properties and phase behavior of sour natural gas and liquid mixtures. This cubic equation of state, which is based on statistical mechanical theoretical grounds, is applied to pure fluids as well as mixtures with quite accurate results. All the thermodynamic property relations of sour gaseous and liquid mixtures are derived and reported in this report. Parameters of this equation of state are derived for different components of sour natural gas systems. The resulting equation of state is tested for phase behavior and other thermodynamic properties of simulated and natural sour gas mixtures. It is shown that the proposed equation of state is simple and predicts the properties of interest with ease and accuracy.

1. Introduction

In the past two decades, a number of subquality natural gas/gas condensate fields have been discovered around the world, Campbell (1976). The major impurities of these subquality natural gas/gas condensate sources consist of N_2 , CO_2 and H_2S . Because H_2S easily dissociates into hydrogen and elemental sulfur, thermodynamic properties and specially phase equilibria of liquid and gaseous systems containing hydrogen, hydrogen sulfide, carbon dioxide, other acidic components, and light hydrocarbons are of much interest to the natural gas and gas condensate production industries (Campbell, 1976; Katz and Lee, 1990; Mansoori and Savidge, 1989).

Transportation, and processing of sour and hydrogen-containing natural gas is of major concern to the industries involved. Carbon dioxide and hydrogen sulfide are considered as being impurities in natural gas and oil and are responsible for corrosion of the flow-line and processing equipment. Separation of these gases from natural gas and oil is usually the most expensive part of natural gas and oil treatment processes. The economical importance of treatment of sour gas has made it important for the gas and oil industry to have accurate equation of state to represent properties of sour gases and liquid mixtures (Katz and Lee, 1990; Edmister and Lee, 1986). Presence of sour gases in crude oil could also cause deposition of heavy organics, such as asphaltene and wax, from oil which would plug the well, pipeline and refining equipment (Mansoori and Jiang, 1985).

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As of yet no satisfactory equation of state has been available to predict the behavior of sour gases and liquids in reservoir, well, pipeline and compression/expansion facilities (Wichert and Aziz, 1972). Recently, experimental and modeling studies on the phase behavior of high H₂S-content natural gas mixtures were reported by Gu et al. (1993). These workers used the Peng-Robinson (PR) equation of state for phase equilibria calculations, but because the PR equation was not accurate for PVT calculation, they used instead a 33-constant super equation of state. By using this equation of state, Li and Guo (1991) studied the supercompressibility and compressibility factors of natural gas mixtures. However, it is not convenient for engineering calculations to use such a complex equation. Morris and Byers (1991) have performed some experimental work to obtain VLE data for binary and ternary systems containing CH₄, CO₂ and H₂S. Afterwards, they used the PR and Soave-Redlich-Kwong (SRK) equations of state for VLE calculations of the same systems and compared their experimental results with these calculations. In 1978, Huron et al. (1978) and in 1979, Evelein and Moore (1979) used the SRK equation of state to study the hydrocarbon systems containing hydrogen sulfide or carbon dioxide. They reported phase equilibria calculations, but did not report other thermodynamic property calculations. On the same subject, some other experimental research works have been reported, such as the works of Morris and Byers (1990), Huang et al. (1985), Robinson et al. (1978), Mraw et al. (1978) and Eakin and Devaney (1975). By reviewing the above literature on equations of state sour gases and liquids, it is concluded that there is no simple and accurate equation of state available for predicting thermodynamic properties of sour and hydrogen-containing gases and liquids.

In this paper we report the development of an accurate equation of state for sour and hydrogen-containing natural gas/gas condensate systems. This equation of state is tested with success for a variety of cases of interest in natural gas engineering for which experimental data are available for comparison. The basic aim of the present paper is to produce a simple two-constant cubic equation of state which is capable of calculating thermodynamic properties and phase behavior of sour natural gases and liquids. This equation of state is designed specially to predict thermodynamic properties and phase equilibria of liquids and

vapors which consist of hydrogen, methane, other light hydrocarbons and acidic components appearing in the natural gas and gas condensate streams.

In the first part of this report we introduce a two-constant cubic equation of state. This cubic equation of state, which is based on statistical mechanical theoretical grounds, is extended to mixtures. Then parameters of this equation of state are derived for different components of sour natural gas systems. The resulting equation of state is tested for phase behavior and other thermodynamic properties of simulated and natural sour gas mixtures. It is shown that the present equation of state, even though it is simple, predicts the properties of interest with ease and accuracy.

