Technical Data Book: Part 5 – Vapor Pressure

API TECHNICAL REPORT TDB-5
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SCOPE

Technical Report TDB-5 provides procedures for calculating the vapor pressure for pure components, petroleum fractions and mixtures that are common in refinery applications. Methods for estimating the Reid vapor pressure and true vapor pressure of mixtures are also presented. Both computer algorithms and figures are presented for estimation of these properties. An estimate of the accuracy and range of application for each method is presented.

Any references to other chapters within this document refer to the corresponding Technical Data Book Chapter which is published as API Technical Report TDB-x, where x is the chapter number.

5-0 Introduction

Vapor pressure is the pressure at which the vapor phase of a substance is in equilibrium with the liquid phase of that substance at a specified temperature. The term is commonly applied to pure substances but it is also used occasionally with mixtures. Apart from the temperature effect, the composition of the vapor and liquid phases (when not pure) also influences the equilibrium pressure. Therefore, to use the term vapor pressure with mixtures, the composition effect is taken into account, either by holding liquid, vapor, or overall composition constant or by focusing attention on a portion of the liquid mixture which is sufficiently close boiling that composition changes with temperature have a negligible effect on pressure.

Specific vapor pressure correlation equations are recommended in Procedures 5A1.1 and 5A1.3. For compounds covered in this section these equations will give more accurate vapor pressures over the range specified for the particular compound than the generalized predictive procedures. The approximate average error to be expected and the range of applicability for each compound for each correlating equation deemed satisfactory are given together with the correlation coefficients in Tables 5A1.2 and 5A1.4. Procedure 5A1.1 is the primary method and is of a form that can be extrapolated slightly above the critical point when necessary. Procedure 5A1.3 is the alternate method which is constrained at the exact critical point and cannot be extrapolated higher.

The experimental vapor pressure-temperature relationships of a number of the more common hydrocarbons and a few important nonhydrocarbons are plotted directly in Figures 5A1.5 through 5A1.15. The scales of most of these figures are the logarithm of the vapor pressure and a modified reciprocal temperature scale $\frac{1}{t+382}$, where t is temperature in degrees Fahrenheit.

An accurate generalized method of predicting pure hydrocarbon vapor pressures is given as Procedure 5A1.16. This procedure requires the critical temperature, critical pressure and acentric factor of a hydrocarbon. A slightly less accurate alternative prediction method is given for pure hydrocarbons if these critical properties are not available. This alternative method, Procedure 5A1.19, requires only the normal boiling point and the Watson K factor and is also applicable to narrow-boiling range petroleum fractions. The procedure, which includes Figures 5A1.20 and 5A1.21, can also be used to convert a known boiling point from one pressure to another. Table 5-0.1 gives average and bias percent errors for each family of compounds tested for Procedures 5A1.16 and 5A1.19.

The Reid vapor pressure (RVP) is the differential pressure exerted by a mixture in psi determined at 100 °F at a feed vapor-to-liquid volume ratio of 4. (Defined and specified in ASTM Method D323, the apparatus and procedures are standardized under the auspices of ASTM). Frequently, the RVP is used to characterize the volatility of gasolines and crude oils. It also provides a convenient approximation of the absolute vapor pressure of a partly vaporized sample at 100 °F. Two figures are given that relate the RVP and ASTM D86 boiling characteristics to true vapor pressure for crude oils over a wide range of temperatures (Figure 5B1.2) and for gasolines and other finished petroleum products (Figure 5B1.1). Procedure 5B1.4 gives a computer method for predicting the Reid vapor pressure for both pure compounds and petroleum fractions.

Note: *A report that documents the basis upon which the material in this chapter has been selected has been published by the American Petroleum Institute as Documentation Report No. 5-93 available from University Microfilms International, Books and Collections, Ann Arbor, Michigan.*

Table 5-0.1 – Comparison of Prediction Methods

Family	No of Cpds	Procedure 5A1.16 (Lee Kesler) Percent Error		Procedure 5A1.19 (Maxwell Bonnell) Percent Error	
		Bias	Average	Bias	Average
n-Alkanes	22	0.5	3.1	–0.9	3.8
Methyl alkanes	16	–0.1	1.8	0.2	1.4
Dimethyl Alkanes	16	–1.2	1.5	0.1	3
Other branched alkanes	20	–1.3	1.6	–0.4	4.6
Cycloalkanes	4	–1.5	2	1.3	3.1
Substd. cyclopentanes	10	–2.9	4	–1.9	2.9
Substd. cyclohexanes	13	1.9	3.5	–3.5	5.4
Decalins/bicyclohexyl	3	10.6	14.7	–4.6	13.7
n-Alkenes	18	–0.3	2.3	–1.5	3.9
Other linear alkenes	13	–0.8	1.2	0.6	1.9
Methyl alkenes	13	–1.1	2.8	1.1	2
Other branched alkenes	10	1.8	3.8	0.4	1.8
Cycloalkenes	4	–2.2	3.7	–1.9	3.6
Alkadienes	13	12.7	14.5	3.9	4.5
Alkynes	8	–1.1	5.3	1	8
n-Alkylbenzenes	14	–1.9	2.9	–0.2	1.9
Substd. Alkylbenzenes	25	–0.6	3.3	1.3	1.9
Aromatics with unsaturated side chains	13	–0.5	3.4	4.7	6
Naphthalenes & tetralin	8	–1.9	3.7	2	3.3
Fused ring aromatics	6	–12.9	13.7	–16.5	17.1
Multiple aromatic rings	6	5.2	12.7	–4	15.6
Indene/indane	2	–6.0	6.1	3.8	4.3
Thiophene/Tetrahydrothiophene	2	2.3	2.6	3	3.7
Nitrogen rings	5	–4.4	5.2	–4.1	10
Total	**264**				

Table 5-0.2 – Computer Methods

Procedure	Description
5A1.19	Prediction of Vapor Pressure of Pure Hydrocarbons and Narrow-Boiling Petroleum Fractions
5B1.1	True Vapor Pressure of Gasolines and Finished Petroleum Products
5B1.2	True Vapor Pressure of Crude Oils
5B1.3	Blending Method for Reid Vapor Pressure
5B1.4	Predictions of Reid Vapor Pressures
5B1.5	VPCRx Predictions

5A Vapor Pressures

5A1 Vapor Pressure of Pure Hydrocarbons and Narrow -Boiling Petroleum Fractions

Procedure 5A1.1 – Vapor Pressures of Pure Compounds

Discussion

This procedure was last updated in 1994. The following equation is recommended for calculating the vapor pressure of any pure compound over the temperature range specified for the compound.

$$\ln P = A + \frac{B}{T} + C \ln T + DT^2 + \frac{E}{T^2} \qquad (5A1.1\text{-}1)$$

Where:

P	=	*vapor pressure of the pure compound, psia*
T	=	*temperature, °R*
A,B,C,D,E	=	*derived coefficients from Table 5A1.2*

Table 5A1.2 gives the coefficients for the above equation together with the applicable temperature range and the maximum and average percent errors from the comparison with experimental data carried out during regression.

Procedure

Use the coefficients from Table 5A1.2 in equation (5A1.1-1) to calculate the vapor pressure within the temperature range specified.

Comments on Procedure 5A1.1

Purpose

This procedure is to be used to calculate the vapor pressure of specific compounds as a function of temperature.

Limitations

This procedure is valid only over the temperature limits listed in Table 5A1.2. The procedure can be extrapolated slightly above the critical temperature where noted by the limits given in Table 5A1.2

Special Comments

The vapor pressures calculated by this procedure in the experimental data range are totally consistent with the vapor pressure plots for common compounds of Figures 5A1.5 through 5A1.13.

Note the errors given in the correlation coefficient tables when using this procedure.

Literature Sources

Procedure 5A1.1 is a modification of the Riedel (272) method and was developed by the project staff at The Pennsylvania State University. It has been thoroughly tested by the project staff and evaluated by the API Technical Data Committee.

Example

Determine the vapor pressure of *n*-octane at a temperature of 100 °F.

The necessary parameters are obtained from Table 5A1.2 for *n*-octane (API ID 23).

A	=	*76.793*
B	=	*–11700.0*
C	=	*–8.8309*
D	=	*0.0000020086*
E	=	*–395420*

and

T	=	*100 °F = 559.67 °R*

Using equation (5A1.1-1)

ln P	=	*–0.62159*
P	=	*0.5371 psia*

The experimental value listed in the pure component properties tables is 0.5373 psia.

Table 5A1.2 – Coefficients for Procedure 5A1.1

API ID	COMPOUND NAME	A	B	C	D	E	TPT	T_{min}	T_{max}	T_c	MAX% ERR	AVE % ERR
794	Oxygen	3.9762E+01	-2.2262E+03	-4.7268E+00	1.7521E-05	6.1941E+03	98	98	305	278	1.8	0.1
781	Hydrogen	-5.4119E+00	-6.5123E+01	2.9071E+00	2.8894E-05	-8.5898E+02	25	25	65	60	6.0	0.9
845	Water	7.8294E+01	-1.4309E+04	-8.5005E+00	1.4311E-06	1.7526E+05	492	492	1280	1165	0.5	0.1
792	Nitrogen dioxide	-1.6165E+02	1.3458E+04	2.3645E+01	-2.9099E-06	-2.4018E+06	471	471	850	776	3.0	0.2
790	Nitric oxide	3.1705E+02	- 1.6068E+04	-4.7164E+01	7.2089E-05	4.6778E+05	197	197	355	324	6.0	0.8
791	Nitrous oxide	1.2458E+02	-1.0689E+04	-1.6248E+01	9.7825E-06	3.8871E+05	328	328	610	557	9.3	1.5
771	Ammonia	3.6274E+01	- 5.3204E+03	-3.3757E+00	2.0131E-06	-2.1404E+05	352	352	800	730	1.2	0.4
777	Chlorine	-2.2517E+00	-1.8808E+03	1.8891E+00	-4.0763E-08	- 3.9663E+05	310	310	825	751	2.8	0.5
783	Hydrogen chloride	6.2968E+01	-6.0643E+03	-7.4857E+00	5.8712E-06	6.3865E+04	286	286	640	584	4.9	0.6
786	Hydrogen sulfide	-4.7322E+01	2.4043E+03	8.1971E+00	-2.0271E-06	-6.9380E+05	338	338	740	672	7.3	1.0
774	Carbon monoxide	9.6853E+01	-4.0476E+03	-1.4175E+01	4 8573E-05	6.6057E+04	123	123	260	239	10.2	0.9
775	Carbon dioxide	3.2930E+02	-2.7968E+04	-4.4992E+01	2.1351E-05	1.8121E+06	390	390	600	548	0.8	0.1
796	Sulfur dioxide	1.8055E+02	-2.0272E+04	- 2.3014E+01	6.2917E-06	1.1892E+06	356	365	850	775	3.3	0.8
	PARAFFINS											
1	Methane	3.3827E+01	-2.4795E+03	-3.6440E+00	9.5742E-06	5.5736E+03	163	163	375	343	0.3	0.0
2	Ethane	4.6348E+01	-4.6773E+03	-51. 827E+00	4.7093E-06	-1.0459E+03	163	163	605	550	0.3	0.0
3	Propane	5.9242E+01	-6.6250E+03	-6.8654E+00	3.8803B-Q6	1.8418E+04	154	154	*150*	666	2.4	0.9
4	*n*-Butane	6.1014E+01	-7.7978E+03	-6.9583E+00	2 8913E-06	-4.6755E+03	243	243	840	765	6.5	0.4
5	Isobutane	1.2790E+02	-1.2856E+04	-1.6433E+01	6.6710E-06	3.9238E+05	204	450	780	735	2.3	1.1
6	*n*-Pentane	7.0115E+01	-8.9802E+03	-8.1965E+00	2.9533E-06	-1.2087E+05	258	265	930	845	4.5	0.8
7	Isopentane	6.7488E+01	-8.9878E+03	-7.7859E+00	2.7146E-06	7.3035E+02	204	320	910	829	0.3	0.1
8	Neopentane	1.1444E+02	-1.3407E+04	-1.4236E+01	4.5590E-06	5.5466E+05	462	462	860	781	3.3	0.2
9	*n*-Hexane	-2.1375E+01	4.2444E+02	4.2014E+00	-4.2319E-08	-1.3639E+06	320	320	1000	913	2.9	0.8
10	2-Methylpentane	5.3718E+01	-8.1541E+03	-5.8437E+00	1.8985E-06	-2.6826E+05	215	360	985	896	4.5	0.2
11	3-Methylpentane	7.5850E+01	-1.0251E+04	-8.8908E+00	2.7105E-06	- 9.9752E+04	198	345	1000	908	4.8	0.8
12	2,2-Dimethylbutane	3.1072E+00	- 2.5556E+03	9.6386E-01	4.8912E-07	- 7.8464E+05	314	365	965	880	0.3	0.1
13	2,3-Dimethylbutane	6.2350E+01	-8.9893E+03	-7.0300E+00	2.1544E-06	-1.5015E+01	261	330	990	900	1.9	0.1
14	*n*-Heptane	1.83SOE+01	-4.3976E+03	-1.0907E+00	8.1020E-07	-1.0534E+06	329	329	1090	972	4.2	0.3
15	2-Methylhexane	8.3161E+01	-1.1851E+04	-9.7568E+00	2.4654E-06	-6.3936E+04	279	400	1050	955	1.9	0.2
16	3-Methylhexane	5.5109E+01	- 8.6225E+03	-6.0086E+00	1.7501E-06	-4.6227E+05	277	410	1000	963	4.9	0.3
20	2,4-Dimethylpentane	5.8563E+01	-8.7835E+03	-6.5031E+00	1.9426E-06	-3.5657E+05	277	380	1030	936	2.8	0.3

