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UNITED STATES DEPARTMENT OF THE INTERIOR BUREAU OF MINES HELIUM ACTIVITY HELIUM RESEARCH CENTER

INTERNAL REPORT

MODIFIED REDLICH-KWONG EQUATIONS FOR HYDROGEN AND FOR NEON

BY

Philip C. Tully

and

Jonnie M. Estes

BRANCH

Fundamental Research

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CONTENTS

				Page
Abstract	. .	•	•	4
Introduction	•	••		5
Selection of coefficients	•	•••	•	6
Results	a .	• •	•	8
Hydrogen	•		•	11
Neon	•	• •	•	12
Other representations of the PVT properties of				
these gases	•	•••	•	27
Virials	•		•	27
Various other equations	•		•	27
Effective critical constants	•		•	28
Summary	•	•••	•	29
Nomenclature	•	• •		31
Acknowledgments	•	• •	٠	32
References				33

ILLUSTRATIONS

<u>Fig</u> . 1.	P vs Z for experimental data and for Z's calculated by the Redlich-Kwong equation	•	9
2.	Percentage absolute difference between experimental Z's for hydrogen and those calculated by the		
	modified Redlich-Kwong equation	• •	11



3.	Percentage absolute difference between experimental	Page
	Z's for hydrogen and those calculated by the original Redlich-Kwong equation	11
4.	Percentage absolute difference between experimental Z's for neon and those calculated by the modified Redlich-Kwong equation	12
5.	Percentage absolute difference between experimental Z's for neon and those calculated by the original Redlich-Kwong equation	12

TABLES

1.	Ranges of experimental conditions over which calculated Z's were compared with experimental Z's	8
2.	Average percentage absolute difference between Z and Z for various forms of the	
	R-K equation	10
3.	Z-modified Redlich-Kwong vs Z for hydrogen	13
4.	Z-modified Redlich-Kwong vs Z for neon	21

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MODIFIED REDLICH-KWONG EQUATIONS FOR HYDROGEN AND FOR NEON

by

Philip C. Tully $\frac{1}{}$ and Jonnie M. Estes $\frac{2}{}$

ABSTRACT

As part of an over-all program to develop a single equation of state for helium and its mixtures to be used in equilibrium thermodynamic consistency calculations, coefficients of the B term of the Redlich-Kwong equation for pure hydrogen and neon are presented. For normal hydrogen, the original Redlich-Kwong (R-K) value $\frac{.08667T_{c}}{P_{c}T}$, is changed to $\frac{.08063T_{c}}{P_{c}T}$. For temperatures from 98° to 423° K and pressures up to 2,950 atmospheres, this gives an average deviation of 0.63 percent from experimental data. For neon, B is changed to $\frac{.1025T_{c}}{P_{c}T}$. For temperatures from 120° to 973° K and pressures up to 2,900 atmospheres, this gives an average deviation of 0.48 percent from experimental data. No changes were made in the value of A for either gas.

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INTRODUCTION

The PVT properties of gaseous hydrogen and neon have been represented by various types of equations. It is well known that these two gases do not obey the law of corresponding states and so cannot be well represented by generalized equations of state.

Virial-form equations have been given for hydrogen by Michels, de Graaff, Wassenaar, Levelt, and Louwerse (9). $\frac{3}{2}$ Equations of this

3/ Underlined numbers in parentheses refer to items in the list of references at the end of this report.

type have been used for neon by Michels, Wassenaar, and Louwerse (10); Holborn and Otto (6); Nicholson and Schneider (11); and Sullivan and Sonntag (14). For both of these gases Gunn, Chueh, and Prausnitz (5) have published "effective critical constants" to be used in conjunction with Pitzer's (12) generalized tables.

Goodwin (4) has published a six-constant "approximate widerange equation" for hydrogen. Ziegler, McWilliams, and Keller (16) have redetermined these constants for temperatures to 300° K and pressures to 100 atmospheres.

McCarty and Stewart (8) have developed an 18-constant modified Benedict-Webb-Rubin equation for neon for temperatures from 25° to 300° K and pressures from 0.1 to 200 atmospheres.

This paper presents a modification of the R-K $(\underline{13})$ equation of state which is specific for hydrogen. A similar specific modification is made for neon.

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This paper presents a modification of the K-K (12) equation of state which is specific for hydrogen. A similar specific modification is made for neon.

The R-K equation is

$$P = RT/(V-b) - a/T^{1/2}V(V+b)$$
(1)

or

$$Z = 1/(1-h) - (A^2/B)h/(1+h)$$
, (2)

where

$$Z = PV/RT , \qquad (3)$$

$$A^{2} = a/R^{2}T^{2.5} = 0.4278 T_{c}^{2.5}/P_{c}T^{2.5}$$
, (4)

$$B = b/RT = 0.0867 T_{o}/P_{o}T , \qquad (5)$$

and

$$h = b/V = BP/Z \qquad (6)$$

Equation 2 can be solved by successive approximations in Z. The work discussed in this paper was done on an IBM 1620 computer. $\frac{4}{}$

4/ Reference to trade names is made for identification only and does not imply endorsement by the Bureau of Mines.

A list of the nomenclature used in this report is appended.

SELECTION OF COEFFICIENTS

Previous papers (2,3) have presented a method for modifying the R-K equation for helium. This modification consists of developing a new coefficient for the B term, and is based on the limiting volume of helium. Similar individualized coefficients are given here for hydrogen and for neon. However, the technique used to determine the new coefficient for helium could not be used for hydrogen and neon because there is no extremely high pressure data for these gases. Although Bridgman's (1) data for hydrogen extend to 13,000 kg/cm²,

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this pressure is not high enough to warrant extrapolation to the limiting volume. We were unable to find any PVT data above 3000 atm for neon.

The selection of the coefficient for hydrogen was based on the data of Michels, de Graaff, Wassenaar, Levelt, and Louwerse (9). The highest (423° K) and lowest (273° K) isotherms at their highest pressure (2,900 atm) were chosen for optimizing the coefficient because we wanted to fit the high pressure data to less than one percent. (The original R-K equation does quite well at low pressures.) Values of Z were calculated at all points along these two isotherms by using numerous B coefficient values near the original (.0867) value. The value of 0.08063 was selected to yield a maximum deviation of < 1 percent at high and low pressures. The optimum value is obviously a function of pressure, but this single value was selected to maintain the simplicity of the equation.

A similar procedure was employed for neon by using the data of Michels, Wassenaar, and Louwerse (10), also at 273° and 423° K. A value of 0.1025 was selected.

The experimental criticals used were $P_c = 12.80$ atm and $T_c = 33.25^{\circ}$ K for hydrogen and $P_c = 26.86$ atm and $T_c = 44.45^{\circ}$ K for neon. This gives

 $B = \frac{.2094}{T} \quad \text{for hydrogen}$ $B = \frac{.1696}{T} \quad \text{for neon.}$

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RESULTS

Compressibility factors calculated by using these two coefficients are compared with experimental data over the ranges shown in table 1.

