Comparison of Generalized Equations of State to Predict Gas-Phase Heat Capacity

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Many engineering calculations require reliable estimation of basic thermodynamic properties of substances. Several methods of calculating them have been compared: for enthalpy (Tarakad and Danner, 1976; Toledo and Reich, 1988); for density and fugacity (Tarakad et al, 1979); and for entropy (Ormanoudis and Stamatoudis, 1988). In addition, the heat capacity at constant pressure, C_p, is an important physical property both from an industrial and an academic viewpoint. There is a general scarcity of experimental data, particularly for polar compounds and for mixtures. Estimation of C_p from generalized equations of state is not expected to be very accurate, since it requires second-order derivatives. There is no comparative study available for predicting heat capacities of real gases reliably.

The heat capacities of gases at zero pressure (ideal gases) are available in the literature (Kobe et al., 1949-1958; *TRC Thermodynamic Tables*, 1985; *Technical Data Book*, 1983). At higher pressures, their heat capacity deviates from that of ideal gas at the same conditions. This residual heat capacity is calculated by substituting the experimental pressure-volume-temperature (P-V-T) data (or the corresponding equation of state) in the following rigorous relationship:

$$\Delta C_p = \int_{\infty}^{V} T\left(\frac{\partial^2 P}{\partial T^2}\right)_v dV - \frac{T\left(\frac{\partial P}{\partial T}\right)_v^2}{\left(\frac{\partial P}{\partial V}\right)_T} - R \qquad \text{(constant } T\text{)} \quad (1)$$

In the case where there is no P-V-T data available for a certain compound or the available data do not cover a given condition, it is imperative to use generalized equations of state to evaluate Eq. 1.

The purpose of this work is to compare the ability to predict heat capacities using eight well known generalized equations of state.

Equations Studied

Eight of the better known generalized equations of state were selected for comparison in Table 1. They use only three values as input: the critical temperature, the critical pressure (or critical volume), and either the acentric factor or the normal boiling point. Critical property values and acentric factors are available in the literature (*TRC Thermodynamic Tables*, 1985; Reid et al., 1977; Daubert and Danner, 1985; Cholinski et al., 1986).

Sources of Heat Capacity Database

A heat capacity database set is needed to test the generalized equations. A literature search shows that very few experimental C_p values at real gas conditions exist. Thus, it was decided to use mostly the published critically evaluated data for C_p (*TRC Thermodynamic Tables*, 1985). Table 2 lists the components and the range of data. The database consists of 9,260 base C_p departure values of 50 substances (2 inorganics, 29 hydrocarbons, and 19 nonhydrocarbon organics). Theses values were classified into 345 groups (regions) to expedite the calculations. Similarly, the corresponding 9,260 calculated C_p departure values are obtained for each tested equation. These are again classified to the previously corresponding 345 groups (regions). Each of the 345 groups of calculated C_p departure is compared with its corresponding base C_p departure group. The group standard fractional deviation, σ_F, is calculated using the following equation:

Table 1. Equations Evaluated in This Study

No.	Equation of State	Abbr.	Input Data Required
1	Lee-Kesler (1975) 3-parameter corresponding states correlation	LK	T_c, P_c, ω or normal *bp*
2	Lee-Erbar-Edmister (1973) eq. of state	LEE	T_c, P_c, ω
3	Sugie-Lu (1970, 1971) eq. of state	SL	T_c, P_c, ω
4	Soave (1972) modification of the Redlich-Kwong eq. of state	RKS	T_c, P_c, ω
5	Barner-Adler (1970) modification of the Joffe eq. of state	JBA	T_c, P_c, ω
6	Yamada (1973) generalization of the BWR eq. of state using 8 parameters	BWR24	T_c, V_c, ω
7	Yamada (1973) generalization of the BWR eq. of state using 16 parameters	BWR44	T_c, V_c, ω
8	Peng-Robinson (1976) eq. of state	PR	T_c, P_c, ω

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Table 2. Number of Values, Temperature and Pressure Range and Literature Sources for Heat Capacity Database