Table 5A1.2 (Continued)

API ID	COMPOUND NAME	A	B	C	D	E	TPT	T_{min}	T_{max}	T_c	MAX% ERR	AVE % ERR
18	2,2-Dimethylpentane	1.5119E+02	-1.9177E+04	- 1.8944E+01	4.4423E-06	8.7572E+05	269	350	1030	937	1.2	0.1
19	2,3-Dimethylpentane	9.4974E+01	-1.3556E+04	-1.1289E+01	2.6213E-06	2.2304E+05		365	1060	967	11.6	0.6
21	3,3-Dimethylpentane	9.6124E+01	-1.3605E+04	-1.1465E+01	2.6966E-06	2.8357E+05	250	345	1060	966	2.9	0.2
22	2,2,3-Trimethylbutane	5.4984E+01	-8.6672E+03	-5.9961E+00	1.7379E-06	-2.7764E+05	447	447	1050	956	1.0	0.1
17	3-Ethylpentane	7.9864E+01	-1.1732E+04	-9.2765E+00	2.2407E-06	-6.5284E+04	278	390	1070	973	0.7	0.1
23	*n*-Octane	7.6793E+01	-1.1700E+04	-8.8309E+00	2.0086E-06	-3.9542E+05	389	*515*	1 125	1024	3.2	0.4
28	2,2-Dimethylhexane	5.4874E+01	-8.6970E+03	-5.9785E+00	1.6700E-06	- 5.7342E+05	274	425	1090	990	0.8	0.1
29	2,3-Dimethylhexane	6.1935E+01	-9.7969E+03	-6.8866E+00	1.7584E-06	-4.8764E+05		*505*	1115	1014	0.6	0.1
30	2,4-Dimethylhexane	5.4351E+01	-8.7655E+03	-5.8896E+00	1.6114E-06	-5.7499E+05		500	1095	996	0.6	0.1
31	2,5-Dimethylhexane	6.2056E+01	-9.6132E+03	-6.9233E+00	1.8230E-06	-4.8486E+05	328	460	1090	990	0.9	0.1
32	3,3-Dimethylhexane	1.3044E+01	- 7.1790E+03	0	0	0	265	693	1012	1012		0.1
33	3,4-Dimethylhexane	9.0387E+01	-1.3569E+04	-1.0613E+01	2.2616E-06	2.3841E+04	295	SIS	1125	1024	0.5	0.1
24	2-Methylheptane	1.2326E+02	-1.7380E+04	-1.4990E+01	3.0524E-06	4.4368E+05		375	1105	1007	1.9	0.2
25	3-Methylheptane	1.0472E+02	-1.5246E+04	-1.2513E+01	2.5833E-06	1.7988E+05	275	390	1015	1015	2.7	0.1
26	4-Methylheptane	7.4219E+01	-1.1371E+04	-8.4932E+00	1.9726E-06	-3.2851E+05	274	450	1110	1011	0.8	0.1
37	2,2,4-Trimethylpentane	6.0368E+01	- 9.5060E+03	-6.6958E+00	1.7786E-06	- 3.2521E+05	298	405	1075	979	5.0	0.4
36	2,2,3-Trimethylpentane	7.3085E+01	- 1.1307E+04	-8.3493E+00	1.9377E-06	-1.6521E+05	290	390	1115	1014	0.6	0.1
38	2,3,3-Trimethylpentane	7.5022E+01	-1.1872E+04	-8.5698E+00	1.8976E-06	-6.6510E+04	310	440	1135	1032	0.7	0.1
39	2,3,4-Trimethylpentane	9.3068E+01	-1.3987E+04	-1.0961E+01	2.3058E-06	1.6588E+05	295	360	1120	1019	2.0	0.2
40	2,2,3,3-Tetramethylbutane	1.2759E+01	-6.8783E+03	0	0	0	673	674	1022	1022		
27	3-Ethylhexane	8.1873E+01	-1.2385E+04	-9.4986E+00	2.1125E-06	-1.8613E+05		510	1120	1018	0.6	0.1
34	2-Methyl-3-ethylpentane	8.1555E+01	-1.2436E+04	-9.4517E+00	2.0862E-06	- 9.98488+04	285	450	1120	1021	0.7	0.1
35	3-Methyl-3-ethylpentane	6.9800E+01	-1.1284E+04	-7.8703E+00	1.7653E-06	-1.7973E+05	328	400	1140	1038	0.6	0.1
41	*n*-Nonane	2.7423E+02	-3.7778E+04	- 3.4697E+01	5.5309E-06	2.9320E+06	395	470	1180	1072	1.4	0.2
42	2-Methyloctane	3.0932E+02	-4.2271E+04	-3.9304E+01	6.1939E-06	3.6281E+06	347	545	1160	1056	1.3	0.3
43	3-Methyloctane	1.5059E+02	-2.1303E+04	-1.8536E+01	3.3714E-06	7.2649E+05	298	485	1200	1062	1.9	0.4
44	4-Methyloctane	-1.8716E+01	1.05161l+03	3.6412E+00	2.8836E-07	-2.3831E+06	288	440	1160	1058	3.1	0.8
46	2,2-Dimethylheptane	-1.5510E+02	1.8030E+04	2.1659E+01	- 2.5250E-06	-4.4601E+06	288	460	1140	1038	1.6	0.4
47	2,6-Dimethylheptane	3.7963E+02	-5.1564E+04	-4.8507E+01	7.4551E-06	5.0373E+06	306	545	1145	1042	2.7	0.4
55	3,3-Diethylheptane	4.5559E+01	-8.6120E+03	-4.6574E+00	1.2128E-06	-7.3508E+05	432	432	1205	1098	0.0	0.0
50	2,2,5-Trimethylhexane	3.2024E+01	-6.1507E+03	-2.9266E+00	1.0430E-06	-1.0391E+06	301	450	1125	1022	0.0	0.0

Table 5A1.2 (Continued)

API ID	COMPOUND NAME	A	B	C	D	E	TPT	T_{min}	T_{max}	T_c	MAX% ERR	AVE % ERR
53	2,4,4-Trimethylhexane	6.7499E+01	-1.0753E+04	-7.6172E+00	1.8336E-06	-4.2139E+05	288	440	1150	1046	0.1	0.0
58	2,2,3,3-Tetramethylpentane	1.1685E+01	-4.4205E+03	-1.5629E-01	3.5604E-07	-1.2300E+06	474	474	1210	1100	0.1	0.0
59	2,2,3,4-Tetramethylpentane	3.4213E+01	-6.9464E+03	-3.1691E+00	9.5568E-07	-8.7465E+05	274	425	1170	1066	0.2	0.0
60	2,2,4,4-Tetramethylpentane	4.1550E+01	-7.5761E+03	-4.1731E+00	1.2086E-06	-7.2071E+05	373	460	1130	1028	0.1	0.0
61	2,3,3,4-Tetramethylpentane	4.1460E+01	-8.1491E+03	-4.0967E+00	1.0504E-06	-7.4630E+05	308	4. 0	1200	1094	0.0	0.0
45	3-Ethylheptane	-8.5096E+01	7.2769E+03	1.2121E+01	-1.7771E-06	-2.8701E+06	285	460	1165	1062	4.0	0.7
56	2,2-Dimethyl-3-ethylpentane	2.5586E+02	-3.5086E+04	-3.2343E+01	5.2895E-06	2.8063E+06	313	440	1165	1062	1.6	0.3
57	2,4-Dimethyl-3-ethylpentane	1.0593E+02	-1.5496E+04	-1.2694E+01	2.5877E-06	9.9535E+04	271	450	1170	1064	1.6	0.4
62	*n*-Decane	1.0673E+02	-1.6454E+04	-1.2659E+01	2.2295E-06	-2.3063E+05	438	515	1225	1113	3.8	0.5
63	2-Methylnonane	-5.2049E+01	6.1934E+03	7.8999E+00	-1.6668E-07	-3.5822E+06	357	500	1205	1098	2.4	0.4
64	3-Methylnonane	2.2831E+02	-3.3136E+04	-2.8491E+01	4.2568E-06	2.3144E+06	339	485	1210	1103	2.3	0.4
65	4-Methylnonane	1.5893E+02	- 2.3989E+04	-1.9413E+01	3.0471E-06	1.0874E+06	314	470	1240	1098	2.2	0.4
66	5-Methylnonane	-1.3683E+02	1.8182E+04	1.8881E+01	-1.4465E-06	-5.3373E+06	334	500	1205	1098	1.7	0.3
501	2,2-Dimethyloctane	-7.9228E+01	7.9789E+03	1.1715E+01	-1.1846E-06	-3.3585E+06		*565*	1190	1084	1.9	0.6
73	*n*-Undecane	9.1338E+01	-1.4110E+04	-1.0691E+01	1.9995E-06	-9.4297E+05	446	580	1265	1150	4.2	0.2
74	*n*-Dodecane	1.7024E+02	-2.5990E+04	-2.0822E+01	2.9759E-06	6.4519E+05	474	515	1300	1185	1.3	0.2
75	*n*-Tridecane	8.3482E+02	-1.3154E+05	-1.0554E+02	1.0785E-05	1.8631E+07	482	600	1285	1216	9.0	1.5
76	*n*-Tetradecane	1.3078E+02	-2.0072E+04	-1.5743E+01	2.3531E-06	-1.0089E+06	502	665	1246	1246	0.3	0.1
77	*n*-Pentadecane	1.9685E+02	-3.0584E+04	-2.4158E+01	3.0811E-06	4.6577E+05	510	690	1330	1272	0.2	0.1
78	*n*-Hexadecane	1.7420E+02	-2.8534E+04	-2.1090E+01	2.5228E-06	8.8111E+04	524	530	1385	1297	5.4	0.3
79	*n*-Heptadecane	-7.5324E+01	1.3948E+04	1.0397E+01	2.1438E-09	-8.1956E+06	531	560	1450	1320	3.3	0.5
80	*n*-Octadecane	4.3311E+02	-6.8776E+04	-5.4134E+01	5.4392E-06	6.1073E+06	542	570	1341	1341	6.5	1.8
81	*n*-Nonadecane	2.4395E+02	-4.1187E+04	-2.9766E+01	2.8843E-06	1.5865E+06	550	665	1385	1361	2.7	0.5
82	*n*-Eicosane	2.1435E+02	-4.1637E+04	-2.5400E+01	1.7283E-06	2.2404E+06	557	620	1450	1381	7.8	1.2
86	*n*-Tetracosane	8.0484E+02	-1.4037E+05	-1.0011E+02	7.8503E-06	1.9191E+07	583	800	1560	1458	4.0	0.7
90	*n*-Octacosane	2.3472E+01	-1.6628E+02	-2.2044E+00	9.0323E-07	-1.0217E+07	602	750	1665	1517	5.1	1.1

Table 5A1.2 (Continued)