2. The equation of state

A new simple two-constant cubic equation of state for hydrocarbons, hydrocarbon mixtures, and other non-associating fluids was introduced earlier by Mohsen-Nia et al. (1993). This equation of state model is based on the statistical mechanical information available for the repulsive thermodynamic functions and the phenomenological knowledge of the attractive potential tail contributions to the thermodynamic properties. This new two-constant-parameter cubic equation is in the following form:

$$Z = (v + 1.3191b)/(v - b) - a/[RT^{3/2}(v + b)] \quad (1)$$

Eq. 1 is cubic in terms of volume and contains only two adjustable parameters. By applying the critical point constraints on the above equation, parameters a and b are determined to be (Mohsen-Nia et al., 1993):

$$a = 0.486989R^2T_c^{5/2}/P_c \quad \text{and} \quad b = 0.064662RT_c/P_c \quad (2)$$

The critical compressibility factor based on this equation of state is calculated to be:

$$Z_c = 1/3 \quad (3)$$

the same as the Redlich-Kwong (RK) equation of state. It is shown that this equation of state is more accurate than the Redlich-Kwong equation, which had been considered to be the best two-constant-parameter cubic equation of state (Mohsen-Nia et al., 1993). For mul-

Table 1
Equation of state constants

Substances	α_1	β_1
Major components of sour natural gas		
H ₂	-0.07099	0.12307
N ₂	-0.02474	0.06393
CO	-0.02281	0.06066
CO ₂	-0.00580	0.01456
H ₂ S	-0.02351	0.04207
CH ₄	-0.03662	0.05957
C ₂ H ₄	-0.02898	0.03865
C ₂ H ₆	-0.02133	0.04504
C ₃ H ₆	-0.00841	0.04624
C ₃ H ₈	-0.01457	0.03657
Components of natural gas in minute quantities		
n-C ₄ H ₁₀	-0.00663	0.03613
i-C ₄ H ₁₀	-0.01373	0.02852
n-C ₅ H ₁₂	-0.00878	0.02251
n-C ₆ H ₁₄	-0.00761	0.01258
n-CH ₁₆	0.00425	0.01342

For two-component mixtures this equation of state assumes the following form (Mohsen-Nia et al., 1993):

$$Z_m = (v + 1.3191b_{Rm}) / (v - b_{Rm}) - \sum_i \sum_j x_i x_j a_{ij} / [RT^{3/2}(v + \sum_i x_i b_{ii})] \quad (4)$$

where b_{Rm} is defined as:

$$b_{Rm} = (3/4) \sum_i \sum_j x_i x_j b_{ij} + (1/4) \sum_i x_i b_{ii} \quad (5)$$

Table 2
Comparison of the proposed, PR and SRK equations of state for density (ρ), enthalpy (H) and entropy (S) predictions of the major pure components of sour natural gas

Substance	T (K)	P (bar)	No. of data points	SRK			PR			Proposed		
				ρ (%)	H (%)	S (%)	ρ (%)	H (%)	S (%)	ρ (%)	H (%)	S (%)
Methane	110-500	10-500	90	2.4	1.3	0.5	5.3	1.0	0.9	1.8	1.2	0.6
Ethane	200-500	1.5-350	80	3.1	1.0	0.5	5.1	0.6	1.3	2.2	1.0	0.5
Ethylene	150-450	10-400	70	3.7	2.6	0.8	4.7	0.8	1.1	1.7	1.1	1.2
Propane	150-560	0.5-500	80	4.5	0.8	0.5	4.6	2.5	0.4	2.5	3.1	0.5
Propylene	100-600	10-400	75	4.0	2.6	2.5	5.0	1.6	2.3	1.6	1.9	2.1
Hydrogen	20-500	0.1-400	70	1.3	0.5	2.4	6.0	2.1	1.7	2.3	0.8	1.2
Nitrogen	74-700	0.75-500	60	2.9	0.8	0.7	4.7	0.8	0.5	2.2	0.8	0.4
CO	80-600	5.0-500	85	1.4	0.5	0.7	5.3	0.6	0.3	1.4	0.5	0.8
CO ₂	250-1000	2.0-500	90	8.0	0.5	1.7	1.8	0.4	0.5	2.1	0.4	0.5
H ₂ S	255-480	1.0-210	80	2.6	2.4	0.2	4.4	3.1	0.4	1.5	1.7	0.1
AAD %				3.4	1.3	1.1	4.7	1.4	0.9	1.9	1.2	0.8