Component	No. of Values	Pres. bar	Temp. (K)	Source
Light Hydrocarbons ($C<5$)				
Methane	339	1-1,000	140-650	TRC Tables
Ethane	323	1-1,000	250-550	TRC Tables
Propane	362	1-700	270-1,200	TRC Tables
n-Butane	276	1-400	280-1,200	TRC Tables
Isobutane	273	1-400	270-1,200	TRC Tables
I-Butene	219	1-1,000	320-1,000	TRC Tables
Isobutene	266	1-1,000	320-1,000	TRC Tables
Propyne	222	1-50	280-1,000	TRC Tables
Propylene	80	1-120	298-473	Bier et al. (1974)
Intermediate Hydrocarbons (C_6-C_8)				
n-Hexane	128	1-30	400-1,000	TRC Tables
n-Heptane	193	1-1,000	440-1,000	TRC Tables
n-Octane	124	1-1,000	480-1,000	TRC Tables
Isooctane	188	1-1,000	440-1,000	TRC Tables
Cyclohexane	226	1-1,000	420-1,000	TRC Tables
Heavy Hydrocarbons (C_9-C_{10})				
Nonane	116	1-20	500-1,000	TRC Tables
Decane	102	1-20	520-1,000	TRC Tables
Aromatic Hydrocarbons				
Quinoline	134	1-1,000	600-1,000	TRC Tables
Isoquinoline	129	1-1,000	600-1,000	TRC Tables
Toluene	189	1-1,000	430-1,000	TRC Tables
o-Xylene	155	1-1,000	490-1,000	TRC Tables
m-Xylene	173	1-1,000	490-1,000	TRC Tables
p-Xylene	173	1-1,000	490-1,000	TRC-Tables
p-Cymene	133	1-1,000	540-1,000	TRC Tables
Naphthalene	136	1-1,000	490-1,000	TRC Tables
Tetraline	139	1-1,000	580-1,000	TRC Tables
Cisdecaline	134	1-1,000	580-1,000	TRC Tables
Transdecaline	147	1-1,000	560-1,000	TRC Tables
Cumene	146	1-1,000	520-1,000	TRC Tables
Alcohols				
Methanol	247	1-1,000	400-1,000	TRC Tables
Ethanol	224	1-1,000	400-1,000	TRC Tables
1-Propanol	215	1-1,000	420-1,000	TRC Tables
2-Propanol	224	1-1,000	420-1,000	TRC Tables
Sulfur Components				
Sulfur Dioxide	223	1-1,000	310-1,000	TRC Tables
Methanethiol	224	1-1,000	340-1,000	TRC Tables
Ethanethiol	190	1-1,000	380-1,000	TRC Tables
Thiophene	172	1-1,000	430-1,000	TRC Tables
Refrigerants				
Diethylether	199	1-1,000	380-1,000	TRC Tables
Freon 23	175	1-40	220-1,000	TRC Tables
Freon 152a	182	0.1-250	220-520	TRC Tables
Methanamine	174	1-50	300-1,000	TRC Tables
Freon 22	167	1-40	240-1,000	TRC Tables
Freon 13	161	1-30	240-1,000	TRC Tables
Freon 21	168	1-50	340-1,000	TRC Tables
Freon 12	159	0.1-40	220-520	TRC Tables
Freon 11	155	1-40	360-1,000	TRC Tables
Freon 114a	168	1-30	300-1,000	TRC Tables
Freon 114	135	1-30	280-1,000	TRC Tables
Freon 113	133	1-30	340-1,000	TRC Tables
Unclassified Components				
Oxygen	150	1-50	110-600	TRC Tables
Acetone	186	1-1,000	400-1,000	TRC Tables

$$\sigma_F = 100 \times \left(\frac{1}{N} \sum \left((\Delta C_{P,\text{calc}} - \Delta C_{P,\text{base}}) / \Delta C_{P,\text{base}} \right)^2 \right)^{1/2}$$