API ID	COMPOUND NAME	A	B	C	D	E	TPT	T_{min}	T_{max}	T_c	MAX% ERR	AVE % ERR
	NAPHTHENES											
101	Cyclopentane	7.8860E+01	-1.1139E+04	9.1663E+00	2.4385E-06	1.7936E+05	323	365	1010	921	4.0	0.6
102	Methylcyclopentane	6.9235E+01	-1.0259E+04	-7.8750E+00	2.0796E-06	-6.9909E+04	235	320	1055	959	2.0	0.1
103	Ethyleyclopentane	3.5173E+01	-6.7688E+03	-3.2937E+00	1.0663E-06	-6.9827E+05	242	330	1125	1025	1.6	0.1
104	1,1-Dimethylcyclopentane	3.7315E+01	-6.2084E+03	-3.7135E+00	1.5840E-06	-7.1444E+05	366	366	1080	985	0.8	0.1
105	cis-1,2-Dimethylcyclopentane	4.8701 E+01	-8.1276E+03	-5.1353E+00	1.5138E-06	-5.2008E+05	395	450	1115	1017	0.1	0.0
106	trans-1,2-Dimethylcyclopentane	4.8807E+01	-7.8438E+03	-5.1929E+00	1.6778E-06	-5.2447E+05	280	360	1095	996	0.2	0.0
107	cis-1,3-Dimethylcyclopentane	-6.2227E.02	6.7460E+04	8.4819E+01	-1.5698E-05	-9.1550E+06	251	475	992	992	3.2	1.2
108	trans-1,3-Dimethylcyclopentane	6.2612E+01	-9.5132E+03	-7.0262E+00	1.9932E-06	-3.0956E+05	251	360	1095	995	0.2	0.0
109	*n*-Propylcyclopentane	-1.9290E+01	-7.8164E+02	4.0133E+00	-4.7027E-07	-1.6638E+06	280	440	1190	1085	0.2	0.0
110	Isopropylcyclopentane	1.6201E+02	-2.2742E+04	-2.0062E+01	3.6929E-06	1.2215E+06	291	375	1175	1067	5.9	0.3
146	Cyclohexane	1.6545E+02	-2.2596E+04	-2.0538E+01	3.9165E-06	1.5144E+06	503	503	1095	996	4.2	0.7
147	Methylcyclohexane	4.1978E+01	-7.6143E+03	-4.1995E+00	1.1892E- 06	-5.3200E+05	264	485	1130	1030	0.9	0.2
148	Ethylcyclohexane	1.0009E+02	-1.4951E+04	-1.1911E+01	2.5016E-06	1.5099E+05	291	410	1205	1096	0.2	0.0
149	1,1-Dimethycyclohexane	8.0576E+00	-3.9419E+03	3.4784E-01	2.1202E-07	-1.0899E+06	431	485	1170	1064	0.1	0.0
150	cis-1,2-Dimethylcylohexane	-1.8289E+01	-9.8315E+02	3.8753E+00	-4.7206E-07	-1.5483E+06	402	470	1200	1091	0.2	0.0
151	trans-1,2-Dimethylcyclohexane	-1.4797E+00	- 2 9696E+03	1.6340E+00	-3.7322E-08	-1.2181E+06	333	440	1180	1073	0.1	0.0
152	cis-1,3-Dimethylcyclohexane	-3.5229E+00	-2.7704E+03	1.9288E+00	-1.5532E-07	-1.2302E+06	356	460	1170	1064	0.4	0.0
153	trans-1,3-Dimethylcyclohexane	-2.0638E+00	-3.0057E+03	1.7475E+00	-1.8037E-07	-1.2516E+06	329	460	1180	1076	1.4	0.1
154	cis-1,4-Dimethylcyclohexane	-2.9807E+00	-2.9255E+03	1.8701E+00	-1.9736E-07	-1.2456E+06	334	400	1185	1077	0.1	0.0
155	trans-1,4-Dimethylcyclohexane	6.4353E+00	-3.8337E+03	5.7787E-01	1.5023E-07	-1.0920E+06	425	425	1165	1062	0.3	0.0
156	*n*-Propylcyclohexane	8.6328E+01	-1.4481E+04	-9.9217E+00	1.7804E-06	0	321	321	1129	1129	2.1	0.4
157	Isopropylcyclohexane	7.7647E+01	-1.3008E+04	-8.8263E+00	1.6545E-06	-2.2675E+05	331	375	1240	1129	3.9	0.1
158	*n*-Butylcyclohexane	9.4624E+01	-1.6090E+04	-1.0948E+01	1.7465E-06	0	357	357	1170	1170	1.7	0.4
163	*n*-Pentylcyclohexane	1.0302E+02	-1.7596E+04	-1.2020E+01	1.8512E-06	0	382	382	1205	1205	10.7	1.2
164	*n*-Hexylcyclohexane	1.3612E+02	-2.2216E+04	-1.6320E+01	2.3371E-06	3.4493E+05	406	406	1236	1236	3.5	0.7
166	*n*-Octylcyclohexane	1.1782E+02	-2.1546E+04	-1.3742E+01	1.7422E-06	0	448	448	1292	1292	5.0	1.6
168	*n*-Decylcyclohexane	2.2865E+02	-3.6584E+04	-2.8165E+01	3.4122E-06	1.4363E+06	488	488	1339	1339	5.1	0.8
179	Cycloheptane	8.3408E+01	-1.2925E+04	-9.6615E+00	1.9926E-06	-1.1286E+04	477	477	1195	1088	0.9	0.1
180	Cyclooctane	8.4262E+01	-1.3713E+04	-9.7188E+00	1.8511E-06	-1.0762E+05	518	518	1265	1152	2.3	0.2
111	1-Methyl-1-ethylcyclopentane	1.2825E+06	- 1.7949E+04	-1.5703E+01	3.3260E-06	5.6921E+05	233	330	1150	1048	1.7	0.1

Table 5A1.2 (Continued)

API ID	COMPOUND NAME	A	B	C	D	E	TPT	T_{min}	T_{max}	T_c	MAX% ERR	AVE % ERR
	OLEFINS											
192	Ethylene	4.5161E+01	-4.1926E+03	-5.0837E+00	5.4583E-06	-1.3941E+04	187	187	560	508.0	8.9	0.6
193	Propylene	6.2835E+01	-6.7973E+03	-7.3821E+00	4.2049E-06	4.0466E+04	158	158	720	658.0	0.2	0.2
194	1-Butene	1.4463E+02	-1.4547E+04	-1.8703E+01	7.1411E-06	5.0169E+05	158	225	830	756	2.1	0.4
195	cis-2-Butene	-2.6281E+02	2.5364E+04	3.7157E+01	-8.1878E-06	-3.5164E+06	242	410	860	784	2.6	0.5
196	trans-2-Butene	-3.2314E+02	3.0875E+04	4.5490E+01	-1.0525E-05	-3.9628E+06	302	440	850	772	2.4	0.5
197	Isobutene	-6.9324E+01	4.8087E+03	1.0982E+01	-2.3641E-06	-1.2083E+06	239	310	825	752	6.0	1.4
198	1-Pentene	-3.8105E+00	-1.4840E+03	1.8865E+00	4.5886E-07	-8.3575E+05	194	300	920	837	6.6	0.3
199	cis-2-Pentene	4.3745E+01	-6.4127E+03	-4.5720E+00	1.9478E-06	-3.9209E+05	219	345	940	855	0.1	0.0
200	trans-2-Pentene	4.4115E+01	-6.7393E+03	-4.5719E+00	1.8326E-06	-3.0799E+05	239	330	940	854	0.2	0.0
201	2-Methyl-1-butene	3.6418E+01	-5.6531E+03	-3.5712E+00	1.7189E-06	-4.2192E+05	244	345	900	837	0.6	0.1
203	2-Methyl-2-butene	2.3137E+01	-4.9060E+03	- 1.6702E+00	1.0476E-06	-4.6056E+05	251	320	930	848	3.4	0.3
202	3-Methyl-1-butene	9.1844E+01	- 1.0947E+04	-1.1206E+01	4.0316E-06	1.9735E+05	188	280	890	811	0.5	0.0
204	1-Hexene	3.5628E+01	-6.0432E+03	-3.4267E+00	1.4302E-06	-5.6499E+05	240	410	1000	907	0.0	0.0
205	cis-2-Hexene	-1.0962E+01	-2.2573E+03	3.0846E+00	-6.1127E-07	-8.5797E+05	238	345	1000	923	1.7	0.1
206	trans-2-Hexene	-9.6301E+00	-1.5257E+03	2.7644E+00	-2.4009E-07	-1.0753E+06	252	375	1000	923	0.2	0.0
207	cis-3-Hexene	1.0675E+02	-1.4082E+04	-1.2963E+01	3.2953E-06	3.3891E+05	244	345	1000	916	1.2	0.1
208	trans-3-Hexene	1.0661E+02	-1.4140E+04	-1.2928E+01	3.2664E-06	3.4015E+05	288	350	1005	916	0.7	0.0
209	2-Methyl-1-pentene	-7.8186E-01	-2.4475E+03	1.5731E+00	-2.5963E-08	-9.2401E+05	247	375	1000	913	0.0	0.0
212	2-Methyl-2-pentene	- 1.0133E+01	-1.9369E+03	2.9290E+00	-6.0052E-07	-9.7344E+05	249	330	1000	925	0.1	0.0
210	3-Methyl-1-pentene	1.2955E+02	-1.5480E+04	-1.6255E+01	4.7487E-06	5.0436E+05	216	300	980	891	1.0	0.1
213	cis-3-Methyl-2-pentene	5.6169E+01	-9.0317E+03	-6.0614E+00	1.5880E-06	-1.6888E+05	249	345	1000	927	0.9	0.1
211	4-Methyl-1-pentene	2.3255E+01	-4.8545E+03	-1.7230E+00	9.5002E-07	- 5.7535E+05	215	330	980	893	0.1	0.0
215	cis-4-Methyl-pentene	1.2874E+01	-3.7286E+03	-3.0876E-01	5.5797E-07	-7.4782E+05	249	375	985	898	0.1	0.0
216	trans-4-Methyl-2-pentene	2.2498E+01	-4.9368E+03	-1.5772E+00	7.5395E-07	-6.1735E+05	238	320	990	902	0.0	0.0
220	2,3-Dimethyl-2-butene	-2.9304E+01	-5.7830E+01	5.5452E+00	-1.2707E-06	-1.2073E+06	358	425	1035	943	0.2	0.0
218	2,3-Dimethyl-1-butene	-3.3874E+00	-2.2991E+03	1.9466E+00	-1.3276E-07	-8.4720E+05	209	345	990	900	0.1	0.0
219	3,3-Dimethyl-1-butene	4.2387E+00	-1.9716E+03	7.0272E-01	8.7222E-07	-8.9696E+05	284	375	950	864	0.6	0.1
217	2-Ethyl-1-butene	-6.1009E+01	3.0795E+03	9.8874E+00	-2.3672E-06	-1.4322E+06	255	375	1015	922	0.2	0.0
221	1-Heptene	3.8560E+01	-6.7946E+03	-3.7807E+00	1.3042E-06	-6.9878E+05	278	390	1060	967	2.8	0.1
222	cis-2-Heptene	1.3502E+02	-1.8954E+04	-1.6515E+01	3.2217E-06	8.9483E+05	295	485	1085	988	3.2	0.3

Table 5A1.2 (Continued)