TABLE	1.	-	Ranges	of	exper	imental	condit	ions	over	which	calculated
			2	Z's	were	compared	with	exper	iment	al Z'	5

Investigator	Temperature range, °K	Approxima range	te pressure , atm
		Min	Max
	HYDROGEN		
Michels, de Graaff, Wassenaar, Levelt, and			
Louwerse (9)	273-423	20 -	<u>1</u> /2425-2950
Do	98-248	5 -	<u>1</u> / 325-1000
Johnston and White (7) .	35-300	1	200
Woolley, Scott and Brickwedde (<u>15</u>)	273-600	20 -	<u>1</u> / 800-1700
· · · · · · · · · · · · · · · · · · ·	NEON		
Michels, Wassenaar, and Louwerse (<u>10</u>)	273-423	25	<u>1</u> /2600-2900
Holborn and Otto (6)	90-673	1	100
Nicholson and Schneider (<u>11</u>)	273-973	10	80
Sullivan and Sonntag (<u>14</u>)	70-120	10	300

 $\frac{1}{1}$ Maximum pressure differs with each isotherm.

STATISTICS S

Compressibility factors effectated by using these the conflictence

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Temperature Argunt Argunt Links and and a second and a se

Johnston and Mutte (2). (j-Jos

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Michels, Wessensen, . . 273-123

Belleven and Ored (D)

Seimelder (12)

Maximum pressure differs wight and i ambass.

Over wide pressure ranges, such as are shown in table 1, plots of P vs Z data for helium, hydrogen, and neon show that dZ/dP goes through a maximum before reaching very high reduced-pressure values (see figure 1). Neither the original R-K equation nor the modifications



Figure 1. P vs Z for Experimental Data and for Z's Calculated by the Redlich-Kwong Equation

suggested here reproduce this change in slope. Therefore, there is increasing divergence between experimental and calculated values at very high pressures.

The maximum deviation is < 1 percent up to 1,050 atm for hydrogen, (with the exception of a few low temperature points) and up to about 1,500 atm for neon. The average percentage absolute differences over these ranges are given in table 2. For the higher pressure points (up to 2,950 atm), the maximum deviations are considerably greater (< 8.8) than 1 percent. However, the "all-points" averages, also given in table 2, are still < 1 percent. In addition, the table



TABLE 2.	-	Averag	ge	perc	enta	ge absol	ute di	ffei	rence	e bei	tween	Zexp
		and	Zc	alc	for	various	forms	of	the	R-K	equat	ion

Coefficient,	Critical constants	Number	Average percentage
<u>B</u> term	used	<u>of points</u>	absolute difference

HYDROGEN

Data of Michels, de Graaf, Wassenaar, Levelt, and Louwerse (9), $98^{\circ} - 423^{\circ}$ K

Optimum pressure range, < 1,050 atm

.08063	Experimental	439	.36
.0867	Experimental	439	1.32
.0867	"Effective" <u>1</u> /	439	1.44
	All points, $< 2,9$	50 atm	
.08063	Experimental	483	.63
.0867	Experimental	483	1.88
.0867	"Effective" <u>1</u> /	483	1.47

NEON

Data of Michels, Wassenaar, and Louwerse (10); Nicholson and Schneider (11); and Holborn and Otto (6); $120^{\circ} - 973^{\circ}$ K

Optimum pressure range, < 1,500 atm

. 1025	Experimental	444	.34
.0867	Experimental	444	1.82
.0867	"Effective" <u>1</u> /	444	1.67

All points, < 2,900 atm.

1025	Francisco		
.1025	Experimental	479	.48
.0867	Experimental	479	2.12
.0867	"Effective" 1/	479	1.91

1/ Developed by Gunn, Chueh, and Prausnitz (5).

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shows the performance of the original R-K equation when two different sets of critical constants are used: (1) the experimental critical constants; and (2) the "effective critical constants" proposed by Gunn, Chueh, and Prausnitz (5), which will be discussed later.

A future paper will discuss the use of these modified equations for mixtures.

Hydrogen

The range of greatest usefulness of the modified equation for hydrogen is shown in figure 2. A similar graph showing how well the

FIGURE 2. - Percentage Absolute Difference Between Experimental Z's for Hydrogen and Those Calculated by the Modified Redlich-Kwong Equation.

unmodified R-K equation fits these same data is shown in figure 3.

FIGURE 3. - Percentage Absolute Difference Between Experimental Z's for Hydrogen and Those Calculated by the Original Redlich-Kwong Equation.

Down to about 40° K, the low temperature, experimental data of Johnston and White (7) are better represented by the modified equation than by the original. However, since the modified equation gives deviations as large as 2.6 percent at 90°, it is not recommended for use below 98°. Woolley, Scott, and Brickwedde (15) state that the available PVT data





FIGURE 2.- Percentage Absolute Difference Between Experimental Z's For Hydrogen And Those Calculated By The Modified Redlich-Kwong Equation.









on hydrogen at high temperatures "do not appear to be very reliable, probably because of penetration of the container by hydrogen." For this reason it is difficult to determine the accuracy of the present equation above 423° K.

A detailed comparison of Z's calculated by the modified R-K equation with those calculated from experimental data on hydrogen is given in table 3. All temperatures are reported to .01° K, and all pressures and compressibility factors are reported to five significant figures. No effort was made to determine whether or not the experimental data justified precisely this number of figures. Not all temperatures and pressures for which we have calculated Z's are included in these tables. We made an arbitrary selection to demonstrate the accuracy of the equation for the temperatures and pressures where it might be applied.

Neon

The modified equation for neon, which changes the numerical coefficient in B from .0867 to .1025, increases the pressure range which can be fitted to < 1 percent from 100 atmospheres to about 1,500 atm. This is shown in figures 4 and 5. Down to 120° K this

- FIGURE 4. Percentage Absolute Difference Between Experimental Z's for Neon and Those Calculated by the Modified Redlich-Kwong Equation.
- FIGURE 5. Percentage Absolute Difference Between Experimental Z's for Neon and Those Calculated by the Original Redlich-Kwong Equation.











<u>т, °к</u>	P, atm	Z _{exp}	Z _{calc}	Z _{exp} -Z _{calc} 1/	Percentage absolute difference
	Michels, de Gr	aaff, Wasso	enaar, Leve	lt, and Louwerse	(<u>9</u>)
	29.671	1.0141	1.0130	0.0011	0.11
	52.722	1.0249	1.0233	.0016	.16
	77.542	1.0363	1.0344	.0019	. 19
	100.73	1.0471	1.0448	.0023	.22
	138.75	1.0648	1.0620	.0027	.26
	165.01	1.0772	1.0740	.0031	.29
	198.12	1.0927	1.0893	.0034	.32
	238.81	1.1118	1.1081	.0037	.33
	336.99	1.1580	1.1542	.0038	. 33
	418.46	1.1963	1.1928	.0035	.29
423.15	513.77	1.2408	1.2385	.0024	. 19
	636.85	1.2981	1.2979	.0002	.01
	707.82	1.3308	1.3324	0017	.13
	781.48	1.3647	1.3683	0036	.26
	961.96	1.4465	1.4568	0102	. 71
	1,138.3	1.5254	1.5436	.0181	1.19
	1,197.0	1.5515	1.5726	0211	1.36
	1,460.6	1.6662	1.7028	0367	2.20
	1,754.6	1.7908	1.8486	0578	3.23
	1,854.4	1.8322	1.8983	0661	3.61
	2,424.1	2.0632	2.1812	1180	5.72
	27.915	1.0140	1.0129	.0011	.11
	49.594	1.0246	1.0230	.0016	.16
	72.937	1.0360	1.0340	.0020	. 19
	94.739	1.0467	1.0443	.0024	.23
	130.48	1.0642	1.0614	.0028	.26
398.15	155.16	1.0764	1.0732	.0032	. 30
	186.27	1.0919	1.0884	.0035	. 32
	224.51	1.1109	1.1071	.0038	. 34
	316.81	1.1570	1.1528	.0042	.36
	439.36	1.2183	1.2146	.0037	.30
	503.72	1.2503	1.2473	.0030	.24