Results and Conclusions

The 345 σ_F values of each equation tested are used in the construction of Tables 3 and 4. Because of large C_p departure errors, the RKS equation is disregarded in further discussions or comparisons. The analysis of results made it necessary to classify the 50 compounds into eight categories: small, intermediate, heavy and aromatic hydrocarbons, alcohols, compounds containing sulfur, refrigerants, and the category of

Table 3. 50% and 85% Confidence

	Confidence Interval	LK Regions		*Lee Regions*		JBA Regions	
		A $Pr<10$ $Tr<4$	*B* $Pr>10$ all Tr	*A* $Pr<1$, $Tr<1.3$ & $1<Pr<10$ $Tr>1.3$	*B* $Pr<1$, $Tr>1.3$ & $1<Pr<10$ $Tr<1.3$	*A* $Pr<7$ $Tr<1.3$	*B* $Pr<7$ $Tr>1.3$
Light Hydrocarbons*,**(C<5)	85%	5-20	21-57	3-23†	8-28†	3-20	4-14
	50%	5-14	21-40	3-13†	8-15†	3-13	4-9
Propyne	85%	23-28	-	17-24	-	22-27	22-27
	50%	23-24	-	17-20	-	22-26	22-26
n-Butane, Isobutane	85%	5-20	21-57	3-23†	8-28†	3-20	4-14
	50%	5-14	21-57	3-13†	8-15†	3-13	4-9
Intermediate Hydrocarbons (C_6-C_8)	85%	17-37	56-107	8-22	12-27	10-25	17-45
	50%	17-30	56-97	8-16	12-25	10-22	17-32
Cyclohexane	85%	9-23	56-107	8-22	12-27	10-25	17-45
	50%	9-19	56-97	8-16	12-25	10-22	17-32
n-Heptane, *n*-octane	85%	17-37	56-107	8-22	12-27	30-42	17-45
	50%	17-30	56-97	8-16	12-25	30-39	17-32
Heavy Hydrocarbons (C_9-C_{10})	85%	49-57	-	25-29	37-44	48-54	57-67
	50%	49-54	-	25-26	37-40	48-52	57-64
*Aromatic Hydrocarbons****	85%	14-36	65-95	9-33	20-47	16-39	17-42
	50%	14-28	65-87	9-21	20-31	16-26	17-34
Tetraline	85%	27-50	65-95	27-58	20-47	40-56	40-56
	50%	27-41	65-95	27-39	20-47	40-42	40-42
Toluene	85%	14-36	65-95	9-33	20-47	14-24	21-35
	50%	14-28	65-95	9-21	20-47	14-22	21-31
Quinoline, Isoquinoline	85%	14-36	65-95	9-33	20-47	24-42	-
	50%	14-36	65-95	9-21	20-47	24-34	-
Alcohols	85%	24-60	38-83	9-27	25-48	42-59	41-75
	50%	24-50	38-66	9-19	25-44	42-50	41-67
Sulfur Components	85%	10-23	37-56	4-28	15-30	7-17	16-31
	50%	10-19	37-42	4-24	15-19	7-11	16-23
Refrigerants	85%	8-28	-	4-17	14-27	9-22	12-32
	50%	8-22	-	4-13	14-23	9-18	12-25
Freon 23	85%	>100	-	>100	>100	>100	>100
	50%		-				
Freon 152a***	85%	26-49	-	21-35	33-39	18-38	44-46
	50%	26-45	-	21-26	33-37	18-22	44-46
Methanamine	85%	8-28	-	4-17	14-27	9-22	12-32
	50%	8-22	-	4-13	14-23	9-18	12-25
Unclassified Components							
Oxygen	85%	3-8	-	9-15	4-9	4-8	5-8
	50%	3-4	-	9-14	4-9	4-6	5-8
Acetone	85%	23-41	50-50	21-23	29-45	33-35	26-47
	50%	23-36	50-50	21-22	29-36	33-34	26-40

* Larger deviations are obtained for saturated hydrocarbons in the region $P_r>7$, $T_r<1.3$.
** Larger deviations are obtained for unsaturated hydrocarbons in the region $1<P<5$ bar.
*** In the region $1<P<5$ bar, most deviation values lie nearer the upper limit of the 85% confidence interval.

unclassified compounds. Each of these categories was subdivided usually into three regions, A, B, and C (defined in Table 3), in the order of decreasing C_p departure prediction ability. Category C (containing all the values besides those of regions A and B) has the worst predictions and is not included in Tables 3 and 4.