API ID	COMPOUND NAME	A	B	C	D	E	TPT	T_{min}	T_{max}	T_c	MAX% ERR	AVE % ERR
223	trans-2-Heptene	-2.1132E+01	4.0113E+02	4.1093E+00	1.2428E-07	-1.5905E+06	295	425	1075	977	2.6	0.4
224	cis-3-Heptene	-5.4011E+01	4.1237E+03	8.5495E+00	-9.7790E-07	-2.0452E+06	246	410	1080	981	2.7	0.5
225	trans-3-Heptene	1.8442E+02	-2.3491E+04	-2.3309E+01	5.0537E-06	1.2722E+06	246	390	1055	972	3.6	0.5
226	2-Methyl-1-hexene	2.5630E+02	-3.2603E+04	-3.2761E+01	6.3826E-06	2.5035E+06	307	470	1065	968	2.9	0.4
227	3-Methyl-1-hexene	-1.8480E+02	1.8799E+04	2.6125E+01	-4.4390E-06	-3.6521E+06	261	425	1045	950	3.6	0.5
228	4-Methyl-1-hexene	7.2808E+01	-1.0546E+04	-8.3730E+00	2.1754E-06	-2.3051E+05	237	390	1000	961	2.0	0.4
241	2-Ethyl-1-pentene	-2.9096E+02	3.2876E+04	3.9967E+01	-6.1438E-06	- 5.6541E+06	302	450	1070	977	1.7	0.5
242	3-Ethyl-1-pentene	7.5261E+01	-1.1256E+04	-8.6226E+00	2.0329E-06	-6.4080E+04	262	410	1050	954	2.0	0.5
256	2,3,3-Trimethyl-1-butene	2.3694E+01	-5.0213E+03	-1.7982E+00	8.9348E-07	-7.2713E+05	294	415	1050	956	0.0	0.0
257	1-Octene	3.5672E+01	-6.7861E+03	-3.3698E+00	1.1012E-06	-9.3687E+05	309	450	1125	1020	1.9	0.1
259	trans-2-Octene	5.1461E+02	-6.7255E+04	-6.6525E+01	1.0720E-05	7.0877E+06	334	520	1140	1039	3.7	0.4
261	trans-3-Octene	3.1329E+02	-4.1937E+04	-3.9971E+01	6.6618E-06	3.7661E+06	294	485	1135	1033	2.2	0.7
263	trans-4-Octene	-1.3954E+01	-8.5591E+01	3.0969E+00	2.1541E-07	-1.8673E+06	323	485	1135	1031	2.7	0.4
269	2-Ethyl-1-hexene	8.4816E+01	-1.2155E+04	-1.0022E+01	2.6694E-06	-2.6204E+05		515	1135	1033	1.6	0.7
276	2,4,4-Trimethyl-1-pentene	1.4372E+00	-3.0957E+03	1.2587E+00	1.2439E-08	-1.0744E+06	323	460	1095	995	5.1	0.3
277	2,4,4-Trimethyl-2-pentene	-4.8449E+01	2.6463E+03	7.9609E+00	-1.4070E-06	-1.8654E+06	300	475	1105	1004	0.3	0.0
278	1-Nonene	2.8668E+01	-6.1469E+03	-2.4234E+00	8.2776E-07	-1.2924E+06	345	425	1115	1068	0.0	0.0
279	1-Decene	5.8278E+01	-9.7125E+03	-6.3613E+00	1.4414E-06	-1.1720E+06	372	440	1220	1111	2.5	0.2
280	1-Undecene	-3.8531E+01	4.3995E+03	6.1206E+00	5.0017E-08	-3.7023E+06	403	*515*	1260	1148	1.4	0.2
281	1-Dodecene	5.3618E+01	-8.6285E+03	-5.8273E+00	1.4304E-06	-2.0671E+06	428	500	1285	1183	2.5	0.2
282	1-Tridecene	7.5610E+02	-1.0864E+05	-9.6850E+01	1.2341E-05	1.2940E+07	450	560	1215	1215	2.2	0.3
283	1-Tetradecene	-1.1292E+01	-2.5951E+02	2.7062E+00	8.6684E-08	-3.8832E+06	469	580	1370	1246	2.7	0.2
284	1-Pentadecene	-2.1392E+01	1.3425E+03	4.0036E+00	-9.6243E-08	-4.5238E+06	485	690	1385	1274	1.2	0.1
285	1-Hexadecene	6.5563E+02	-1.0294E+05	-8.2708E+01	8.6110E-06	1.2658E+07	500	*590*	1385	1300	2.2	0.3
286	1-Heptadecene	3.4158E+02	-4.9875E+04	-4.3021E+01	5.3198E-06	2.4452E+06	512	700	1440	1325	4.6	1.1
287	1-Octadecene	-6.7481E+02	6.9200E+03	8.7131E+01	-7.7180E-06	-2.4308E+07	523	630	1346	1346	4.5	0.3
288	1-Nonadecene	-1.2373E+02	1.9652E+04	1.6837E+01	-1.0657E-06	-9.5428E+06	534	750	1500	1368	0.0	0.0
289	1-Eicosene	1.0046E+02	-1.6767E+04	-1.1651E+01	1.4612E-06	-3.3776E+06	543	720	1440	1388	0.5	0.1
310	Cyclopentene	5.1199E+01	-7.7606E+03	5.4969E+00	1.8863E-06	-2.1217E+05	249	300	1000	913	0.1	0.0
315	Cyclohexene	1.3765E+01	-4.0382E+03	-4.4456E-01	6.2202E-07	-8.8825E+05	305	360	1110	1009	0.2	0.0
511	Cycloheptene	-2.0534E+02	1.8714E+04	2.9159E+01	-5.4123E-06	-3.4466E+06	391	415	1150	1076	3.0	0.2
512	Cyclooctene	-7.1036E+02	8.3655E+04	9.5371E+01	-1.4284E-05	-1.2310E+07	385	485	1138	1138	3.5	0.6

Table 5A1.2 (Continued)

API ID	COMPOUND NAME	A	B	C	D	E	TPT	T_{min}	T_{max}	T_c	MAX% ERR	AVE % ERR
	DIOLEFINS AND ACETYLENES											
318	Cyclopentadiene	1.3009E+01	-5.8344E+03	0	0	0	339	485	913	913		
292	1,3-Butadiene	5.4800E+01	-6.9074E+03	-6.1491E+00	2.8746E-06	-1.1478E+05	296	296	840	765	4.1	0.7
299	2-Methyl-1,3-butadiene	2.4493E+01	-5.4640E+03	-1.7274E+00	3.2614E-07	-3.4081E+05	229	280	960	871	0.3	0.1
298	3-Methyl-1,2-butadiene	3.8924E+01	-7.1018E+03	-3.6571E+00	7.0194E-07	-2.2982E+05	287	320	970	882	0.4	0.1
293	1,2-Pentadiene	2.7552E+01	-6.1271E+03	-2.0689E+00	8.1259E-08	-3.4386E+05	245	290	990	900	0.4	0.1
294	cis-1,3-Pentadiene	3.0552E+01	-6.4927E+03	-2.4652E+00	1.1738E-07	-2.8797E+05	238	310	990	898	1.1	0.1
295	trans-1,3-Pentadiene	1.0455E+01	-4.5965E+03	3.0418E-01	-7.1449E-07	-4.3895E+05	334	334	990	900	0.1	0.0
296	1,4-Pentadiene	-2.2440E+01	- 8.9438E+02	4.7644E+00	-1.8951E-06	-7.6044E+05	225	300	950	862	0.1	0.0
297	2,3-Pentadiene	5.2518E+01	-8.4935E+03	-5.5160E+00	1.2173E-06	-1.5813E+05	266	320	985	895	0.3	0.0
521	1,3-Cyclohexadiene	7.7919E+01	-1.1612E+04	-8.9729E+00	2.0577E-06	4.5362E+04	290	340	1105	1004	2.9	0.2
300	2,3-Dimethyl-1,3-butadiene	5.0477E+01	-8.6258E+03	-5.2431E+00	1.1458E-06	- 2.0312E+05	355	355	1040	947	0 9	0.1
302	1,5-Hexadiene	-4.7748E+01	4.6466E+03	7.5104E+00	-6.6340E-08	-1.9113E+06	238	390	1005	913	0.4	0.0
522	trans,trans-2,4-Hexadiene	1.7644E+02	-2.3195E+04	-2.2111E+01	4.5170E-06	1.4376E+06	411	485	1060	963	1.8	0.2
523	1,5-Cyclooctadiene	1.0039E+02	-1.0669E+04	-1.2523E+01	3.4328E-06	-1.5056E+06	367	530	1275	1161	0.1	0.0
322	Acetylene	-2.1783E+01	-7.2296E+01	4.7923E+00	-1.5196E-06	-3.5081E+05	346	346	610	*555*	2.5	0.4
323	Methylacetylene	-2.9216E+01	1.4637E+03	5.4266E+00	-2.3842E-07	- 9.0124E+05	307	307	780	724	2.4	0.6
324	Dimethylacetylene	3.1080E+01	- 5.6888E+03	-2.6926E+00	1.1461E-06	-3.6593E+05	434	434	935	852	1.0	0.1
329	3-Methyl-1-butyne	1.8034E+02	-1.9023E+04	-2.3463E+01	7.9515E-06	8.1725E+05	330	400	915	834	3.3	0.5
327	1-Pentyne	6.6000E+01	-7.1490E+03	-8.0047E+00	4.9909E-06	-4.8217E+05	301	400	866	866	3.2	0.4
330	1-Hexyne	3.5369E+02	-4.1129E+04	-4.6241E+01	1.0443E-05	3.3180E+06	254	400	1020	929	5.1	0.9
527	2-Hexyne	-1.8608E+01	-3.5564E+02	3.9321E+00	-4.8475E-07	-1.4014E+06	331	400	1085	988	1.8	0.3
528	3-Hexyne	-2.2432E+01	-1.3006E+03	4.6763E+00	-1.1609E-06	-1.0475E+06	306	400	1075	979	3.8	0.7
	AROMATICS											
335	Benzene	6.1987E+01	-9.5276E+03	-6.8729E+04	1.7690E-06	-2.6942E+05	502	502	1110	1012	1.6	0.3
336	Toluene	7.9179E+01	-1.2541E+04	-9.0609E+00	1.8911E-06	-2.4490E+01	321	440	1125	1065	3.0	0.3
337	Ethylbenzene	8.8275E+01	-1.4406E+04	-1.0180E+01	8.2860E-07	9.9386E+04	321	425	1200	1111	0.8	0.1
339	m-Xylene	9.2449E+01	-1.5084E+04	-1.0716E+01	1.9216E-06	1.8459E+05	406	450	1220	1111	3.7	0.2
338	o-Xylene	7.4341E+01	-1.2661E+04	-8.3543E+00	1.5845E-06	-2.1492E+05	446	446	1245	1135	2.2	0.3
340	p-Xylene	1.0073E+02	-1.5935E+04	-1.1840E+01	2.1494E-06	2.8395E+05	516	516	1220	1109	7.6	0.4
341	*n*-Propylbenzene	1.0930E+02	-1.7478E+04	-1.2917E+01	2.1422E-06	3.2754E+05	312	425	1200	1149	*5.5*	0.4

Table 5A1.2 (Continued)

API ID	COMPOUND NAME	A	B	C	D	E	TPT	T_{min}	T_{max}	T_c	MAX% ERR	AVE % ERR
346	1,2,3-Trimelhylbenzene	2.5635E+01	-6.4754E+03	-1.9801E+00	7.0513E-07	-1.4022E+06	446	515	1315	1196	0.2	0.0
347	1,2,4-Trimethylbenzene	4.9075E+01	-9.7805E+03	-5.0110E+00	1.0618E-06	-8.2929E+05	413	500	1285	1168	8.4	0.6
344	m-Ethyltoluene	-5.3727E+01	3.1001E+03	8.5867E+00	-1.2002E-06	-2.4581E+06	320	470	1260	1147	0.3	0.0
343	o-Ethyltoluene	-6.4313E+01	4.5408E+03	9 9613E+00	-1.3794E-06	-2.7048E+06	346	475	1290	1172	0.3	0.0
345	p-Ethyltoluene	1.7605E+02	-2.6318E+04	-2.1658E+01	3.3576E-06	1.5292E+06	379	515	1265	1152	16.6	1.1
349	*n*-Butylbenzene	5.7955E+01	-1.0520E+04	-6.23728+00	1.2674E-06	-9.8531E+05	334	420	1285	1189	8.0	0.7
350	Isobutylbenzene	8.6630E+01	-1.3918E+04	-1.0057E+01	1.9637E-06	-3.9224E+05	399	530	1285	1170	0.0	0.0
351	sec-Butylbenzene	-2.1250E+02	2.5796E+04	2.9108E+01	-3.5519E-06	-6.0236E+06	356	530	1315	1196	1.1	0.2
352	tert-Butylbenzene:	-1.0401E+02	1.0717E+04	1.5025E+01	-1.8836E-06	-3.7613E+06	387	530	1 305	1188	0.4	0.0
360	m-Diethylbenzene	-2.7331E+01	3.5372E+02	5.0066E+00	-4.7443E-07	-2.4567E+06	341	530	1310	1193	1.3	0.1
359	o-Diethylbenzene	-3.0283E+01	7.5753E+02	5.3867E+00	-5.2878E-07	-2.5316E+06	435	560	1320	1202	0.1	0.0
361	p-Diethylbenzene	4.7689E+01	-9.3006E+03	-4.8767E+00	1.0649E-06	-1.1367E+06	415	530	1300	1184	0.0	0.0
357	m-Cymene	2.0183E+02	-3.1084E+04	-2.4843E+01	3.3305E-06	2.2729E+06	377	530	1300	1183	2.7	0.6
356	o-Cymene	2.5931E+02	-4.0364E+04	-3.2146E+01	3.9366E-06	3.8537E+06	363	530	1310	1192	2.9	0.6
358	p-Cymene	-3.5369E+01	1.4886E+03	6.0257E+00	-5.1235E-07	-2.4943E+06	369	460	1290	1176	7.6	1.4
364	2-Ethyl-m-xylene	1.2303E+02	-2.0068E+04	-1.4626E+01	2.1723E-06	4.0666E+05	462	500	1325	1208	0.5	0.1
367	2-Ethyl-p-xylene	2.9676E+02	-4.4962E+04	-3.7098E+01	4.7548E-06	4.2669E+06	395	530	1310	1193	3.6	0.8
362	3-Ethyl-o-xylene	-3.9455E+01	1.7522E+03	6.5988E+00	-6.7995E-07	-2.7568E+06	403	500	1345	1224	0.2	0.1
365	4-Ethyl-m-xylene	2.4789E+02	-3.8952E+04	-3.0650E+01	3.8091E-06	3.5170E+06	378	470	1315	1197	6.3	0.7
363	4-Ethyl-o-xylene	1.3327E+02	- 2.1586E+04	-1.5947E+01	2.3447E-06	6.5677E+05	371	470	1320	1201	0.1	0.1
366	5-Ethyl-m-xylene	-2.9799E+01	6.8722E+02	5.2938E+00	-3.2605E-07	-2.4775E+06	340	475	1300	1179	8.0	0.8
369	1,2,3,5 Tetramethylbenzene	7.1404E+01	-1.3163E+04	-7.8927E+00	1.3286E-06	-6.7016E+05	449	515	1345	1222	9.6	0.4
370	1,2,4,5-Tetramethylbenzene	9.2028E+01	-1.5886E+04	-1.0592E+01	1.70558-06	-2.7704E+05	634	634	1335	1215	0.2	0.0
371	*n*-Pentylbenzene	5.9796E+01	- 1.0507E+04	-6.5266E+00	1.34808-06	-1.3374E+06	357	560	1345	1224	1.8	0.2
372	*n*-Hexylbenzene	1.0156E+01	-3.3984E+03	-1.1324E-01	5.9445E-07	-2.7424E+06	382	600	1380	1256	1.8	0.2
541	m-Diisopropylbenzene	-3.2576E+00	-5.3558E+03	2.1799E+00	-6.9405E-07	-1.4833E+06	378	450	1355	1231	0.5	0.1
542	p-Diisopropylbenzene	6.1845E+02	-9.2604E+04	-7.8451E+01	8.77908-06	1.1382E+07	461	580	1365	1240	3.7	0.8
373	*n*-Heptylbenzene	1.9594E+02	-3.1177E+04	-2.4005E+01	3.07878-06	1.4098E+06	405	640	1385	1285	2.0	0.2
374	*n*-Octylbenzene	4.7696E+02	-7.0777E+04	-6.0463E+01	7.4948E-06	7.0461E+06	427	560	1312	1312	7.4	0.7
384	Styrene	-1.6555E+00	- 2.5457E+03	1.5959E+00	1.8197E-07	-1.6733E+06	437	437	1260	1145	0.2	0.0
	alpha-Methylstyrene	1.0975E+03	-1.4791E+05	-1.4246E+02	2.1009E-05	1.8637E+07	450	530	1295	1177	8.3	1.6