TABLE 3. - Z-Modified Redlich-Kwong vs Zexp for hydrogen

<u>1</u>/ Apparent arithmetic errors which appear in this column are due to rounding.

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	· 8040			
		1.1118*		
			72.337	

CARLE 3. - E-Modified Radifen-Kwong vs Laxa for hydrogen

Apparent arithmetic errors which appear in this column are one

21
<u>T, °K</u>	P, atm	Zexp	Z calc	Z _{exp} -Z _{calc} 1/	Percentage absolute difference
	Michels, de	Graaff, Wass	enaar, Lev	elt, and Louwerse	(9)
	598.95	1.2975	1.2961	0.0014	0.11
	665.82	1.3304	1.3306	0002	.02
	735.25	1.3646	1.3665	0019	.14
	838.16	1.4147	1.4200	0053	.37
	905.56	1.4472	1.4551	0079	. 54
398.15	1,072.2	1.5271	1.5423	0152	.99
	1,363.7	1.6636	1.6954	0318	1.91
	1,656.8	1.7972	1.8499	0528	2.94
	1,751.6	1.8393	1.8999	0606	3.29
	2,295.0	2.0760	2.1868	1108	5.34
	2,952.5	2.3489	2.5342	1853	7.89
	26.157	1.0138	1.0127	.0011	.11
	46.463	1.0242	1.0226	.0016	.15
	68.324	1.0355	1.0335	.0020	. 19
	88.743	1.0461	1.0437	.0024	.23
	122.21	1.0635	1.0606	.0029	.28
	164.29	1.0856	1.0821	.0036	.33
	210.22	1,1098	1,1058	.0040	.36
	296 57	1,1557	1,1512	.0044	.38
373 15	411 27	1 2168	1,2126	.0042	.34
575.15	560 78	1 2962	1 2939	0023	.18
	688 65	1 3638	1.3642	- 0004	.03
	785 35	1 4144	1 4177	0034	.24
	1 005 6	1 5282	1.5405	0123	.81
	1 280 7	1 6670	1 6946	- 0276	1.66
	1 647 7	1 8460	1 9012	0551	2.99
	2 163 6	2 0883	2 1920	- 1037	4.97
	2,105.0	2.0005	2.1720	- 1765	7.45
	2,791.0	2.3099	2.9404	. 1705	7.15
	24.397	1.0135	1.0125	.0010	.10
0/0 15	43.332	1.0238	1.0223	.0015	.15
348.15	63.713	1.0349	1.0329	.0020	.19
	82.738	1.0454	1.0430	.0024	.23

TABLE 3. - Z-Modified Redlich-Kwong vs Z_{exp} for hydrogen

(Con.)

<u>1</u>/ Apparent arithmetic errors which appear in this column are due to rounding.

			838.16	
	1.5954			
			SEAC. 88	

TABLE 3. - . Z-Modified Reditch-Kwong vs Zawn for hudrogen

/ Apparent atitimetic errors which appear in this column are due to rounding.

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TABLE 3	B Z-Modifi	led Redlich-	Kwong vs Z	for hydrogen	
		14	(Con.)		
T, °K	P, atm	^Z exp	Z _{calc}	Z _{exp} -Z _{calc} 1/	Percentage absolute difference
	Michels, de	Graaff, Wass	senaar, Levo	elt, and Louwerse	(9)
	113.93	1.0626	1.0596	0.0030	0.28
	153.12	1.0844	1.0809	.0036	. 33
	195.87	1.1084	1.1044	.0040	. 36
	276.25	1.1538	1.1493	.0045	.39
	383.07	1.2147	1.2102	.0046	.38
	522.47	1.2944	1.2911	.0032	.25
2/ 0 15	641.82	1.3623	1.3614	.0009	.07
540.15	732.21	1.4134	1.4149	0015	.11
	938.46	1.5285	1.5379	0094	. 62
	1,196.8	1.6696	1.6932	0236	1.41
	1,457.7	1.8083	1.8505	0422	2.33
	1,542.7	1.8526	1.9017	0491	2.65
	2,031 1	2.1011	2.1971	0960	4.57
	2,628.7	2.3917	2.5585	1668	6.98
	22.638	1.0132	1.0122	.0010	.09
	46.479	1.0268	1.0253	.0015	. 15
	65.669	1.0379	1.0359	.0020	. 19
	90.195	1.0522	1.0497	. 0024	.23
	123.70	1.0719	1.0689	.0030	.28
	160.10	1.0936	1.0900	.0036	. 33
	269.41	1.1597	1.1551	.0046	.40
	374.59	1.2242	1.2195	.0047	. 39
323.15	520.67	1.3142	1.3108	.0034	.26
	642.27	1.3890	1.3880	.0010	.07
	796.12	1.4827	1.4866	0039	.26
	870.54	1.5276	1.5345	0069	.45
	999.77	1.6049	1.6179	0130	.81
	1,111.8	1.6711	1.6906	0195	1.17
	1,232.2	1.7411	1.7688	0278	1.59
	1,496.4	1.8918	1.9407	0489	2.58
	1,896.6	2.1138	2.2016	0878	4.15
	2,462.7	2.4140	2.5708	1568	6.50
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<u>1</u>/ Apparent arithmetic errors which appear in this column are due to rounding.