For reasons mentioned elsewhere (Mohsen-Nia et al., 1993), the mixing rule for parameter b when it appears in the repulsive (positive) term of the equation of state is different from that of the attractive (negative) term. For unlike-interaction parameters a_{ij} and b_{ij} , we use the following combining rules:

$$b_{ij} = (b_{ii}^{1/3} + b_{jj}^{1/3})^3 / 8 \quad (6)$$

$$a_{ij} = (1 - k_{ij})(a_{ii}a_{jj})^{1/2} \quad (7)$$

where parameter k_{ij} is defined as the coupling parameter which can be determined using some mixture data. The theoretical foundations for the choice of the above mixing and combining rules are discussed elsewhere (Mohsen-Nia et al., 1993). The above cubic equation of state was applied for calculation of thermodynamic properties of hydrocarbons and other non-associating fluids and fluid mixtures. It was shown that this two-constant cubic equation of state and its mixture version are far superior to the RK equation of state, which is also a two-constant cubic equation. However, the better accuracies achieved by this simple cubic equation of state is not still sufficient enough to be used for engineering design calculations.

In order to improve the accuracy of the present equation of state to the level that it could be used for engineering design calculations, it is necessary to make parameters a and b temperature-dependent similar to the many modifications of the Van der Waals and RK equations of state (Mansoori and Savidge, 1989;

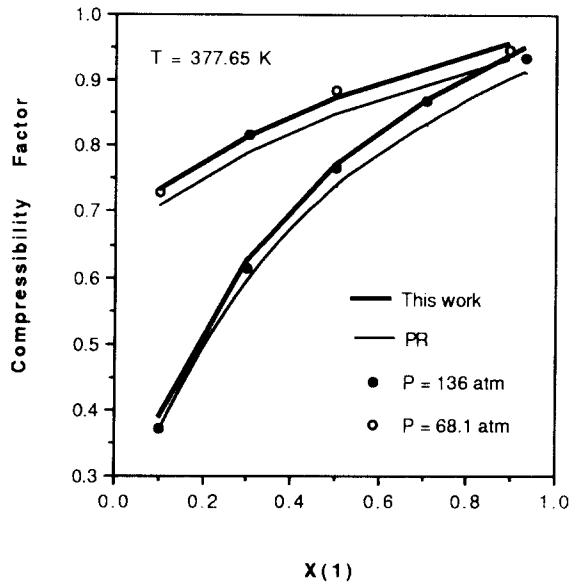


Fig. 1. Comparison of the calculated compressibility factor of the mixture of (methane (1) + hydrogen sulfide (2)) with the experimental data (Sage and Lacey, 1955) as calculated by the proposed and PR equations of state ($k_{ij}=0$) at different mole fractions at 377.65 K and two different pressures of 136 and 68.1 atm.

Edmister and Lee, 1986; Hall et al., 1983; Chorn and Mansoori, 1988). For this purpose we replace parameters a and b with the following temperature-dependent expressions:

$$a = a_c \alpha(T_r) \quad \text{and} \quad b = b_c \beta(T_r) \quad (8)$$

where:

$$a_c = 0.486989R^2T_c^{5/2}/P_c \quad \text{and} \quad (9)$$

$$b_c = 0.064662RT_c/P_c \quad (9)$$

The dimensionless temperature-dependent parameters $\alpha(T_r)$ and $\beta(T_r)$, while being different, reduce to unity at the critical point:

$$\alpha(T_r = 1) = \beta(T_r = 1) = 1 \quad (10)$$

There have been a variety of empirical functional forms for α and β reported in the literature. However, in line with the variational and perturbation molecular theories of fluids (Mansoori and Canfield, 1970), we may use the following polynomial expression for $\beta(T_r)$:

$$\beta(T_r)^{1/3} = \frac{[1 + \beta_1/T_r + \beta_2/T_r^2 + \dots]}{[1 + \beta_1 + \beta_2 + \dots]} \quad (11)$$