Table 5A1.2 (Continued)

API ID	COMPOUND NAME	A	B	C	D	E	TPT	T_{min}	T_{max}	T_c	MAX% ERR	AVE % ERR
389	1-Methyl-3-ethenyl benzene	-2.1703E+03	2.5248E+05	2.9086E+02	-5.4092E-05	-3.3446E+07	336	515	1183	1183	1.7	0.4
388	1-Methyl-2-ethenyl benzene	-2.7461E+02	2.8475E+04	3.8134E+01	-6.8722E-06	-5.6163E+06	368	500	1305	1186	0.4	0.1
390	1-Methyl-4-ethenyl benzene	8.7244E+01	-1.5193E+04	-9.9434E+00	1.5044E-06	-6.2113E+04	430	530	1200	1197	1.1	0.3
375	*n*-Nonylbenzene	3.7849E+02	-5.8980E+04	-4.7432E+01	5.4828E-06	5.3461E+06	448	560	1440	1334	1.7	0.3
376	*n*-Decylbenzene	3.5173E-01	-1.9389E+03	1.1753E+00	2.3903E-07	-4.4175E+06	466	600	1490	1355	0.1	0.0
377	*n*-Undecylbenzene	1.1213E+02	- 2.3702E+04	-1.2607E+01	8.3827E-07	-1.7541E+05	482	690	1500	1375	1.2	0.2
378	*n*-Dodecylbenzene	2.1147E+02	-3.8097E+04	-2.5483E+01	2.4995E-06	1.8263E+06	497	600	1530	1394	10.5	1.7
379	*n*-Tridecylbenzene	4.4541E+02	-7.3142E+04	-5.5467E+01	5.3272E-06	6.8857E+06	510	150	1550	1409	2.0	0.4
342	Isopropylbenzene	3.5939E-01	-3.0770E+03	1.3672E+00	7.6358E-08	-1.6308E+06	319	410	1250	1136	3.9	0.2
348	1,3,5-Trimethylbenzene	2.5101E+01	-6.2916E+03	-1.9092E+00	7.3647E-07	-1.3395E+06	411	515	1260	1147	0.6	0.2
422	Ethynylbenzene	1.3790E+01	-8.3131E+03	0	0	0	411	558	1170	1170		
385	cis-1-Propenylbenzene	-1.1679E+02	8.4411E+03	1.7160E+01	-2.6842E-06	-2.7238E+06	381	530	1330	1208	1.9	0.1
386	trans-1-Propenylbenzene	1.4545E+01	-9.6346E+03	0	0	0	438	587	1206	1206		
544	m-Divinylbenzene	7.696413+02	-9.7506E+04	-1.0078E+02	1.8371E-05	1.0290E+07	371	545	1370	1246	7.5	1.6
395	2-Phenyl-1-butene	1.5035E+01	-1.0057E+04	0	0	0		624	1199	1199		
	DIAROMATICS AND OTHER HYDROCARBON RINGS											
383	Cyclohexylbenzene	6.0591E+02	-9.1917E+04	-7.6632E+01	8.0701E-06	1.0863E+07	504	510	1470	1339	4.4	0.9
184	cis-Decahydronaphthalene	5.2792E+01	-9.7044E+03	-5.6255E+00	1.2065E-06	-1.1190E+06	414	414	1385	1264	6.7	0.8
185	trans-Decahydronaphthalene	-9.3751E+01	8.9050E.03	1.3668E+01	1.6269E-06	-3.1603E+06	437	455	1360	1237	8.2	0.6
446	1,2,3,4-Tetrahydronaphthalene	1.4086E+.01	-5.7527E+03	-3.9853E-01	2.6827E-07	-1.6909E+06	427	427	1425	1296	5.6	1.2
466	Indane	1.1487E+02	-1.9191E+04	-1.3535E+01	1.9911E-06	5.4241E+09	399	560	1355	1233	0.9	0.2
463	Indene	2.0834E+01	-4.4476E+03	-1.5385E+00	8.8505E-07	-2.0178E+06	489	489	1360	1237	0.9	1.8
396	Biphenyl	1.9452E+02	-3.4314E+04	-2.3404E+01	2.3028E-06	2.4115E+06	616	630	1560	1421	11.8	1.7
427	Naphthalene	-2.4462E+01	-2.1250E+02	4.5702E+00	-2.9416E-07	-2.6466E+06	636	636	1480	1347	10.6	0.7
428	1-Methylnaphthalene	1.5216E+02	-2.7975E+04	-1.7999E+01	1.9032E-06	1.6998E+06	437	470	1530	1390	9.0	1.6
429	2-Methylnaphthalene	3.3276E+01	-8.4334E+03	-2.9343E+00	6.4520E-07	-1.7047E+06	554	554	1500	1370	2.6	0.2
553	2,6-Dimethylnaphthalene	-5.4115E+01	1.4314E+04	7.0441E+00	1.4163E-06	-7.3976E+06	690	690	1540	1399	0.1	0.0
554	2,7-Dimethylnaphthalene	7.0013E+01	-1.4772E+04	-7.5713E+00	9.9456E-07	-8.5093E+05	664	664	1540	1400	11.7	1.2
430	1-Ethylnaphthalene	3.6830E+01	-9.9996E+03	-3.2399E+00	3.6090E-07	-1.6319E+06	467	580	1535	1397	10.9	0.5
436	1-*n*-Butylnaphthalene	1.5741E+01	-1.3219E+04	0	0	0	456	696	1426	1426		
474	Anthracene	-3.6757E+02	6.3213E+04	4.7152E+01	-2.7038E-06	-1.7186E+07	880	885	1730	1571	5.6	0.5
479	Triphenylene	2.2720E+02	-5.1833E+04	-2.6517E+01	1.5260E-06	4.9532E+06	848	848	1783	1783	6.1	4.5

Table 5A1.2 (Continued)

API ID	COMPOUND NAME	A	B	C	D	E	TPT	T_{min}	T_{max}	T_c	MAX% ERR	AVE % ERR
480	Benzanthracene	2.2020E+02	-4.8606E+04	-2.5784E+01	1.4896E-06	4.0929E+06	780	780	1762	1762	0.1	0.1
482	Naphthacene	4.0745E+02	-9.0633E+04	-4.8509E+01	2.4366E-06	1.4798E+07	1134	1134	1777	1777	0.2	0.0
475	Phenanthrene	2.6281E+02	-4.7316E+04	-3.2012E+01	2.9491E-06	4.1851E+06	670	670	1720	1565	0.9	0.2
476	Pyrene	-3.6338E+01	1.4079E+03	5.8834E+00	0	-5.2642E+06	763	763	1850	1685	1.3	0.5
478	Chrysene	2.9931E+02	-6.5780E+04	-3.5427E+01	1.9395E-06	8.1802E+06	956	956	1762	1762	0.3	0.1
472	Acenaphthene	-5.7592E+01	2.5840E+03	8.9947E+00	-9.0751E-07	-3.4254E+06	660	660	1590	1446	0.1	0.0
473	Fluorene	7.3631E+02	-1.2307E+05	-9.2447E+01	9.2571E-06	1.8478E+07	698	765	1200	1566	1.9	0.4
183	Bicyclohexyl	4.1288E+02	-6.3964E+04	-5.1859E+01	5.8333E-06	7.0303E+06	498	535	1440	1309	0.8	0.3
473	Fluoranthene	1.2980E+02	-2.7058E+04	-1.5111E+01	1.6081E-06	6.4537E+05	690	690	1790	1629	0.6	0.2
420	cis-1,2-Diphenylethene	4.4801E+02	-7.0751E+04	-5.6152E+01	5.8022E-06	7.5281E+06	496	640	1550	1411	9.9	5.0
403	1,1-Diphenylethane	-3.8636E+02	5.4491E+04	5.0940E+01	-4.7364E-06	-1.2377E+07	459	640	1395	1395	1.3	0.4
404	1,2-Diphenylethane	-1.9555E+02	2.1198E+04	2.7021E+01	-3.1592E-06	-6.2984E+06	584	600	1404	1404	1.3	0.2
425	1,3-Diphenylbenzene	1.7843E+02	-3.7234E+04	-2.0875E+01	1.5510E-06	1.9698E+06	648	648	1830	1665	0.6	0.1
426	1,2-Diphenylbenzene	4.3879E+02	-8.0834E+04	-5.3736E+01	4.0377E-06	1.0677E+07	593	710	1760	1604	0.2	0.8
	AROMATIC AMINES											
746	Pyridine	4.6438E+01	-8.8989E+03	-4.6438E+00	1.0092E-06	-5.3724E+05	417	425	1200	1116	1.5	0.2
881	Isoquinoline	-2.8891E+01	-4.4146E+02	5.2051E+00	-3.7166E-07	-2.7598E+06	539	539	1565	1446	0.7	0.2
749	Quinoline	-5.3503E+01	5.4848E+03	8.1295E+00	-3.5963E-07	-4.1793E+06	465	545	1500	1408	0.5	0.2
750	Dibenzopyrrole	-1.2548E+03	2.4043E+05	1.5662E+02	-8.7255E-06	-5.7646E+11	932	932	1780	1618	3.8	0.8
751	Acridine	3.3950E+01	-1.3307E+04	-2.5771E+00	-4.8322E-08	-1.4544E+06	690	690	1629	1629	22.4	2.2
	OTHER AMINES											
748	Indole	3.0407E+02	-4.8684E+04	-3.7600E+01	3.7960E-06	3.8898E+06	493	505	1565	1422	11.7	1.6
	SULFUR COMPOUNDS											
891	Thiophene	4.5017E+01	-7.5427E+03	-4.6098E+00	1.3661E-06	-5.6175E+05	423	423	1125	1043	8.5	0.9
892	Tetrahydrothiophene	-9.1578E+00	-2.3512E+03	2.7316E+00	-3.1228E-07	-1.3177E+06	319	425	1250	1138	2.1	0.1
828	Methyl mercaptan	9.4479E+01	-1.0061E+04	-1.1680E+01	4.4715E-06	-6.4479E+04	270	325	930	846	14.6	3.1
776	Carbonyl sulfide	-4.1386E+01	1.9196E+03	7.2808E+00	-1.4956E-06	-6.6358E+05	242	242	750	682	7.3	1.5
831	Ethyl mercaptan	1.0346E+02	-1.3387E+04	-1.2516E+01	3.3404E-06	4.3498E+05	225	345	990	898	6.3	0.4