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TABLE :	3 Z-Modifi	ed Redlich-I	wong vs Ze:	xp for hydrogen	
		((Con.)		
T, °K	P, atm	Zexp	Zcalc	$Z_{exp}-Z_{calc} \frac{1}{2}$	Percentage absolute difference
	Michels, de	Graaff, Wass	senaar, Leve	elt, and Louwerse (<u>9</u>)
	20.877	1.0127	1.0119	0.0008	0.08
	42.849	1.0260	1.0246	.0014	.13
	70.697	1.0431	1.0411	.0020	. 19
	97.295	1.0597	1.0571	.0025	. 24
	121.26	1.0747	1.0718	.0029	.27
	175.51	1.1094	1.1057	.0037	.33
	295.25	1.1878	1.1831	.0047	.39
	395.70	1.2547	1.2500	.0047	.37
298.15	495.16	1.3213	1.3175	.0038	.28
	591.06	1.3855	1.3833	.0022	.16
	733.15	1.4799	1.4818	0020	. 13
	921.87	1.6040	1.6137	0097	.61
	1,138.5	1.7435	1.7661	0226	1.29
	1,385.2	1.8982	1.9402	0421	2.22
	1,760.3	2.1264	2.2054	0790	3.72
	2,294.4	2.4375	2.5833	1457	5.98
	2,946.3	2.7976	3.0441	2466	8.81
	10 116	1 0122	1 0115	0007	07
	39 217	1.0122	1.0115	.0007	.07
	6/ 675	1.0250	1.0230	.0011	• 11
	88 967	1.0415	1.0590	.0017	.1/
	110 85	1.0570	1.0554	.0022	. 21
	160.34	1.0724	1.0097	.0026	. 24
	226 31	1.1002	1.1029	.0034	. 31
	220.51	1.1545	1.1404	.0041	.35
273 15	/37 10	1.2100	1.2112	.0047	.38
273.15	530 56	1.3033	1.3009	.0043	. 33
	559.50	1.3003	1.3//3	.0032	. 23
	009.79	1.4/5/	1.4750	.0001	.01
	1 0/3 2	1.0010	1.0080	0064	.40
	1 272 6	1.7439	1.7615	01/6	1.01
	1,2/2.0	2 1200	1.9384	0350	1.84
	1,022.3	2.1390	2.2085	0695	3.25
	2,123.1	2.4621	2.5956	1335	5.42
	2,730.1	2.8358	3.0690	2332	8.22

1/ Apparent arithmetic errors which appear in this column are due to rounding.

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Apparant arithmetic strong which appear in this column are due to rounding.

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TABLE	3 Z-Modifie	d Redlich-	Kwong vs Z _e	xp for hydrogen	
		T Cours	(Con.)		
<u>T, °K</u>	P, atm	Zexp	Zcalc	Zexp ^{-Z} calc ¹ /	Percentage absolute difference
	Michels, de G	raaff, Wass	senaar, Leve	elt, and Louwerse	(<u>9</u>)
	7.1755 28.480 48.181 88.667	1.0050 1.0189 1.0323 1.0608	1.0045 1.0182 1.0312 1.0589	0.0005 .0007 .0011 .0019	0.05 .07 .11 .18
248.1	123.46 186.62 235.16 335.48	1.0859 1.1332 1.1708 1.2503	1.0836 1.1301 1.1671 1.2459	.0023 .0031 .0037 .0044	.21 .28 .32 .35
	425.92 609.50 845.19 1,005.6	1.3233 1.4723 1.6619 1.7885	1.3190 1.4706 1.6688 1.8048	.0043 .0017 0069 0163	. 55 . 11 . 41 . 91
223.1	$\begin{array}{r} 6.5000\\ 25.779\\ 60.785\\ 80.087\\ 111.43\\ 168.24\\ 5\\ 211.87\\ 302.08\\ 461.19\\ 549.73\\ 642.12\\ 764.49\\ 911.69\\ \end{array}$	1.0046 1.0177 1.0430 1.0574 1.0818 1.1277 1.1645 1.2431 1.3866 1.4672 1.5512 1.6616 1.7928	1.0043 1.0173 1.0421 1.0563 1.0803 1.1256 1.1619 1.2397 1.3829 1.4645 1.5505 1.6652 1.8040	.0004 .0004 .0009 .0011 .0015 .0021 .0026 .0034 .0036 .0027 .0007 0036 0112	.04 .04 .09 .10 .14 .18 .23 .28 .26 .18 .04 .22 .63
198.1	5.8140 28.994 54.203 99.146 5 149.44 224.48 340.09 488.11 570.93	1.0042 1.0205 1.0394 1.0757 1.1196 1.1897 1.3047 1.4570 1.5429	1.0039 1.0203 1.0393 1.0756 1.1192 1.1887 1.3024 1.4543 1.5411	.0003 .0001 .0001 .0001 .0003 .0010 .0023 .0028 .0018	.03 .01 .01 .01 .03 .03 .08 .18 .19 .12

<u>1</u>/ Apparent arithmetic errors which appear in this column are due to rounding.

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 Apparent arithmetic scrore which appear in this culum are due to rounding.

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		(Con	.)	<u>p</u>	
		And a second			Percentage
т, °К	P, atm	Zexp	Zcalc	$\frac{Z_{exp}-Z_{calc}}{2}$ 1/	absolute <u>difference</u>
	Michels, de G	raaff, Was	senaar, Lev	elt, and Louwers	se (<u>9</u>)
198.15	681.22	1.6568	1.6576	-0.0008	0.05
170.15	814.64	1.7931	1.7995	0064	.36
	6.6416	1.0046	1.0045	.0001	.01
	25.460	1.0175	1.0181	0005	. 05
	47.491	1.0342	1.0353	0011	. 11
	86.595	1.0668	1.0688	0020	. 18
173.15	130.20	1.1076	1.1099	0023	.21
	195.12	1.1742	1.1764	0021	. 18
	295.28	1.2865	1.2871	0006	.04
	424.46	1.4394	1.4379	.0015	. 10
	594.89	1.6443	1.6432	.0011	.07
	713.93	1.7864	1.7885	0021	. 12
	5.9055	1.0036	1.0038	0002	.02
	30.241	1.0194	1.0213	0019	.18
	55.176	1.0387	1.0418	0031	. 30
	94.388	1.0738	1.0786	0048	.44
153.15	143.55	1.1249	1.1307	0058	.51
	203.71	1.1954	1.2010	0055	.46
	311.07	1.3344	1.3371	0026	.20
	436.39	1.5056	1.5048	.0008	.05
	523.40	1.6258	1.6239	.0019	. 12
	630.30	1.7728	1.7718	.0010	.05
	6.3094	1.0034	1.0037	0003	.03
	27.293	1.0151	1.0179	0028	.27
	49.651	1.0312	1.0359	0047	.46
	102.44	1.0799	1.0882	0083	.77
138 15	181.54	1.1750	1.1846	0095	.81
150.15	276.98	1.3106	1.3167	0062	.47
	389.35	1.4818	1.4830	0012	.08
	468.11	1.6042	1.6026	.0016	. 10
	565.62	1.7553	1.7524	.0029	.16
123.15	5.6428	. 99918	1.0026	0034	. 34

TABLE 3. - Z-Modified Redlich-Kwong vs Z for hydrogen

<u>1</u>/ Apparent arithmetic errors which appear in this column are due to rounding.