Table 3 gives the 50% and 85% confidence intervals containing the 50% and 85% smaller σ_F values, respectively. Compounds that give statistical different results from those of the group classified are listed separately, and their results are not included in the group results.

Table 4 gives the number of σ_F values falling in each σ_F interval.

Analyzing the results of Tables 3 and 4 it is observed that in general none of the equations tested predicts C_p departures very accurately. This is in contrast with the relatively good results obtained by some of them when used to calculate enthalpy departures (Tarakad and Danner, 1976), entropy departures (Ormanoudis and Stamatoudis, 1988), and density and fugacity (Tarakad et al., 1979). The relatively greater errors in C_p predictions are apparently a result of the second-order derivative and of the ratio of two derivatives in Eq. 1. A close observation of Tables 3 and 4 gives the following for each category of components (the 85% confidence interval is given in parentheses):

Small Hydrocarbons. Relatively better predictions are given

Intervals for C_p Departures

BWR24 Regions		BWR44 Regions		PR Regions		SL Regions	
A all *Pr* *Tr*>1.3	*B* all *Pr* *Tr*<1.3	*A* *Pr*<7 *Tr*<1.3	*B* *Pr*<7 *Tr*>1.3	*A* all *Pr* *Tr*<1.3	*B* all *Pr* *Tr*>1.3	*A* *Pr*>0.4 *Tr*>1	*B* *Pr*<0.4 *Tr*>1
2-14	5-35	7-22	7-22	3-23	10-44	4-24	26-53
2-7	5-13	7-13	7-13	3-15	10-30	4-14	26-45
12-17	5-35	24-38	7-22	16-31	10-44	10-26	26-53
12-15	5-13	24-34	7-13	16-18	10-30	10-16	26-45
2-14	5-35	7-22	7-22	21-47	10-44	4-24	26-53
2-7	5-13	7-13	7-13	21-39	10-30	4-14	26-45
16-40	21-62	19-42	31-55	9-25	12-41	6-31	-
16-26	21-44	19-37	31-40	9-19	12-30	6-24	-
12-26	12-26	10-32	21-37	9-25	12-41	6-31	-
12-17	12-17	10-21	21-23	9-19	12-41	6-24	-
16-40	21-62	19-42	31-55	9-25	12-41	6-31	-
16-26	21-44	19-37	31-40	9-19	12-41	6-24	-
52-64	69-92	47-60	58-74	16-25	49-60	>100	-
52-58	69-86	47-60	58-61	16-22	49-53		-
15-45	14-61	18-50	18-50	8-28	17-37	5-23‡	30-111‡
15-33	14-47	18-36	18-36	8-21	17-28	5-18‡	30-78‡
15-45	14-61	18-50	18-50	8-28	17-37	5-23‡	30-111‡
15-33	14-47	18-36	18-36	8-21	17-28	5-18‡	30-78‡
14-28	14-61	18-50	18-50	8-28	17-37	5-23‡	30-111‡
14-22	14-47	18-36	18-36	8-21	17-28	5-18‡	30-78‡
15-45	14-61	18-50	18-50	8-28	17-37	5-23‡	30-111‡
15-33	14-47	18-36	18-36	8-21	17-28	5-18‡	30-78‡
24-66	31-123	11-74	11-74	15-36	33-73	12-61	-
24-53	31-91	11-60	11-60	15-25	33-58	12-38	-
8-27	14-29	13-27	16-34	13-34	13-34	8-31	31-40
8-18	14-27	13-16	16-27	13-25	13-25	8-16	31-34
8-25	8-43	7-35	20-38	6-29	25-42	9-21	18-69
8-16	8-34	7-27	20-31	6-21	25-37	9-16	18-44
8-25	8-43	7-35	20-38	>100	>100	>100	>100
8-16	8-34	7-27	20-31				
-	21-75	7-35	20-38	6-29	25-42	9-21	18-69
-	21-56	7-27	20-31	6-21	25-37	9-16	18-44
33-37	57-62	43-48	47-54	6-29	46-52	9-21	18-69
33-35	57-60	43-46	47-51	6-21	46-49	9-16	18-44
5-8	3-20	9-16	15-18	9-16	26-31	8-15	-
5-8	3-6	9-11	15-18	9-10	26-31	8-15	-
12-27	15-44	17-31	12-35	8-19	20-50	6-18	34-38
12-21	15-30	17-23	12-25	8-11	20-43	6-17	34-38