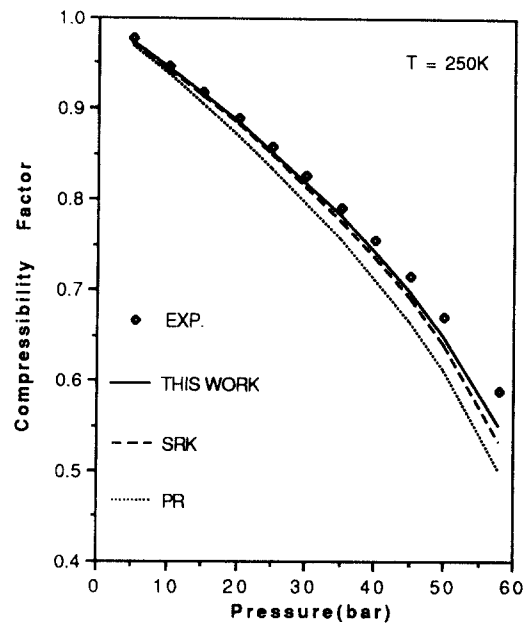


Fig. 2. Comparison of the calculated compressibility factor of the mixture of (methane + carbon dioxide) with the experimental data (Bailey et al., 1989) as calculated by the proposed, SRK and PR equations of state ($k_{ij}=0$) at different pressures at 250 K and $x_{\text{CO}_2}=0.4761$.

Table 3

Comparison between the experimental (Bailey et al., 1989) and calculated compressibility factors for (nitrogen + carbon-dioxide) system at $x_{\text{N}_2} = 0.553$ using the proposed, PR and SRK equations of state ($k_{ij}'s=0$)

T (K)	P (bar)	Z exp.	SRK	PR	Proposed
300.10	318.29	0.8870	0.9311	0.8629	0.9146
320.06	372.49	0.9736	1.0169	0.9439	0.9997
288.79	287.52	0.8326	0.8763	0.8113	0.8603
273.19	245.07	0.7500	0.7923	0.7322	0.7769
260.02	209.51	0.6736	0.7127	0.6574	0.6978
250.06	183.18	0.6123	0.6467	0.5955	0.6321
242.95	165.10	0.5680	0.5967	0.5484	0.5821
241.99	162.69	0.5620	0.5897	0.5418	0.5751
241.03	160.45	0.5564	0.5828	0.5353	0.5682
240.00	157.98	0.5502	0.5753	0.5282	0.5607
239.82	157.57	0.5492	0.5740	0.5270	0.5594
Overall % deviations			5.1	3.2	2.7

Table 4

Compositions (in mole fractions) of three different samples of sour natural gas used in the calculations reported in Table 5

Components	Sample A	Sample B	Sample C
N ₂	0.0000	0.0052	0.0081
CH ₄	0.7130	0.7458	0.8303
CO ₂	0.0000	0.2016	0.0744
C ₂ H ₆	0.0900	0.0474	0.0130
H ₂ S	0.1970	0.0000	0.0735
C ₃ H ₈	0.0000	0.0000	0.0007

Table 5

Comparison between the experimental (Katz and Lee, 1990; Buxton and Campbell, 1967; Satter and Campbell, 1963) and calculated compressibility factors for the three sour natural gas samples of Table 4 using the proposed, PR and SRK equations of state all with $k_{ij,s} = 0$

Sample	T (K)	P (bar)	Compressibility Factor (Z)			
			Exp.	SRK	PR	Proposed
A	311.93	70.72	0.830	0.820	0.790	0.830
A	327.87	70.72	0.856	0.855	0.825	0.857
A	311.93	139.65	0.714	0.709	0.665	0.711
A	327.87	139.65	0.762	0.765	0.721	0.767
B	310.93	70.72	0.865	0.861	0.831	0.864
B	310.93	139.65	0.778	0.782	0.738	0.785
B	310.93	208.58	0.778	0.791	0.737	0.791
C	310.93	112.0	0.821	0.823	0.783	0.826

Then for simplicity, and as a first approximation, we use the following form for $\beta(T_r)$:

$$\beta(T_r) = (1 + \beta_1/T_r)^3 / (1 + \beta_1)^3 \tag{12}$$

where β_1 is a constant. Eq. 12 satisfies the basic theoretical conditions for $\beta(T_r)$ at the critical point, i.e.,