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TABLE 3. - X-Modified Radifab. Swong vs 3 ... for hydrogen

Apparent antimetto arrera which appear in this column are due to round to:

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TABLE 3.	- Z-Modifie	ed Redlich-K	wong vs Z	for hydrogen	
					D
				1 /	Percentage
Т, °К	P, atm	Zexp	Zcalc	$Z_{exp} - Z_{calc} \frac{1}{2}$	difference
	E Cen	<u> </u>			
	Michels, de	e Graaff, Wa	ssenaar, L	evelt, and Louwer	rse (<u>9</u>)
	11 057	1 0020	1 0055	0.0017	0.17
	2/ 31/	1.0058	1.0033	-0.0017	65
	24.514	1.0000	1.0135	- 0094	.05
	74 690	1.0100	1.0200	- 0134	1 28
100 15	122 01	1.0434	1 1278	0134	1.20
123.15	201 15	1 2083	1.1270	01/4	1 38
	201.15	1.2005	1.2250	0107	85
	209.04	1.5555	1,5000	0115	.05
	341.05	1.4445	1.4020	0002	
	411.23	1.5082	1.5/21	0039	.25
	498.98	1./234	1.7240	0006	.03
	7.9670	1.0013	1.0027	0014	. 14
	22.316	1.0052	1.0094	0043	.43
	55.345	1.0232	1.0338	0106	1.03
	102.33	1.0690	1.0858	0168	1.57
113.15	143.52	1.1249	1.1433	0184	1.64
	216.35	1.2464	1.2615	0151	1.21
	261.76	1.3301	1.3412	0111	.84
	308.66	1.4199	1.4264	0065	.46
	383.66	1.5663	1.5660	.0003	.02
	all all a chart as	a service and			
	7.2712	.99934	1.0008	0015	. 15
	31.162	1.0016	1.0096	.0079	. 79
	61.248	1.0172	1.0326	0154	1.51
	91.635	1.0464	1.0670	0206	1.97
103.15	127.96	1.0962	1.1194	0232	2.12
	192.36	1.2110	1.2309	0199	1.64
	232.84	1.2929	1.3082	0153	1.18
	274.92	1.3819	1.3918	0098	.71
	342.84	1.5294	1.5306	0012	.08
	6.9217	99821	99976	00155	. 16
	11.566	.99715	1,0001	0030	.30
	29.547	.99649	1,0052	0087	.87
98.15	47,235	1.0017	1.0157	0140	1.40
20.15	69.428	1,0162	1.0360	0197	1.94
	101 60	1.0521	1.0768	- 0247	2.35
	120.09	1.0791	1.1050	0259	2.40

<u>1</u>/ Apparent arithmetic errors which appear in this column are due to rounding.

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Apparent artitmatic errors which appear in this column are due to rounding.

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DIST.L I		(Con.)	ex	<u>p</u>	
T, °K	P, atm	Z _{exp}	Z _{calc}	Z _{exp} -Z _{calc} 1/	Percentage absolute difference
	Michels, de	Graaff, Was	senaar, Le	velt, and Louwerse	<u>(9</u>)
98.15	151.31 218.10	1.1332	1.1584 1.2881	-0.0252 0179	2.22 1.41
	257.73 322.04	1.3588 1.5068	1.3706 1.5089	0118 0022	.87 .14
	20.000	Johnston	and White	(7)	
	1.0000 10.000 20.000	1.0001 .99416	.99956 .99672	.0006 0026 0064	.06 .26
90.00	30.000	.98726 .98793	.99732 1.0012	0101 0132	1.02 1.34
	80.000 100.00	1.0142 1.0388	1.0374 1.0658	0232	2.29
	150.00 200.00	1.1315 1.2430	1.1562 1.2629	0247 0198	2.19

TABLE 3. - Z-Modified Redlich-Kwong vs Z for hydrogen

1/ Apparent arithmetic errors which appear in this column are due to rounding.

modification gives a better fit to experimental data than the original equation. Below this temperature, however, the original equation should be used. All indications are that this modified equation can be used at temperatures much higher than 423° K and pressures higher than the 100 atm shown in figure 4.

A detailed comparison of experimental Z's with those calculated by this modification is shown in table 4, which was compiled on the same basis as table 3.

			151.31 218.10 257.73 322.04	
	ottaW bas			
.05 .26 .55				
		8820.1 - 4141-1 0245.1		

Apparent arithmetic artists which appear in this column are due

and ilication gives a better fit is experimental data than the original equation. Soluw this temperature, however, the original equation should be used. All indications are that this modified equation can be used at temperatures can't higher than 512° E and pressures higher class the 100 are shown to from 6

A detailed comparison of experimental 2's with those colculated by this modification is shown in eable 6, which was compiled on the same basis as table 3.

T, °K	P, atm	Zexp	^Z calc	Zexp ^{-Z} calc ¹ /	Percentage absolute difference
	Milipie	Nicholson a	and Schneide	er (<u>11</u>)	
973.15	20.000 40.000 60.000 80.000	1.0030 1.0065 1.0100 1.0135	1.0033 1.0067 1.0100 1.0134	-0.0004 0002 0001 .0001	0.04 .02 .01 .01
873.15	20.000 40.000 60.000 80.000	1.0034 1.0072 1.0111 1.0150	1.0037 1.0074 1.0111 1.0148	0004 0002 0000 .0001	.03 .02 .00 .01
773.15	20.000 40.000 60.000 80.000	1.0038 1.0081 1.0125 1.0168	1.0041 1.0083 1.0124 1.0166	0003 0001 .0000 .0002	.03 .01 .00 .02
		Holborn	and Otto ((<u>5</u>)	
673.09	$1.3157 \\ 26.316 \\ 52.632 \\ 78.947 \\ 105.26$	1.0001 1.0063 1.0128 1.0194 1.0259	1.0003 1.0062 1.0124 1.0186 1.0248	0002 .0001 .0004 .0008 .0011	.02 .01 .05 .08 .11
573.10	1.3157 26.316 52.632 78.947 105.26	1.0001 1.0075 1.0152 1.0229 1.0306	1.0004 1.0071 1.0142 1.0214 1.0286	0002 .0004 .0009 .0015 .0020	.02 .04 .09 .14 .20
473.12	1.315726.31652.63278.947105.26	1.0002 1.0086 1.0178 1.0270 1.0364	1.0004 1.0083 1.0167 1.0252 1.0337	0002 .0003 .0011 .0018 .0027	.02 .03 .10 .17 .26

TABLE 4. - Z-Modified Redlich-Kwong vs Z for neon

<u>1</u>/ Apparent arithmetic errors which appear in this column are due to rounding.

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CARLE 4. - Z-Modified Reditah Swong ve 2 ... for neer

1/ Appacent arithmetic errors which appear in this column are due to rounding.