Table 5A1.2 (Continued)

API ID	COMPOUND NAME	A	B	C	D	E	TPT	T_{min}	T_{max}	T_c	MAX% ERR	AVE % ERR
	OXYGENATED COMPOUNDS											
709	Methanol	7.5938E+01	-1.2791E+04	-8.3164E+00	1.8644E-06	1.5234E+05	316	316	1015	923	5.9	0.7
710	Ethanol	1.4653E+02	-2.2041E+04	-1.7506E+01	2.7145E-06	1.1282E+06	286	350	1015	925	4.9	0.5
712	Isopropanol	3.6628E+01	-9.9305E+03	-2.6438E+00	-8.8636E-07	-3.9992E+05	334	334	1005	915	8.5	1.6
716	tert-Butanol	1.0610E+03	-1.2218E+05	-1.4068E+02	2.7969E-05	1.2121E+07	538	538	1000	911	11.5	1.4
766	Methyl tert-butyl ether	1.1704E+02	-1.5083E+04	-1.4339E+01	3.5469E-06	5.0444E+05	296	310	985	895	8.4	1.3
893	tert-Butyl ethyl ether	9.1566E+01	1.2885E+04	-1.0829E+01	2.6472E-06	1.7640E+05	322	322	1015	925	8.0	4.6
865	Diisopropyl ether	9.8330E+01	1.2567E+04	-1.1937E+01	3.4765E-06	5.0529E+04	338	338	990	900	23.5	2.7
767	Methyl tert-pentyl ether	1.0204E+02	-1.4571E+04	-1.2173E+01	2.6056E-06	3.5891E+05		285	1060	961	1.6	0.4

Procedure 5A1.3 – Alternate Calculation Procedure for the Vapor Pressures of Pure Compounds

Discussion

This procedure was last updated in 1994.The following alternative equation is recommended for calculating the vapor pressure of any pure compound over the temperature range specified for the compound. This equation is useful when an exact match at the critical point is desired.

$$\ln P_r = aX_1 + bX_2 + cX_3 + dX_4 \qquad (5A1.3\text{-}1)$$

Where:

$$X_1 = \frac{(1 - T_r)}{T_r} \qquad (5A1.3\text{-}2)$$

$$X_2 = \frac{(1 - T_r)^{1.5}}{T_r} \qquad (5A1.3\text{-}3)$$

$$X_3 = \frac{(1 - T_r)^{2.6}}{T_r} \qquad (5A1.3\text{-}4)$$

$$X_4 = \frac{(1 - T_r)^{5}}{T_r} \qquad (5A1.3\text{-}5)$$

T_r	=	*T/T_c = reduced temperature*
P_r	=	*P/P_c = reduced pressure*
T_c	=	*critical temperature, in °R*
P_c	=	*critical pressure, in psia*
T	=	*temperature, in °R*
P	=	*vapor pressure of compound, in psia*

Table 5A1.4 gives the coefficients for the above equation together with the applicable temperature range and the maximum and average percent errors from the comparison with the experimental data carried out during regressions. Compounds shown without coefficients had insufficient data to use this method.

Procedure

Step 1: *Obtain the critical temperature and pressure of the compound from The pure component properties tables.*

Step 2: *Calculate the reduced temperature at the desired conditions using the definitions above.*

Step 3: Use the coefficients in Table 5A1.4 in equations (5A1.3-1) through (5A1.3-5) to calculate the reduced vapor pressure within the range specified. Vapor pressure is calculated by multiplying the reduced vapor pressure by the critical pressure.

Comments on Procedure 5A1.3

Purpose

This alternate procedure is to be used to calculate the vapor pressure of specific compounds as a function of temperature.

Limitations

This procedure is valid over the temperature limits listed in Table 5A1.4. The procedure will exactly match the critical temperature and pressure used in the equation. *However, the equation cannot be extrapolated to temperatures above the critical point.*

Special Comments

The vapor pressures calculated by this procedure in the experimental data range are generally consistent with the vapor pressure plots for common compounds of Figures 5A1.5 through 5A1.15.

Note the errors given in the correlation coefficient tables when using this procedure.

The triple point temperature and critical temperature listed in Table 5A1.4 are taken from the 1992 version of the pure component properties tables. Therefore, slight discrepancies may be found for some compounds.

Literature Sources

Procedure 5A1.3 is a linearized form of the Wagner (341) method developed by Shen-Tu (294). It has been tested by the project staff at the Pennsylvania State University and evaluated by the API Technical Data Committee.

Example

Determine the vapor pressure of *n*-octane at a temperature of 100 °F.

The necessary parameters are obtained from Table 5A1.4 for *n*-octane (compound number 36).

a	=	*–8.0092*
b	=	*1.8442*
c	=	*–3.2907*
d	=	*–3.5457*

From the pure component properties tables, T_c = 563.99 °F. The reduced temperature is:

$$T_r = \frac{T}{T_c} = \frac{559.7°R}{1023.66°R} = 0.5467$$

Using equations (5A1.3-2) through (5A1.3-5)

X_1	=	*0.82904*
X_2	=	*0.55815*
X_3	=	*0.23374*
X_4	=	*0.034993*

Using equation (5A1.3-1)

$$\ln P_r = -6.5039$$

$$P_r = 0.001498$$

From the pure component properties tables, the critical pressure is 361.1 psia. Therefore, the predicted vapor pressure is

$$P = 0.001498 \times 361.1\ psi = 0.5409\ psia$$

The experimental value listed in the pure component properties tables is 0.5373 psia.

Table 5A1.4 – Coefficients for Procedure 5A1.3

API ID	COMPOUND NAME	A	B	C	D	TPT	T_{min}	T_{max}	T_c	MAX% ERR	AVE % ERR
794	Oxygen	-6.0896E+00	1.3376E+00	-8.4623E-01	-1.2860E+00	98	98	278	278	2.0	0.2
781	Hydrogen	-4.7322E+00	5.5473E-01	1.5353E+00	-1.1391E+00	25	25	60	60	6.0	0.8
845	Water	-7.8310E+00	1.7399E+00	-2.2505E+00	-1.9828E+00	492	492	1165	1165	0.4	0.0
792	Nitrogen dioxide	-1.1099E+01	1.5091E+00	2.6896E+00	-8.2478E+00	471	471	776	776	2.9	0.3
790	Nitric oxide	-8.9298E+00	2.0806E+00	-4.5693E+00	-7.1463E+00	197	197	324	324	6.0	0.8
791	Nitrous oxide	-6.6642E+00	1.2408E+00	-1.5644E+00	-2.6768E+00	328	328	557	557	9.3	1.5
771	Ammonia	-6.9459E+00	6.7727E-01	-8.4450E-01	-3.3340E+00	352	352	730	730	1.2	0.4
777	Chlorine	-5.5127E+00	-5.7031E-01	7.2610E-01	-3.6002E+00	310	310	751	751	2.8	0.5
783	Hydrogen chloride	-6.2600E+00	1.0205E-01	1.0793E+00	-4.8162E+00	286	286	584	584	4.6	0.6
786	Hydrogen sulfide	-5.7185E+00	-4.9282E-01	1.0044E+00	-4.5547E+00	338	338	672	672	7.3	1.0
774	Carbon monoxide	-6.2604E+00	1.5811E+00	-1.5740E+00	-9.4265E-01	123	123	239	239	10.1	0.9
775	Carbon dioxide	-6.9903E+00	1.3912E+00	-2.2046E+00	-3.3649E+00	390	390	548	548	0.8	0.1
796	Sulfur dioxide	-6.8929E+00	1.3119E+00	-3.5225E+00	-6.8654E-01	356	365	775	775	3.8	1.7
	PARAFFINS										
1	Methane	-5.9999E+00	1.2027E+00	-5.3098E-01	-1.3447E+00	163	163	343	343	0.1	0.0
2	Ethane	-6.4812E+00	1.4042E+00	-1.2166E+00	-1.7143E+00	163	163	550	550	0.1	0.0
3	Propane	-6.8092E+00	1.6377E+00	-1.8173E+00	-1.8094E+00	154	154	666	666	2.7	0.9
4	*n*-Butane	-7.0524E+00	1.6779E+00	-2.0398E+00	-2.0630E+00	243	243	765	765	6.5	0.4
5	Isobutane	-6.7710E+00	1.0669E+00	-9.2013E-01	-3.8903E+00	204	225	735	735	1.6	1.2
6	*n*-Pentane	-7.2048E+00	1.3503E+00	-1.5540E+00	-4.2828E+00	258	282	845	845	6.5	0.8
7	Isopentane	-7.1383E+00	1.5320E+00	-1.8896E+00	-2.7290E+00	204	320	829	829	0.3	0.1
8	Neopentane	-6.9677E+00	1.5464E+00	-1.9563E+00	-2.6057E+00	462	462	781	781	3.2	0.2
9	*n*-Hexane	-7.3505E+00	9.2745E-01	-7.3208E-01	-6.7135E+00	320	320	913	913	5.8	1.0
10	2-Melhylpenlane	-7.2196E+00	1.1799E+00	-1.8207E+00	-3.4355E+00	215	360	896	896	4.5	0.2
11	3-Melhylpenlane	-7.5334E+00	1.9625E+00	-2.4600E+00	-3.3503E+00	198	360	908	908	4.8	0.8
12	2,2-Dimethylbutane	-6.3510E+00	-5.6836E-01	6.2620E-01	-5.6283E+00	314	365	880	880	0.3	0.1
13	2,3-Dimethylbutane	-7.4163E+00	2.0361E+00	-2.6077E+00	-2.5619E+00	261	330	900	900	1.9	0.2
14	*n*-Heptane	-7.4103E+00	7.2958E-01	-1.3081E+00	-5.9210E+00	329	329	972	972	4.6	0.4

Table 5A1.4 (Continued)

API ID	COMPOUND NAME	A	B	C	D	TPT	T_{min}	T_{max}	T_c	MAX% ERR	AVE % ERR
15	2-Methylhexane	-7.6340E+00	1.6113E+00	-2.4895E+00	-3.7538E+00	279	400	955	955	1.9	0.2
16	3-Methylhexane	-7.5791E+00	1.5257E+00	-2.2947E+00	-3.9555E+00	277	410	963	963	4.9	0.3
20	2,4-Dimethylpentane	-7.4134E+00	1.3732E+00	-2.9030E+00	-3.9837E+00	277	380	936	936	2.8	0.3
18	2,2-Dimethylpentane	-7.9269E+00	2.9114E+00	-3.9363E+04	-1.6685E+00	269	350	937	937	0.9	0.1
19	2,3-Dimethylpentane	-7.5582E+00	1.8933E+00	-2.9051E+00	-2.1990E+00		365	967	967	11.5	0.6
21	3,3-Dimethylpentane	-7.4396E+00	1.8922E+00	-2.6619E+00	-2.2083E+00	250	345	966	966	3.2	0.2
22	2,2,3-Trimethylbutane	-7.2314E+00	1.5238E+00	-2.0270E+00	-3.1147E+00	447	447	956	956	0.9	0.1
17	3-Ethylpentane	-7.4995E+00	1.5385E+00	-2.4277E+00	-3.4699E+00	278	390	973	973	0.6	0.1
23	*n*-Octane	-8.0092E+00	1.8442E+00	-3.2907E+00	-3.5457E+00	389	515	1024	1024	3.1	0.3
28	2,2-Dimethylhexane	-7.5996E+00	1.4415E+00	-2.3822E+00	-4.2077E+00	274	425	990	990	0.7	0.1
29	2,3-Dimethylhexane	-7.6339E+04	1.3702E+00	-1.1946E+00	-4.4756E+00		505	1014	1014	0.5	0.1
30	2,4-Dimethylhexane	-7.6060E+00	1.3858E+00	-2.3160E+00	-4.2674E+00		500	996	996	0.6	0.1
31	2,5-Dimethylhexane	-7.7783E+00	1.6637E+00	-2.6848E+00	-4.0525E+00	328	460	990	990	0.9	0.1
32	3,3-Dimethylhexane	NOT APPLICABLE									
33	3,4-Dimethylhexane	-7.6399E+00	1.5311E+00	-2.4620E+00	-3.8625E+00		515	1024	1024	0.4	0.1
24	2-Methylheptane	-7.9107E+00	1.8799E+00	-3.4029E+00	-2.7230E+00	295	375	1007	1007	1.9	0.2
25	3-Methylheptane	-7.9117E+00	1.9291E+00	-3.3038E+00	-3.0229E+00	275	390	1015	1015	2.7	0.1
26	4-Methylheptane	-7.8699E+00	1.7730E+00	-3.0201E+00	-3.6452E+00	274	450	1011	1011	0.8	0.1
37	2,2,4-Trimethylpentane	-7.4717E+00	1.5074E+00	-2.2532E+00	-3.5291E+00	298	405	979	979	5.0	0.3
36	2,2,3-Trimethylpentane	-7.4620E+00	1.5755E+00	-2.3591E+00	-3.4372E+00	290	390	1014	1014	0.5	0.1
38	2,3,3-Trimethylpentane	-7.4312E+00	1.5376E+00	-2.1927E+00	-3.2220E+00	310	440	1032	1032	0.6	0.1
39	2,3,4-Trimethylpentane	-7.6819E+00	1.9464E+00	-2.9862E+00	-2.4654E+00	295	360	1019	1019	2.1	0.2
40	2,2,3,3-Tetramethylbutane	NOT APPLICABLE									
27	3-Ethylhexane	-7.8126E+00	1.7109E+00	-2.8235E+00	-3.7955E+00		510	1018	1018	0.6	0.1
34	2-Methyl-3-ethylpentane	-7.6293E+00	1.6051E+00	-2.5337E+00	-3.6245E+00	285	450	1021	1021	0.6	0.1
35	3-Methyl-3-ethylpentane	-7.5992E+00	1.7830E+00	-2.4927E+00	-3.0867E+00	328	400	1038	1038	0.2	0.1
41	*n*-Nonane	-9.5734E+00	5.7040E+00	-8.9745E+00	3.3386E+00	395	420	1072	1072	3.9	0.6
42	2-Methyloctane	-9.4111E+00	5.6052E+00	-9.1179E+00	3.9544E+00	347	545	1056	1056	1.4	0.3
43	3-Melhyloctane	-8.3900E+00	2.6425E+00	-4.2868E+00	-3.0994E+00	298	485	1062	1062	1.8	0.4
44	4-Melhyloctane	-7.5061E+00	1.1774E+01	-5.4096E-01	-8.9404E+00	288	440	1058	1058	3.2	0.8