† Region *A* (P_r<10, T_r>1.3) and *B* (P_r<10, T_r<1.3).
‡ Region *A* (P_r>1.8, T_r>1) and *B* (P_r<1.8, T_r>1).

by Eq. BWR24 in region $A(\sigma_F = 2\text{-}14)$ and by Eq. JBA in region $B(\sigma_F = 4\text{-}14)$.

Intermediate Hydrocarbons. Equation LEE offers the best results ($\sigma_F = 8\text{-}22$) in region A. All equations give much larger error in region B.

Heavy Hydrocarbons. Based on only two components, Eq. PR offers the best results ($\sigma_F = 16\text{-}25$) in region A. All the equations give large errors in region B.

Aromatic Hydrocarbons. Equation SL is the best ($\sigma_F = 5\text{-}23$) in region A (here defined as $P_r > 1.8, T_r > 1$).

Alcohols. Best results are obtained by Eq. LEE ($\sigma_F = 9\text{-}27$) in region A.

Components Containing Sulfur. The best results in region A are obtained by Eq. JBA ($\sigma_F = 7\text{-}17$).

Refrigerants. Equation LEE gives the best results in region A ($\sigma_F = 4\text{-}17$). Table 4 shows that only few times (3 out of 44)σ_F has a value higher than 20.

Unclassified. The best equations for oxygen in region A are the LK, JBA and BWR24 ($\sigma_F < 9$). In region B, the best equations are the LEE and JBA ($\sigma_F < 9$). The best predictions for acetone are given in region A by SL and PR ($\sigma_F = 6\text{-}19$).

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Table 4. Number of σ_F Values Falling in Each Interval of σ_F