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TABLE 4	Z-Modifie	ed Redlich-	Kwong vs Z	for neon	
		(Con.)	<u></u>	
					Percentage
T, °K	P, atm	Zexp	Zcalc	$\frac{Z_{exp}-Z_{calc}}{2}$ 1/	absolute <u>difference</u>
	Miche	els, Wassena	aar, and Lou	uwerse (<u>10</u>)	
	37.568 61.434 86.687 114 21	1.0146 1.0236 1.0332 1.0436	1.0130 1.0214 1.0303 1.0400	0.0016 .0022 .0030 .0036	0.16 .22 .29 .34
	132.69 155.22 192.63 229.82	1.0508 1.0594 1.0738 1.0880	1.0467 1.0548 1.0683	.0041 .0046 .0054 .0060	.39 .44 .50
	268.87 304.07 353.51	1.1030 1.1167 1.1356	1.0963 1.1094 1.1278	.0067 .0074 .0078	.61 .66 .68
423.15	415.64 503.86 599.41 688.32	1.1938 1.2306 1.2648	1.1313 1.1848 1.2215 1.2560	.0084 .0090 .0090 .0088	.72 .75 .74 .70
	772.51 825.92 950.25 1,154.0	1.2971 1.3172 1.3643 1.4412	1.2887 1.3097 1.3585 1.4391	.0083 .0075 .0057 .0020	.64 .57 .42 .14
	1,479.7 1,762.9 2,039.7 2,210.0	1.5620 1.6651 1.7642 1.8245	1.5689 1.6824 1.7934 1.8619	0068 0172 0291 0374	.44 1.04 1.65 2.05
	2,635.5 35.339 57 781	1.9733 1.0144 1.0232	2.0332 1.0128	0598 .0016 .0021	3.03 .15 21
	81.523 112.90 140.17	1.0327 1.0452 1.0561	1.0298 1.0415 1.0518	.0029 .0037 .0043	.28 .35 .40
398.15	161.54 181.06 215.99 252.67	1.0647 1.0726 1.0867 1.1017	1.0599 1.0674 1.0808 1.0951	.0047 .0052 .0059 .0066	.44 .49 .54 .60
	309.79	1.1249	1.1175	.0074	.66

<u>1</u>/ Apparent arithmetic errors which appear in this column are due to rounding.

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Apparent arithmetic errors which appear in this column are due

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		(<u>Con.</u>)		
T, °K	P, atm	Zexp	Zcalc	Z _{exp} -Z _{calc} 1/	Percentage absolute difference
	Michels, Was	senaar, and	Louwerse (<u>10</u>)	
398.15	473.26 562.97 683.43 775.69 892.58 1,122.6 1,468.2 1,657.6 1,927.4 2,079.9	1.1917 1.2283 1.2773 1.3147 1.3620 1.4542 1.5905 1.6640 1.7672 1.8249	1.1828 1.2193 1.2688 1.3070 1.3558 1.4524 1.5988 1.6795 1.7947 1.8598	0.0089 .0090 .0086 .0077 .0062 .0017 0084 0155 0275 0349	0.75 .74 .67 .59 .46 .12 .53 .93 1.56 1.91
	2,482.4 33.109 54.126 76.345 100.57 131.23 151.23 202.15 267.31 310.72 442.56	1.9754 1.0140 1.0227 1.0319 1.0422 1.0550 1.0635 1.0852 1.1132 1.1132 1.1319 1.1891	2.0320 1.0126 1.0207 1.0293 1.0388 1.0510 1.0590 1.0796 1.1064 1.1245 1.1804	0566 .0014 .0020 .0026 .0034 .0040 .0046 .0056 .0068 .0074 .0086	2.87 .14 .20 .25 .32 .38 .43 .52 .62 .62 .65 .72
373.15	526.34 639.01 725.20 834.58 1,049.8 1,300.9 1,551.5 1,805.1 1,948.7 2,327.5 2,894.5	$1.2253 \\ 1.2743 \\ 1.3115 \\ 1.3588 \\ 1.4510 \\ 1.5574 \\ 1.6618 \\ 1.7660 \\ 1.8243 \\ 1.9762 \\ 2.1976$	1.2166 1.2658 1.3038 1.3523 1.4487 1.5621 1.6758 1.7913 1.8569 2.0298 2.2891	.0087 .0085 .0077 .0064 .0023 0047 0140 0253 0325 0536 0916	.71 .67 .59 .47 .16 .30 .84 1.44 1.78 2.71 4.17
348.15	30.881	1.0137	1.0123	.0014	. 14

TABLE 4. - Z-Modified Redlich-Kwong vs Z for neon

1/ Apparent arithmetic errors which appear in this column are due to rounding.

 Apparent artthmetic errors which appear in this column are due to rounding.

23

TABLE 4	Z-Modifi	ed Redlich-	Kwong vs Z	for neon	
		(<u>C</u>	on.)		
					Percentage
T, °K	P, atm	Z	Z,	Z -Z 1/	absolute
		exp	_calc	exp calc ='	difference
	Miche	ls, Wassena	ar, and Lou	werse (<u>10</u>)	
	50.475	1.0222	1.0202	0.0019	0.19
	71.182	1.0312	1.0287	.0025	.25
	98.538	1.0432	1.0400	.0032	.31
	122.30	1.0538	1.0499	.0039	.37
	157.90	1.0698	1.0650	.0047	.44
	188.30	1.0835	1.0781	.0054	.50
	220.20	1.0980	1.0919	.0061	.55
	269.85	1.1206	1.1137	.0068	.61
	339.93	1.152/	1.1450	.0077	.67
010 15	439.26	1.1986	1.1902	.0084	. 70
348.15	562.26	1.2558	1.2472	.0086	.68
	667.82	1.3044	1.2968	.0077	.59
	776.24	1.3546	1.3482	.0064	.47
	943.06	1.4315	1.4280	.0035	. 24
	1,210.8	1.5536	1.5575	0038	.25
	1,444.8	1.6586	1.6713	0127	.76
	1,682.0	1.7637	1.7871	0234	1.32
	1,810.4	1.8226	1.8528	0303	1.66
	2,1/1.5	1.9762	2.0267	0505	2.56
	2,704.8	2.2010	2.2883	0873	3.97
	28.652	1.0133	1.0120	.0013	.13
	53.146	1.0244	1.0224	.0020	.20
	73.369	1.0337	1.0311	.0026	.25
	91.354	1.0420	1.0390	.0030	.29
	118.00	1.0546	1.0508	.0038	.36
	146.30	1.0679	1.0635	.0044	.41
323.15	174.43	1.0813	1.0763	.0050	.46
010.15	203.93	1.0955	1.0899	.0056	.52
	254.90	1.1202	1.1137	.0065	.58
	314.61	1.1494	1.1421	.0073	.63
	452.95	1.2176	1.2097	.0080	. 65
	583.32	1.2825	1.2749	.0076	.59
	717.71	1.3493	1.3432	.0061	.46
	903.14	1.4414	1.4386	.0027	.19

1/ Apparent arithmetic errors which appear in this column are due to rounding.

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TABLE 4. - 2-Modified Budlich-Moong vs 2 app for neon

Apparent arithmatic errors which appear in this column are due to rounding.