Table 6

The percentage deviations of pressures and vapor compositions from the experimental data (Mraw et al., 1978; Wichterle and Kobayashi, 1972; Sagara et al., 1972) for seven different binary mixtures by using the proposed, PR and SRK equations of state all with $k_{ij}'s = 0$

Systems (1) + (2)	T Range (K)	No. of data points	P % Deviation			y ₁ % Deviation		
			SRK	PR	Proposed	SRK	PR	Proposed
(CH ₄ + C ₂ H ₆)	158-189	26	3.3	2.5	2.5	0.5	0.2	0.1
(CH ₄ + H ₂ S)	230-311	20	20.0	21.3	20.4	14.8	16.7	15.3
(CH ₄ + CO ₂)	183-230	25	19.2	20.3	17.7	9.9	10.3	9.6
(H ₂ + CH ₄)	103-143	12	24.4	16.2	19.4	4.2	5	2
(H ₂ + C ₂ H ₄)	173-198	16	22.1	38	4.9	2.2	3	0.2
(H ₂ + C ₂ H ₆)	173-223	16	15.8	29.2	7.6	1.5	3.5	1.4
(CO ₂ + H ₂ S)	233-316	21	17.0	17.1	17.1	22.6	23.2	22
Overall % deviations			20.3	24.1	14.9	9.3	10.3	8.4

$\beta(T_r) \rightarrow 1$ at $T_r \rightarrow 1$. This functional form will remain finite and positive for all possible temperature ranges. For symmetry and simplicity we also use the same functional form for parameter $\alpha(T_r)$, i.e.:

$$\alpha(T_r) = (1 + \alpha_1/T_r)^3 / (1 + \alpha_1)^3 \tag{13}$$

where α_1 is a constant. Eq. 13 also satisfies the basic theoretical conditions for $\alpha(T_r)$ at the critical point, i.e., $\alpha(T_r) \rightarrow 1$ at $T_r \rightarrow 1$. It can also be inferred from the equation of state, that as the temperature tends to infinity, the attractive term of the equation of state, $-a/[RT^{3/2}(v+b)]$, must approach to zero. The form of $\alpha(T_r)$ considered in this work is conducive to this requirement.

The constants α_1 and β_1 have been determined for the components of the sour natural gas and gas-condensate mixtures as reported in Table 1. These constants were found by minimization of vapor pressures and saturation liquid densities.

For ease of calculations, we have correlated parameters α_1 and β_1 of the major components of natural gas (see Table 1) to their acentric factor in the following forms:

$$\alpha_1 = -0.036139 + 0.14167\omega;$$

$$\beta_1 = 0.0634 - 0.18769\omega$$

$$\text{for } -0.22 \leq \omega \leq 0.18 \tag{14}$$

These correlations are for ω in the range of $-0.22 \leq \omega \leq 0.18$ and they do not hold very well for parameters of the components of natural gas which are in minute quantities (C₄ to C₇₊). Because of the very small concentrations of these components in natural

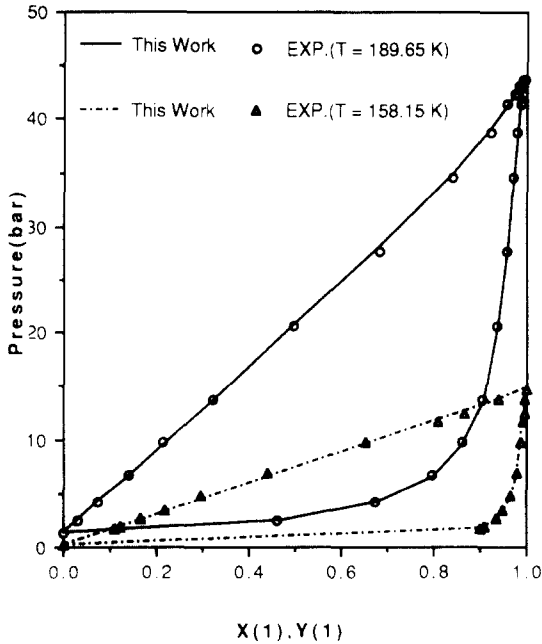


Fig. 3. Comparison of the calculated equilibrium pressure-composition diagram of (methane + ethane) system by the proposed equation of state ($k_{ij}=0$) with the experimental data (Wichterle and Kobayashi, 1972) at two different temperatures of 189.65 and 158.15 K.