Table 5A1.4 (Continued)

API ID	COMPOUND NAME	A	B	C	D	TPT	T_{min}	T_{max}	T_c	MAX% ERR	AVE % ERR
46	2,2-Dimethylheptane	-8.3130E+00	2.8225E+00	-4.7470E+00	-1.1444E+00	288	460	1038	1038	3.9	0.4
47	2,6-Dimethylheptane	-8.7147E+00	4.1852E+00	-7.9870E+00	2.4437E+00	306	460	1042	1042	2.6	0.4
55	3,3-Diethylpentane	-7.5953E+00	1.2707E+00	-1.7405E+00	-4.3033E+00	432	432	1098	1098	0.1	0.0
50	2,2,5-Trimethylhexane	-7.3528E+00	6.0866E+01	-1.5526E+00	-5.6168E+00	301	450	1022	1022	0.1	0.0
53	2,4,4-Trimethylhexane	-7.9562E+00	2.1012E+00	-2.9705E+00	-3.3584E+00	288	440	1046	1046	0.2	0.0
58	2,2,3,3-Tetramethylpentane	-6.6669E+04	-1.3750E-01	-6.1430E+01	-5.1209E+00	474	474	1100	1100	0.1	0.0
59	2,2,3,4-Tetramethylpentane	-7.1800E+00	6.9628E-01	-1.4066E+00	-4.6793E+00	274	425	1066	1066	0.2	0.0
60	2,2,4,4-Tetramethylpentane	-7.2701E+00	8.5893E-01	-1.5987E+00	-4.5870E+00	373	460	1028	1028	0.1	0.0
61	2,3,3,4-Tetramethylpentane	-7.3160E+00	9.8271E-01	-1.6426E+00	-4.1716E+00	308	450	1094	1094	0.1	0.0
45	3-Ethylheptane	-5.9957E+00	-3.3308E+00	2.5136E+00	-9.1893E+00	285	460	1062	1062	4.0	0.7
56	2,2-Dimethyl-3-ethylpentane	-9.4211E+00	6.5025E+00	-9.2966E+00	4.1670E+00	313	440	1062	1062	1.7	0.3
57	2,4-Dimethyl-3-ethylpentane	-8.0840E+00	2.4302E+00	-3.3816E+00	-3.5183E+00	271	450	1064	1064	1.6	0.4
62	*n*-Decane	-8.4734E+00	2.0043E+00	-3.9338E+00	-4.5270E+00	438	515	1113	1113	3.8	0.5
63	2-Methylnonane	-7.7440E+00	-1.6747E-02	-4.7601E+01	-1.0900E+01	357	500	1098	1098	2.3	0.4
64	3-Methylnonane	-8.9914E+00	3.7850E+00	-6.5288E+00	-4.7406E-02	339	485	1103	1103	2.3	0.4
65	4-Methylnonane	-8.6347E+00	2.7567E+00	-5.0510E+00	-1.4461E+00	314	470	1098	1098	2.3	0.4
66	5-Methylnonane	-7.4288E+00	-8.7050E+00	1.3069E+00	-1.4122E+01	334	500	1098	1098	1.7	0.3
501	2,2-Dimethyloctane	-7.1779E+00	-6.5430E+00	-5.7430E-01	-7.0784E+00		570	1084	1084	1.7	0.8
73	*n*-Undecane	-8.6767E+00	1.8339E+00	-3.6173E+00	-6.5674E+00	446	580	1150	1150	4.2	0.2
74	*n*-Dodecane	-9.1638E+00	2.8127E+00	-5.5268E+00	-4.1247E+00	474	530	1185	1185	5.4	0.2
75	*n*-Tridecane	-1.1558E+01	9.5675E+00	-1.7808E+01	2.3910E+01	482	600	1216	1216	3.2	1.5
76	*n*-Tetradecane	-9.5592E+00	2.6739E+00	-5.3261E+00	-7.2218E+00	502	665	1246	1246	0.4	0.1
77	*n*-Pentadecane	-9.8836E+00	2.9809E+00	-5.8999E+00	-7.3690E+00	510	690	1272	1272.0	0.2	0.1
78	*n*-Hexadecane	-1.0158E+01	3.4349E+00	-7.2350E+00	-4.7220E+00	524	530	1297	1297	5.9	0.3
79	*n*-Heptadecane	-8.7518E+00	-1.2524E+00	6.3922E-01	-2.1323E+01	531	560	1320	1320	4.9	0.7
80	*n*-Octadecane	-1.1302E+01	6.3651E+00	-1.2451E+01	2.7902E-01	542	580	1341	1341	6.6	1.9
81	*n*-Nonadecane	-1.0079E+01	2.7305E+00	-7.8556E+00	-5.3836E+00	550	720	1361	1361	2.8	0.5
82	*n*-Eicosane	-9.2912E+00	7.3641E-01	-8.1737E+00	-4.5461E-01	557	635	1381	1381	8.0	1.2
86	*n*-Tetracosane	-1.4429E+01	1.2024E+01	-2.1555E+01	1.1216E+01	583	805	1458	1458	4.0	0.8
90	*n*-Octacosane	-1.1449E+01	2.0664E+00	-7.4138E+00	1.5477E+01	602	750	1517	1517	5.7	1.2

Table 5A1.4 (Continued)

API ID	COMPOUND NAME	A	B	C	D	TPT	T_{min}	T_{max}	T_c	MAX% ERR	AVE % ERR
	NAPHTHENES										
101	Cyclopentane	-7.2042E+00	2.2227E+00	-2.8579E+00	-1.2980E+00	323	365	921	921	3.9	0.6
102	Methylcyclopentane	-7.1157E+00	1.5063E+00	-2.0252E+00	-2.9670E+00	235	320	959	959	2.0	0.1
103	Ethylcyclopentane	-7.2608E+00	1.3487E+00	-1.8819E+00	-3.7286E+00	242	330	1025	1025	1.5	0.1
104	1,1-Dimethylcyclopentane	-7.4646E+00	1.5596E+00	-1.2479E+00	-5.1494E+00	366	366	985	985	1.2	0.4
105	cis-1,2-Dimethylcyclopentane	-7.2375E+00	1.2744E+00	-1.5586E+00	-4.1959E+00	395	450	1017	1017	0.2	0.0
106	trans-1,2-Dimethylcyclopentane	-7.3997E+00	1.5794E+00	1.7321E+00	-4.1363E+00	280	360	996	996	0.3	0.0
107	cis-1,3-Dimethylcyclopentane	-3.3344E+00	-8.9599E+00	1.0303E+01	-1.5107E+01	251	330	992	992	3.5	1.3
108	trans-1,3-Dimethylcyclopentane	-7.5680E+00	2.0220E+00	-2.2671E+00	-3.5069E+00	251	360	995	995	0.4	0.0
109	*n*-Propylcyclopentane	-6.0536E+00	-1.3961E+00	2.3830E-01	-5.7723E+00	280	440	1085	1085	0.1	0.0
110	Isopropylcyclopentane	-8.1892E+00	3.3014E+00	-4.2468E+00	-1.3269E+00	291	414	1067	1067	2.1	0.5
146	Cyclohexane	-7.0110E+00	1.5792E+00	-2.2610E+00	-2.4011E+00	503	503	996	996	4.3	0.7
147	Methylcyclohexane	-7.1204E+00	1.4340E+00	-1.9015E+00	-3.3273E+00	264	390	1030	1030		0.2
148	Ethylcyclohexane	-8.1385E+00	2.9387E+00	-3.3728E+00	-2.5752E+00	291	291	1087	1087	2.4	0.4
149	1,1-Dimethycyclohexane	-6.2907E+00	-4.3323E-01	-3.4330E-01	-4.8567E+00	431	485	1064	1064	0.2	0.0
150	cis-1,2-Dimethylcylohexane	-5.9784E+00	-1.0686E+00	-9.1999E-02	-4.8359E+00	402	470	1091	1091	0.3	0.0
151	trans-1,2-Dimethylcyclohexane	-6.2918E+00	-4.6416E-01	-4.3416E-01	-4.4298E+00	333	440	1073	1073	0.3	0.0
152	cis-1,3-Dimethylcyclohexane	-6.1474E+00	-7.3699E-01	-3.4479E-01	-4.5670E+00	356	460	1064	1064	0.5	0.0
153	trans-1,3-Dimethylcyclohexane	-5.9773E+00	-1.0532E+00	-1.9120E-01	-4.8365E+00	329	460	1076	1076	1.4	0.1
154	cis-1,4-Dimethylcyclohexane	-5.9207E+00	-1.1984E+00	4.9520E-02	-5.0241E+00	334	400	1077	1077	0.1	0.0
155	trans-1,4-Dimethylcyclohexane	-6.2135E+00	-6.7727E-01	-1.1209E-01	-4.9714E+00	425	425	1062	1062	0.3	0.0
156	*n*-Propylcyclohexane	-7.7909E+00	1.7018E+00	-2.6649E+00	-3.0125E+00	321	321	1129	1129	2.1	0.4
157	Isopropylcyclohexane	-7.8041E+00	2.0024E+00	-2.8297E+00	-3.4032E+00	331	375	1129	1129	3.5	0.1
158	*n*-Butylcyclohexane	-7.9517E+00	1.7251E+00	-3.1034E+00	-3.2207E+00	357	357	1170	1170	1.7	0.4
163	*n*-Pentylcyclohexane	-8.3175E+00	1.8554E+00	-3.1882E+00	-3.6684E+00	382	382	1205	1205	10.7	1.2
164	*n*-Hexylcyclohexane	-8.9066E+00	2.7450E+00	-4.5050E+00	-3.4153E+00	406	406	1236	1236	3.5	0.7
166	*n*-Octylcyclohexane	-9.1014E+00	1.7971E+00	-3.7743E+00	-4.1296E+00	448	448	1292	1292	5.0	1.6
168	*n*-Decylcyclohexane	-1.0751E+01	4.7710E+00	-7.1455E+00	-4.0370E+00	488	488	1339	1339	5.1	0.8
179	Cycloheptane	-7.3231E+00	1.8407E+00	-2.2637E+00	-3.4498E+00	477	477	1088	1088	0.7	0.1
180	Cyclooctane	-7.7603E+00	2.2756E+00	-2.7048E+00	-3.3449E+00	518	518	1152	1152	2.3	0.2
111	1-Methyl-1-ethylcyclopentane	-8.6283E+00	3.8981E+00	-4.4013E+00	-1.6947E+00	233	330	1048	1048	1.7	0.1

Table 5A1.4 (Continued)