TADLE	4 Z-MOd II I	ed Kedlich-	e	xp ror neon	
		(((<u>ion.</u>)		
<u>T, °K</u>	P, atm	Zexp	Z _{calc}	$\frac{Z_{exp}-Z_{calc}}{Z_{exp}-Z_{calc}}$	Percentage absolute difference
	Miche	ls, Wassena	ar, and Louw	verse (<u>10</u>)	
	1,120.0	1.5483	1.5515	-0.0032	0.21
	1,337.2	1.6538	1.6654	0115	70
323.15	1,557.7	1.7597	1.7814	0217	1 24
	1,682.7	1.8191	1.8474	0283	1 56
	2,013.2	1.9739	2.0219	0480	2 43
	2,512.7	2.2028	2.2861	0833	3.78
	06 / 0/	1 0 1 0 0	1,4069		
	20.424	1.0129	1.0116	.0013	.13
	48.997	1.0237	1.0217	.0020	.19
	07.01/	1.0325	1.0301	.0024	.23
	92.974	1.0450	1.0419	.0031	.30
	114.82	1.0557	1.0522	.0036	. 34
	134.68	1.0655	1.0616	.0039	.37
	160.52	1.0785	1.0741	.0044	.41
	187.61	1.0923	1.0874	.0050	.45
	211.96	1.1048	1.0994	.0053	.48
000 15	289.18	1.1451	1.1386	.0065	.57
298.15	373.29	1.1894	1.1824	.0071	.59
	477.39	1.2450	1.2378	.0071	.57
	572.54	1.2959	1.2895	.0064	.49
	828.89	1.4338	1.4316	.0022	. 15
	1,028.4	1.5408	1.5441	0033	.22
	1,228.4	1.6467	1.6576	0109	.66
	1,425.7	1.7501	1.7702	0201	1.15
	1,547.6	1.8132	1.8400	0267	1.47
	1,853.9	1.9701	2.0155	0454	2.30
	2,317.4	2.2020	2.2813	0793	3.60
	2,824.1	2.4487	2.5721	1234	5.04
	24,194	1 0123	1 0111	0012	10
	50.228	1.0250	1 0233	.0012	. 12
	76.959	1.0385	1 0363	.0017	. 1/
273.15	99.321	1 0502	1 0/73	.0022	.21
	123.06	1 0626	1.0473	.0028	.2/
	146.61	1.0752	1.071/	.0033	.31
1/ 1			1.0/14	.0050	. 30

1/ Apparent arithmetic errors which appear in this column are due to rounding

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TABLE 4. - Z-Modified Radiful-Juong vs Z ... for neon

Apparent artifimetic arrors which appass in this column are du to rounding

TABLE 4 Z-Modified Redlich-Kwong vs Z for neon						
(<u>Con.</u>)						
<u>T, °K</u>	P, atm	Z exp	Z _{calc}	$\frac{Z_{exp}-Z_{calc}}{2}$	Percentage absolute difference	
Michels, Wassenaar, and Louwerse (10)						
273.15	171.27 209.65 263.68 318.99 434.66 599.38 728.12 935.85 1,118.5 1,299.1 1,410.9 1,691.7 2,118.2 2,586.7 2,865.7	1.0885 1.1096 1.1397 1.1708 1.2373 1.3331 1.4087 1.5305 1.6366 1.7407 1.8044 1.9623 2.1970 2.4482 2.5945	1.0843 1.1047 1.1342 1.1650 1.2315 1.3291 1.4069 1.5344 1.6476 1.7601 1.8299 2.0058 2.2731 2.5670 2.7416	$\begin{array}{c} 0.0042\\ .0049\\ .0055\\ .0058\\ .0059\\ .0040\\ .0018\\0039\\0109\\0195\\0255\\0255\\0435\\0761\\1189\\1471\end{array}$	$\begin{array}{c} 0.39\\ .44\\ .48\\ .49\\ .47\\ .30\\ .13\\ .26\\ .67\\ 1.12\\ 1.41\\ 2.22\\ 3.46\\ 4.86\\ 5.67\end{array}$	
Holborn and Otto (6)						
223.16	1.315726.31652.63278.947105.26	1.0004 1.0131 1.0272 1.0418 1.0570	1.0006 1.0130 1.0266 1.0409 1.0558	0002 .0002 .0006 .0008 .0011	.02 .02 .06 .08 .11	
173.17	1.315726.31652.63278.947105.26	$1.0003 \\ 1.0123 \\ 1.0258 \\ 1.0405 \\ 1.0562$	$ \begin{array}{r} 1.0006\\ 1.0126\\ 1.0269\\ 1.0426\\ 1.0596 \end{array} $	0003 0004 0011 0021 0035	.03 .04 .10 .20 .33	
Sullivan and Sonntag (<u>14</u>)						
120.0	10.114 29.444 50.451	1.0014 1.0054 1.0117	1.0012 1.0058 1.0138	.0001 0004 0021	.01 .04 .21	

to rounding.

	4.2315		

TABLE 4. - 2-Madified Rediler-Awong va 2 - .4 SIEAT

Apparent arithmetic errors which appear in this column are due

3.6

	<u>Con.</u>)		
tm Z exp	Z calc	Z _{exp} -Z <u>l</u> /	Percentage absolute <u>difference</u>
Sulliva	in and Sonnta	g (<u>14</u>)	
5761.0206301.0385561.0760071.1599791.2386	1.0256 1.0485 1.0941 1.1889 1.2735	-0.0049 0100 0181 0290 0349	0.48 .96 1.68 2.50 2.82
	tm <u>Z</u> <u>exp</u> Sulliva 576 1.0206 30 1.0385 56 1.0760 07 1.1599 79 1.2386	$\frac{\text{(Con.)}}{\text{2}}$	$\frac{1}{12} \frac{1}{12} \frac$

TABLE 4. - Z-Modified Redlich-Kwong vs Z

Apparent arithmetic errors which appear in this column are due to 1/ rounding.

OTHER REPRESENTATIONS OF THE PVT PROPERTIES OF THESE GASES

Virials

The virial-form equations mentioned in the Introduction naturally give a far better fit to the discrete isotherms they represent than do the two modified equations. No two-constant equation developed for a wide temperature range can be expected to achieve the same degree of accuracy as a six-constant equation designed to fit a single isotherm. The usefulness of these modified R-K equations lies in their ability to predict data over large ranges of pressure and temperature. Within certain limitations, they are also useful for mixtures.

Various Other Equations

The six-constant equations of Goodwin (4) and of Ziegler, McWilliams, and Keller (16) for hydrogen have been used to calculate volumes which were compared with experimental volumes taken from Michels, de Graaff,

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1/ Apparent arithmetic writte which oppast in this column are one to rounding.

OTHER ANTERSENTATIONS OF THE FVT INCORTING

EL BLENV

The vertal-form_gquartions mentioned to the Introduction naturally give a far better tit to the discrete isothorms they represent than do the two modified equations. No two-constant equation developed for a wide temperature range can be expected to achieve the same depres of accuracy as a sis-constant equalion designed to iff a single isotherm. The usefulness of these modified R-K equations lies in their ability to predict data over isige ranges of pressure and temperature. Within certain limitations, there are also useful for mixings.

Variation (thing Squarton)

The six-constant equalities of Gooderia (§) and of Siegler, McWillitane, and Seller (16) for hydrogen have been wood to calculate volumes which were compared with experimental volumes taken from Michels, de Graaff, Wassenaar, Levelt, and Louwerse (9) and from Johnston and White (7). Because the work of Ziegler, McWilliams, and Keller consisted of a redetermination of Goodwin's constants, their equation gave a lower average percentage absolute deviation, as might have been expected. For temperatures of 100° K and below, their equation fits experimental data better than our modified R-K; above 100° the modified R-K fits better.