gas streams, application of correlations 14 and 15 for these components will not cause any appreciable error

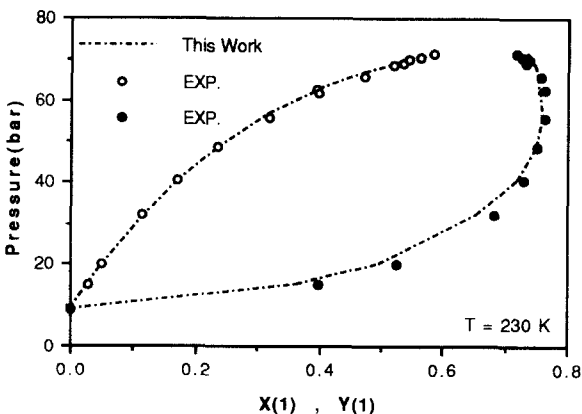


Fig. 4. Comparison of the calculated equilibrium pressure-composition diagram of (methane + carbon dioxide) system by the proposed equation of state ($k_{ij}=0.07$) with the experimental data (Mraw et al., 1978) at 230 K.

in the computation of the natural gas thermodynamic properties. Formulation of equation of state of hydrocarbon mixtures containing appreciable amounts of heavier hydrocarbons requires the application of the continuous thermodynamics and C_{7+} fraction characterization techniques (Mansoori and Savidge, 1989; Chorn and Mansoori, 1988; Du and Mansoori, 1986, 1988), which is outside the scope of the present report.

One of the requirements of equations of state for industrial applications is their analytic representation of thermodynamic functions. Such properties of fluids (like entropy, enthalpy and fugacity) are of direct interest in energy balance and phase behavior calculations in industrial practice. The analytic expressions of these functions are as the following:

$$\begin{aligned}
 H_m - H_{mig}/RT = & (Z_m - 1) - 2.3191Tb_{Rm}'/(v - b_{Rm}) \\
 & - a_m' \ln[v/(v + b_{Am})]/Rb_{Am}T^{1/2} \\
 & + [b_{Am}'/RT^{1/2}]\{(a_m/b_{Am}^2) \ln[v/(v + b_{Am})] \\
 & + a_m/[b_{Am}(v + b_{Am})]\} \\
 & + (1.5a_m/b_{Am}RT^{3/2}) \ln[v/(v + b_{Am})] \quad (15)
 \end{aligned}$$

$$\begin{aligned}
 S_m - S_{mig}/R = & \ln Z_m + 2.319 \ln[(v - b_{Rm})/v] \\
 & - 2.3191Tb_{Rm}'/(v - b_{Rm}) \\
 & - [a_m'/(b_{Am}T^{1/2})] \ln[v/(v + b_{Am})] \\
 & + [a_m b_{Am}'/T^{1/2}]\{(1/b_{Am}^2) \ln[v/(v + b_{Am})] \\
 & + 1/(b_{Am}v + b_{Am}^2)\} \\
 & + [a_m/(2b_{Am}T^{3/2})] \ln[v/(v + b_{Am})] \quad (16)
 \end{aligned}$$

$$\begin{aligned}
 \ln f_i = & -2.31915 \ln(1 - b_{Rm}/v) \\
 & + 2.3191[d(nb_{Rm})/dn_i]/(v - b_{Rm}) \\
 & + [d(nb_{Am})/dn_i][a/(b_{Am}v + b_{Am}^2) \\
 & + (a/b_{Am}^2) \ln(1 + b_{Am}/v)]/(RT^{3/2}) \\
 & - [d(n^2 a_{Am})/dn_i] \ln[(1 + b_{Am}/v)]/ \\
 & RT^{3/2}nb_{Am} - \ln Z_m \quad (17)
 \end{aligned}$$

In the above equations, $H_m - H_{mig}/RT$ and $S_m - S_{mig}/R$ are the mixture enthalpy departure function and mixture entropy departure function, respectively, and f_i is the fugacity of component i in a multicomponent mixture; b_{Am} and a_m , are defined by Eqs. 18 and 19; parameters a' and b' refer to (da/dT) and (db/dT) , respectively. Expressions for the other