	Intervals of σ_F	LK Regions		Lee Regions		JBA Regions		BWR24 Regions		BWR44 Regions		PR Regions		SL Regions	
		A	*B*	*A*	*B*	*A*	*B*	*A*	*B*	*A*	*B*	*A*	*B*	*A*	*B*
Total Number of σ_F		59	11	30	29	34	22	32	38	34	22	36	32	38	16
Light Hydrocarbons (C<5)	0–5	2	0	3	0	4	3	10	5	0	0	2	0	2	0
	6–10	9	0	10	6	9	8	11	6	2	8	5	1	6	0
	11–15	17	0	7	10	6	6	5	10	12	5	12	3	10	0
	16–20	12	0	5	4	9	2	2	2	10	3	8	1	8	2
	>20	19	11	5	9	6	3	4	15	10	6	9	27	12	14
Total Number of σ_F		30	9	20	10	13	18	21	18	13	18	21	13	26	–
Intermediate Hydrocarbons (C_6–C_8)	0–5	0	0	0	0	0	0	0	0	0	0	0	0	0	–
	6–10	0	0	1	0	1	0	0	0	0	0	3	0	1	–
	11–15	0	0	7	1	2	0	0	0	0	0	3	1	5	–
	16–20	4	0	9	1	2	2	3	0	1	0	6	1	4	–
	>20	26	9	3	8	8	16	18	18	12	18	9	11	16	–
Total Number of σ_F		8	–	4	4	4	4	4	4	4	4	4	4	4	4
Heavy Hydrocarbons (C_9–C_{10})	0–5	0	–	0	0	0	0	0	0	0	0	0	0	0	0
	6–10	0	–	0	0	0	0	0	0	0	0	0	0	0	0
	11–15	0	–	0	0	0	0	0	0	0	0	0	0	0	0
	16–20	0	–	0	0	0	0	0	0	0	0	0	2	0	0
	>20	8	–	4	4	4	4	4	4	4	4	4	2	4	4
Total Number of σ_F		61	15	40	21	31	23	36	40	31	23	38	34	32	11
Aromatic Hydrocarbons (with 1 or 2 rings)	0–5	0	0	0	0	0	0	0	0	0	0	0	0	1	0
	6–10	0	0	2	0	0	0	0	0	0	0	3	0	1	0
	11–15	3	0	7	0	0	0	1	1	0	0	6	0	7	0
	16–20	5	0	9	1	4	1	3	3	1	1	9	6	11	0
	>20	53	15	22	20	27	22	32	36	30	22	20	28	12	11
Total Number of σ_F		24	8	12	12	12	12	16	16	12	12	16	16	16	–
Alcohols	0–5	0	0	0	0	0	0	0	0	0	0	0	0	0	–
	6–10	0	0	1	0	0	0	0	0	0	0	0	0	0	–
	11–15	0	0	1	0	0	0	0	0	1	0	1	0	2	–
	16–20	0	0	4	0	0	0	0	0	0	0	3	0	3	–
	>20	24	8	6	12	12	12	16	16	11	12	12	16	11	–
Total Number of σ_F		21	4	15	6	8	12	16	9	8	12	7	18	12	4
Sulfur Components	0–5	0	0	2	0	0	0	0	0	0	0	0	0	0	0
	6–10	1	0	1	0	2	0	3	0	0	0	0	0	1	0
	11–15	4	0	2	2	4	0	3	1	3	0	0	1	4	0
	16–20	6	0	3	2	1	4	4	2	1	2	2	4	3	0
	>20	10	4	7	2	1	8	6	6	4	10	5	13	4	4
Total Number of σ_F		82	–	44	38	45	32	35	47	45	32	45	35	27	20
Refrigerants	0–5	0	–	3	0	0	0	0	0	0	0	0	0	0	0
	6–10	1	–	13	0	2	0	3	2	4	0	7	0	3	0
	11–15	7	–	17	2	16	2	9	3	3	0	3	0	7	0
	16–20	12	–	8	11	12	5	14	5	7	2	10	0	12	2
	>20	62	–	3	25	15	25	9	37	31	30	25	35	5	18
Total Number of σ_F		5	–	2	3	3	2	3	2	2	3	2	3	2	2
Oxygen	0–5	3	–	0	1	1	1	1	1	0	0	0	0	0	0
	6–10	2	–	1	1	2	1	2	0	1	0	1	1	1	0
	11–15	0	–	1	1	0	0	0	0	1	1	0	0	1	0
	16–20	0	–	0	0	0	0	0	1	0	2	1	0	0	0
	>20	0	–	0	0	0	0	0	0	0	0	0	2	0	2
Total Number of σ_F		7	1	4	4	4	3	5	3	3	5	3	5	4	3
Acetone	0–5	0	0	0	0	0	0	0	0	0	0	0	0	0	0
	6–10	0	0	0	0	0	0	0	0	0	0	1	0	1	0
	11–15	0	0	0	0	0	0	2	1	0	1	1	0	0	0
	16–20	0	0	0	0	0	0	0	0	1	0	1	1	3	0
	>20	7	1	4	4	4	3	3	2	2	4	0	4	0	3

Notation

N = number of points
P = pressure, bar
P_C = critical pressure, bar
R = ideal gas constant, J/(mol·K)
ΔC_p = heat capacity departure (real-ideal), J/(mol·K)
$\Delta C_{P,\text{base}}$ = heat capacity departure of database, J/(mol·K)
$\Delta C_{P,\text{calc}}$ = calculated heat capacity departure, J/(mol·K)
T = temperature, K
T_C = critical temperature, K
V = volume, m^3/mol

Greek letter

ω = acentric factor, dimensionless

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