McCarty and Stewart's (8) equation for neon gives a better fit to experimental data than the modified R-K does in the temperature and pressure ranges for which their 18-constant equation was developed. At pressures and/or temperatures above this range the modified R-K fits experimental data better.

Effective Critical Constants

Gunn, Chueh, and Prausnitz (5) say "...Effective critical constants for helium and normal hydrogen have been determined by fitting experimental volumetric data for these gases to the generalized tables of Pitzer (12). The effective critical temperature and pressure are found to depend on the temperature and on the molecular mass in a simple manner ...".

For hydrogen they give

$$T_{c} = \frac{43.6}{1 + \frac{21.8}{(1.008)(T)}}$$
 and $P_{c} = \frac{20.2}{1 + \frac{44.2}{(1.008)(T)}}$

Similar equations are indicated for neon.

Of the various methods (other than virials) for representing

Wessenser, Levelt, and Louverse (2) and from Johnston and White (1) Because the work of Slegier, McWilliams, and Kaller consisted of a redetermination of Goodwin's constants, their equation gave a lower average percentage absolute deviation, as might have buon expected. Ear comportnurses of 100° K and below, their equation fits expected mental data better than our modified S-K; above 100° the modified X-K firs better.

Madarty and Simmart's (2) equation for neon gives a better fit to experimental data then the modified R-E does in the tempereture and pressure targes for which their 18-constant equation was developed. At pressure and/or traperatures stove this range the modified R-E fits experimental data batter.

Affective Critical Constants

Guna, Church, and Frammitz (5) say " ...Effective critical constants for helium and dormal hydrogen have been determined by fitting experimental volumentric darm for these gases to the generalized tables of Filmet (12). The effective critical temperature and pressure are found to depend on the temperature and on the molecular mass in a sizele mather ..."

For hydrogen they give

$$\frac{43.6}{1 + \frac{21.8}{(1.003)(1)}} \quad and \quad T_c = \frac{20.2}{1 + \frac{46.2}{(1.003)(1)}}.$$

Similar dyuncions are indicated for neon.

Of the various methods (other than virials) for representing

the low-temperature $(35^{\circ} - 150^{\circ} \text{ K})$ PVT properties of hydrogen which we investigated, the Gunn, Chueh, and Prausnitz method fits the experimental data best. When this method is used on neon in the temperature range from $70^{\circ} - 120^{\circ}$ K, it gives about as good a fit to experimental data as McCarty and Stewart's equation does. Both of these methods for predicting volumetric data fit the values of Holborn and Otto (6) (which were available when the two methods were developed) better than the data of Sullivan (14) (which were not available, and which deviate slightly from those of Holborn and Otto). In the present report, no work was done on neon below 70° K.

Although Gunn, Chueh, and Prausnitz (5) said nothing about the use of their effective critical constants at temperatures and pressures higher than the range of Pitzer's tables, we investigated the use of these constants in conjunction with the original R-K equation at higher T's and P's. In general, this procedure gave a better fit to experimental data than did the original R-K, but a poorer fit than the modified equations (See table 2).

SUMMARY

Specific modifications of the R-K equation are developed for hydrogen and for neon. The numerical coefficient in B is changed to .08063 for hydrogen and to .1025 for neon. The equation for hydrogen is recommended for temperatures from 98° to 423° K with pressures to 1,050 atm. The neon modification is recommended for

the low-temperature (35" - 130" K) PVT properties of hydrogen which we investigated, the Cuon, Chuch, and Prauanics mathod fite the experimental data best. When this mathod is used on neon in the temperature range from 70" - 130° K, it given about as good a fit to experimental data as McCarty and Stewart's equation does. Noth of these methods for predicting volumetric data fit the values of Bobborn and Date (§) (which were swallable when the two methods net evaluable, and which deviate alightly from those of Holborn and Pato). In the present report, no work was done on neon helo 70° K.

Although Gunn, Chush, and Fransmits (3) said nothing about the use of their effective critical constants at temperatures and pressures bigher than the range of Firzer's tables, we investigated the use of these constants in conjunction with the original S-K equation at higher T's and P's. In general, this procedure gave a better fit to experimental data than did the original R-K, but a

SUMMARY

Specific modifications of the N-K equation are developed for hydrogen and for noon. The measured coefficient in 2 is changed to .05063 for hydrogen and to .1025 for neon. The equation for hydrogen is recommended for temperatures from 98° to 423 ° K with pressures to 1.050 atm. The neon modification is recommended for

temperatures from 120° to 973° K with pressures up to about 1,500 atm. Good performance is indicated above 973° K.

For temperatures lower than these, the use of the "effective critical constants" of Gunn, Chueh, and Prausnitz, in conjunction with Pitzer's tables, is suggested.

P . Pressore, aug.

R = universal mas constant

R-K = Rudlinh-Kaussig

T - comperatione, depress helvin

- I. " relaical comperature
- V = molai volume, on /s note
- 2 compressibility factor, 70/R1

comperatures from 120° to 973° E with pressures up to about 1,300 atm. Good performance is indicated above 973° K.

For températures lover that these, the use of the "effective eritical constants" of Coun, Chush, and Frenshitz, in conjunction with fitzer's tables, is suggested.

NOMENCLATURE

A	=	parameter	of	Redlich-Kwong	equation
а	=	parameter	of	Redlich-Kwong	equation
В	=	parameter	of	Redlich-Kwong	equation
b	=	parameter	of	Redlich-Kwong	equation
h	=	BP Z			

K = Kelvin temperature

- P = pressure, atm
- P_{c} = critical pressure
 - R = universal gas constant
- R-K = Redlich-Kwong
 - T = temperature, degrees Kelvin
 - $T_{c} = critical temperature$
 - $V = molal volume, cm^3/g mole$
 - Z = compressibility factor, PV/RT

NUMBERST

A = parameter of Reditch-Nuong equation a = parameter of Reditch-Nuong equation 3 = parameter of Reditch-Ewong equation b = parameter of Reditch-Ewong equation b = $\frac{3\Gamma}{2}$

- X = Kelvin temperature
 .
- P. = oritical pressure
- in = universal gas constant
 - B-R Reditch-Knong
- T = tearmaracure, degrace Relvin
 - T . Critlesi Lamberstore
 - V = molal voluma, cm /g mola
- Z = compressibility factor, 2V/RT
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The authors wish to acknowledge the valuable assistance of Miss Jo Battle, Librarian of the Helium Research Center and her staff, who ordered many of the reprints needed for this report.

We also wish to acknowledge the untiring efforts of Mr. Billy Joe King who was Digital Computer Systems Operator for the Branch of Automatic Data Processing, Helium Activity, when this work was done.

Dram, &. D., P. L. Chuch, and J. K. Fraunalth. Prediction of Thermodynamic Properties of Dense Gas Mixtures Containing One re Mars of the Coantam Games. AJCh? J., v. 12, No. 3, 1960.

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