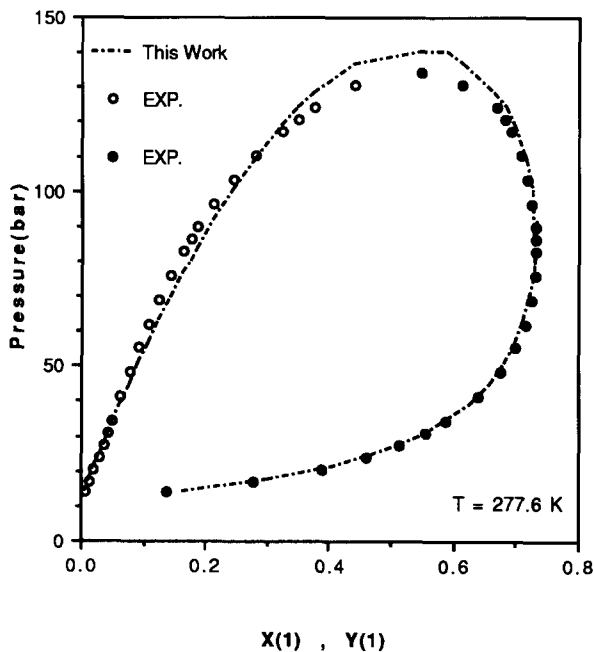


Fig. 5. Comparison of the calculated equilibrium pressure-composition diagram of (methane + hydrogen sulfide) system by the proposed equation of state ($k_{ij}=0.055$) with the experimental data (Reamer et al., 1951) at 277.6 K.

thermodynamic functions can be easily derived from the above equations.

$$b_{Rm} = \sum_i x_i b_{ii} \tag{18}$$

$$a_m = \sum_i \sum_j x_i x_j a_{ij} \tag{19}$$

3. Results and Discussion

In order to test the accuracy and applicability of the present equation of state it is first used for density, enthalpy and entropy calculations of the major pure components of the sour natural gas at different temperatures and pressures. Table 2 shows results of these calculations using the present equation of state along with the SRK and PR equations. According to this table even though predictions by the SRK and PR equations are some times better than the present equation, overall the present equation of state is more accurate than the SRK and PR equations.

We have used the proposed equation of state for calculation of compressibility factors of binary

mixtures of methane-hydrogen sulfide at $T=377.65$ K and at two different pressures. Fig. 1 shows the results of this calculation by using the present equation of state along with the PR equation (all with $k_{ij}=0$). According to this figure, the results of calculations by the proposed equation of state are generally closer to the experimental data than the PR equation.

Another compressibility factor calculation was performed for a methane-carbon dioxide mixture ($x_{CO_2}=0.4761$) at 250 K and at different pressures. Fig. 2 shows results of this calculation based on the present equation of state along with those obtained from the PR and SRK equations (all with $k_{ij}=0$). According to this figure, the proposed equation of state is more accurate than the other equations reported.

A third set of compressibility factor calculations were performed for the nitrogen-carbon dioxide ($x_{CO_2}=0.447$)

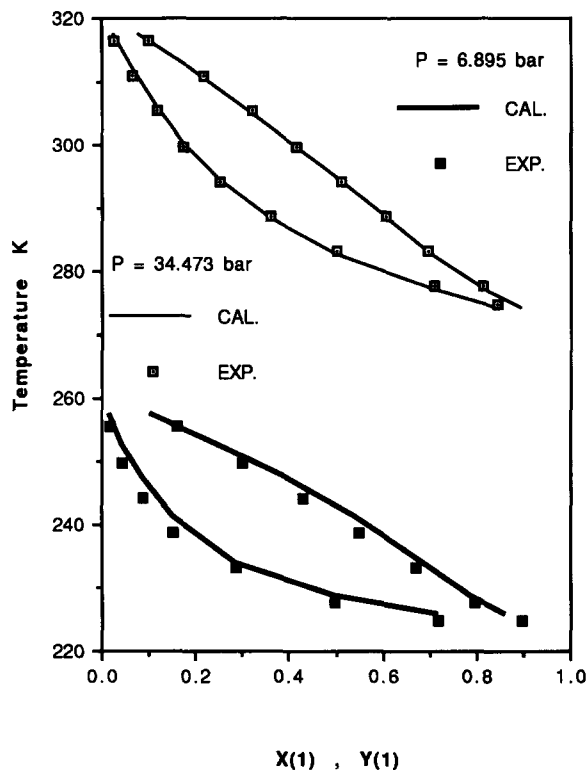


Fig. 6. Comparison of the calculated equilibrium temperature-composition diagram of (carbon dioxide + hydrogen sulfide) system by the proposed equation of state ($k_{ij}=0.08$) with the experimental data (Sobocinski and Kurata, 1959) at two different pressures of 6.895 and 34.473 bar.

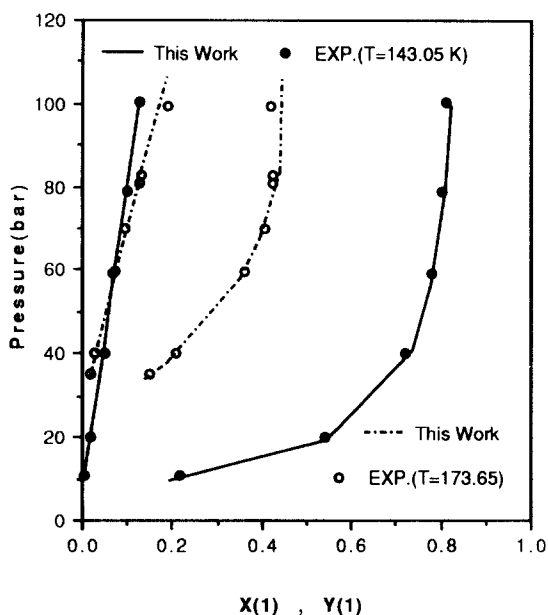


Fig. 7. Comparison of the calculated equilibrium pressure–composition diagram of (hydrogen + methane) system by the proposed equation of state ($k_{ij}=0.144$) with the experimental data (Sagara et al., 1972) at two different temperatures of 143.05 and 173.65 K.

mixture at constant volume (isochore) and at different temperatures and pressures. Table 3 shows the results of this calculation as compared with the results of the PR and SRK equations of state (all with $k_{ij}=0$). According to this table, the compressibility factors calculated by the proposed equation are closer to the experimental data than the other equations.

A fourth set of compressibility factor calculations were performed for three different sour natural gas mixtures. Table 4 shows the compositions of these sour natural gas mixtures. The results of these calculations are reported in Table 5. According to this table, the compressibilities calculated using the proposed equation of state are much closer to the experimental data than the PR equation. The results obtained by using the SRK equation are equally accurate as those obtained by using the proposed equation of state.

The proposed equation of state is used for the vapor–liquid equilibria (VLE) calculations of seven different binary sour and hydrogen-containing fluid mixtures for which experimental data are available. Table 6 compares results of the VLE calculations using the present equation of state, PR equation and SRK equation

assuming k_{ij} 's = 0 for all the equations. According to this table, the proposed equation of state appears to be superior to the other equations for the mixtures tested.

Figs. 3–7 show the results of the VLE calculations along with the experimental data for five different binary mixtures comprising the major components of sour natural gas systems. According to these figures, the proposed equation of state can predict thermodynamic properties of sour and hydrogen-containing vapor and liquid mixtures with good accuracy.

The calculations and comparisons reported here indicate that the proposed equation of state is quite suitable for property prediction of sour and hydrogen-containing natural gas and liquid systems of interest in the oil and gas industries. One major advantage of this equation of state is its sound theoretical basis in the choice of its mixing and combining rules and the functional forms of $\alpha(T_r)$ and $\beta(T_r)$ as reported by Eqs. 12 and 13. These theoretically correct choices make the proposed equation of state more suitable for extrapolation purposes than the empirical equations, beyond the ranges of the available experimental data on which equation of state parameters are based upon.

4. Notations:

a	parameter in equation of state
b	parameter in the equation of state
f	fugacity
H	enthalpy
k_{ij}	coupling parameter
n	total number of moles
P	pressure
PR	Peng-Robinson equation of state
R	Universal gas constant
RK	Redlich-Kwong equation of state
S	entropy
SRK	Soave-Redlich-Kwong equation of state
T	absolute temperature
T_r	$= T/T_c$
v	molar volume
Z	compressibility factor
Greek letters	
α	parameter in equation of state
α_1	constant
β	parameter in equation of state

β_1	constant
ρ	density
π	3.1415927
ω	acentric factor

Subscripts

A	attractive
c	critical
i, j	component indices
ij	property of i - j interaction
ig	ideal gas
m	mixture
r	reduced
R	repulsive

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