API ID	COMPOUND NAME	A	B	C	D	TPT	T_{min}	T_{max}	T_c	MAX% ERR	AVE % ERR
	OLEFINS										
192	Ethylene	-6.3778E+00	1.3298E+00	-1.1667E+00	-2.0209E+00	187	187	508	508	8.9	0.6
193	Propylene	-6.7920E+00	1.7836E+00	-2.0451E+00	-1.5370E+00	158	158	658	658	5.2	0.3
194	1-Butene	-6.9041E+00	1.3587E+00	-1.3839E+00	-3.7388E+00	158	225	756	756	2.4	0.5
195	cis-2-Butene	-5.6603E+00	-2.4078E+00	4.1414E+00	-1.2357E+01	242	410	784	784	2.7	0.5
196	trans-2-Butene	-5.8093E+00	-2.3370E+00	4.3312E+00	-1.1290E+01	302	440	772	772	2.4	0.5
197	Lsobutene	-6.9577E+00	1.5333E+00	-1.7919E+00	-3.1555E+00	139	310	752	752	5.9	1.5
198	1-Pentene	-6.6117E+00	7.2041E-02	2.8003E-04	-5.4313E+00	194	300	837	837	6.5	0.3
199	cis-2-Pentene	-7.0402E+00	1.0734E+00	-1.3928E+00	-4.2267E+00	219	345	855	855	0.1	0.0
200	trans-2-Pentene	-7.0624E+00	1.0993E+00	-1.4920E+00	-3.5048E+00	239	330	854	854	0.2	0.0
201	2-Methyl-1-butene	-6.2824E+00	-5.3623E-11	1.0768E-01	-5.3009E+00	244	345	837	837	1.6	0.2
203	2-Methyl-2-butene	-6.7790E+00	-5.0865E-02	-7.6497E-02	-4.5105E+00	251	320	848	848	4.8	0.4
202	3-Methyl-1-butene	-7.5385E+00	2.4642E+00	-2.7102E+00	-2.1163E+00	188	280	811	811	0.4	0.0
204	1-Hexene	-7.0432E+00	6.6593E-01	-1.1001E+00	-4.6837E+00	240	410	907	907	0.1	0.0
205	cis-2-Hexene	-6.1989E+00	-1.1327E+00	1.1080E-01	-3.9506E+00	238	345	923	923	1.8	0.1
206	trans-2-Hexene	-6.3219E+00	-6.9647E-01	-1.8343E-01	-5.1568E+00	252	375	923	923	0.3	0.0
207	cis-3-Hexene	-7.3370E+00	1.6018E+00	-2.6743E+00	-2.4128E+00	244	345	916	916	1.4	0.2
208	trans-3-Hexene	-7.1677E+00	1.1247E+00	-2.2739E+00	-2.7112E+00	288	350	916	916	1.9	0.2
209	2-Methyl-1-pentene	-6.1749E+00	-7.7941E-01	-1.0829E-01	-5.1637E+00	247	375	913	913	0.1	0.0
212	2-Methyl-2-pentene	-5.8685E+00	-1.4501E+00	1.4690E-01	-4.8744E+00	249	330	925	925	0.1	0.0
210	3-Methyl-1-pentene	-8.1907E+00	3.6301E+00	-3.9140E+00	-1.7788E+00	216	300	891	891	1.0	0.1
213	cis-3-Methyl-2-pentane	-6.6132E+00	6.7872E-02	-1.0110E+00	-3.3631E+00	249	345	927	927	1.6	0.2
211	4-Methyl-1-pentene	-6.7536E+00	-4.9179E-01	-9.6829E-01	-4.0163E+00	215	360	893	893	0.3	0.0
215	cis-4-Methyl-pentane	-6.5083E+00	-1.0529E-01	-5.1997E-01	-4.8199E+00	249	375	898	898	0.3	0.0
214	trans-4-Methyl-2-pentene	-6.3717E+00	-5.3834E-01	-1.7498E-01	-4.9325E+00	238	320	902	902	0.0	0.0
220	2,3-Dimethyl-2-butene	-5.3711E+00	2.4854E+00	1.0360E+00	-5.4731E+00	358	425	943	943	0.2	0.0
218	2,3-Dimethyl-1-butene	-6.1707E+00	-6.5957E-01	-1.2203E-01	-4.5305E+00	209	345	900	900	0.2	0.0
219	3,3-Dimethyl-1-butene	-7.0054E+00	1.0865E+00	-8.9787E-01	-5.4246E+00	284	375	864	864	0.6	0.1
217	2-Ethyl-1-butene	-5.1486E+00	-2.9578E+00	1.0517E+05	-5.1585E+00	255	375	922	922	0.3	0.0
221	1-Heptene	-7.3881E+00	9.8515E-01	-1.0789E+05	-4.4550E+00	278	390	967	967	2.7	0.1

Table 5A1.4 (Continued)

API ID	COMPOUND NAME	A	B	C	D	TPT	T_{min}	T_{max}	T_c	MAX% ERR	AVE % ERR
222	cis-2-Heptene	-7.7327E+00	2.5399E+00	-4.1801E+00	-4.3588E-01	295	360	988	988	3.2	0.3
223	trans-2-Heptene	-7.0747E+00	-2.8493E-01	6.6695E-01	-7.4489E+00	295	425	977	977	2.7	0.4
224	cis-3-Heptene	-6.4089E+00	1.0834E+00	7.5264E-01	-7.4601E+00	246	410	981	981	2.8	0.5
225	trans-3-Heptene	-8.5703E+00	3.8880E+00	-5.0094E+00	-1.2593E+00	246	390	972	972	3.4	0.5
226	2-Methyl-1-hexene	-8.9261E+00	5.5300E+00	-8.0614E+00	3.7861E+00	307	410	968	968	2.8	0.4
227	3-Methyl-1-hexene	-5.6609E+00	-3.3325E+00	3.8975E+00	-1.1505E+01	261	425	950	950	3.7	0.5
228	4-Methyl-1-hexene	-7.4476E+00	1.5406E+00	-2.5204E+00	-3.7526E+00	237	390	961	961	2.1	0.4
241	2-Ethyl-1-pentene	-5.1843E+00	-4.9345E+00	6.8783E+00	-1.6294E+01	302	450	977	977	2.0	0.6
242	3-Ethyl-1-pentene	-7.3213E+00	1.3386E+00	-2.6381E+00	-2.8113E+00	262	410	954	954	2.0	0.5
256	2,3,3-Trimethyl-1-butene	-6.7721E+00	5.4902E-01	-1.0611E+00	-4.3662E+00	294	415	956	956	0.2	0.0
257	1-Octene	-7.4840E+00	6.5826E-01	-1.5963E+00	-5.3229E+00	309	450	1020	1020	1.8	0.1
259	trans-2-Octene	-9.2337E+00	6.0185E+00	-8.8635E+00	4.4257E+00	334	334	1039	1039	3.6	0.4
261	trans-3-Octene	-7.5839E+00	1.4573E+00	-2.8339E+00	-2.3495E+00	294	365	1033	1033	2.6	0.7
263	trans-4-Octene	-6.9197E+00	-4.4603E-01	2.3423E-01	-8.1553E+00	323	485	1031	1031	2.7	0.4
269	2-Ethyl-1-hexene	-8.5361E+00	2.8257E+00	-2.6560E+00	-4.4395E+00		515	1033	1033	1.6	0.7
276	2,4,4-Trimethyl-1-pentene	-6.4322E+00	-4.4727E-01	-6.2444E-01	-4.6331E+00	323	460	995	995	5.2	0.3
277	2,4,4-Trimethyl-2-pentene	-5.5337E+00	-2.4617E+00	9.9019E-01	-6.6826E+00	300	475	1004	1004	0.3	0.0
278	1-Nonene	-7.5932E+00	5.4163E-01	-1.8725E+00	-5.6752E+00	345	425	1068	1068	0.1	0.0
279	1-Decene	-8.0511E+00	1.1002E+00	-2.5630E+00	-6.3981E+00	372	440	1111	1111	2.5	0.2
280	1-Undecene	-7.9898E+00	5.1187E-02	-7.4932E-01	-1.0880E+01	403	515	1148	1148	1.3	0.2
281	1-Dodecene	-8.7446E+00	1.5336E+00	-3.0453E+00	-8.4121E+00	428	165	1183	1183	2.5	0.2
282	1-Tridecene	-1.1880E+01	1.0130E+01	-1.6477E+01	1.2024E+01	450	560	1215	1215	1.2	0.5
283	1-Tetradecene	-9.3064E+00	2.1364E+00	-4.4706E+00	-7.6343E+00	469	580	1246	1246	2.8	0.2
284	1-Pentadecene	-9.9234E+00	3.5165E+00	-7.0033E+00	-3.7698E+00	485	690	1274	1274	0.9	0.1
285	1-Hexadecene	-1.2067E+01	9.3320E+00	-1.6469E+01	1.1060E+01	500	590	1300	1300	1.8	0.4
286	1-Heptadecene	-1.0367E+01	3.4425E+00	-5.6927E+00	-1.2503E+01	512	698	1325	1325	4.9	1.1
287	1-Octadecene	-7.6489E+00	-5.1771E+00	7.3975E+00	-3.4050E+01	523	630	1346	1346	3.2	0.5
288	1-Nonadecene	-1.0665E+01	3.5702E+00	-7.7410E+00	-6.7841E+00	534	750	1368	1368	0.2	0.0
289	1-Eicosene	-1.0681E+01	3.1302E+00	-7.1951E+00	-9.0428E+00	543	720	1388	1388	0.6	0.1
310	Cyclopentene	-7.0012E+00	1.5627E+00	-1.7049E+00	-2.8503E+00	249	300	913	913	0.3	0.1

Table 5A1.4 (Continued)

API ID	COMPOUND NAME	A	B	C	D	TPT	T_{min}	T_{max}	T_c	MAX% ERR	AVE % ERR
315	Cyclohexene	-6.4299E+00	-1.1783E-01	2.0202E-01	-5.4665E+00	305	360	1009	1009	0.9	0.2
511	Cycloheptene	4.3108E-01	-1.7050E+01	1.6693E+01	-1.4823E+01	391	455	1076	1076	2.8	2.7
512	Cyclooctene	-1.5655E+01	1.8012E+05	-1.2686E+01	-2.1927E+00	385	485	1138	1138	2.7	0.7
	DIOLEFINS AND ACETYLENES										
318	Cyclopentadiene					NOT APPLICABLE					
292	1,3-Butadiene	-6.8720E+00	1.3005E+00	-1.3957E+00	3.2192E+00	296	296	765	765	4.1	0.7
299	2-Methyl-1,3-butadiene	-5.6062E+00	-9.7723E-01	-3.3583E-01	-3.1876E+00	229	280	871	871	0.3	0.1
298	3-Methyl-1,2-butadiene	-5.8803E+00	-5.7620E-01	-1.0669E+00	-2.7695E+00	287	320	882	882	0.6	0.0
293	1,2-Pentadiene	-5.1992E+00	-1.6766E+00	-3.2254E-01	-3.2839E+00	245	245	900	900	0.4	0.1
294	cis-1,3-Pentadiene	-5.2454E+00	-1.4339E+00	-6.8396E-01	-2.8231E+00	238	310	898	898	1.1	0.1
295	trans-1,3-Pentadiene	-4.5958E+00	-2.5675E+00	3.1282E-01	-3.2227E+00	334	334	900	900	0.2	0.0
296	1,4-Pentadiene	-4.0365E+00	-3.5363E+00	1.3981E+00	-4.4192E+00	225	300	862	862	0.4	0.0
297	2,3-Pentadiene	-6.2683E+00	-2.4076E-02	-1.6313E+00	-2.7310E+00	266	320	895	895	0.3	0.0
521	1,3-Cyclohexadiene	-8.4177E+00	4.5254E+00	-4.6981E+00	-1.1653E+00	290	340	1004	1004	6.8	0.6
300	2,3-Dimethyl-1,3-butadiene	-6.3186E+00	5.2374E-01	-1.4003E+00	-2.9240E+00	355	355	947	947	0.9	0.1
302	1,5-Hexadiene	-6.6008E+00	-4.0775E-01	1.6305E+00	-9.6753E+00	238	390	913	913	0.4	0.0
522	trans,trans-2,4-Hexadiene	-7.5544E+00	2.0044E+00	-2.9647E+00	-2.3653E+00	411	485	963	963	1.9	0.2
523	1,5-Cyclooctadiene	-9.1295E+00	4.8970E+00	-3.1453E+00	-1.0016E+01	367	530	1161	1161	0.1	0.0
322	Acetylene	-7.3515E+00	2.8334E+00	-4.5075E+00	6.8797E+00	346	346	555	555	2.4	0.4
323	Methylacetylene	-6.8198E+00	6.2814E-01	-8.7570E-02	-6.4802E+00	307	307	724	724	2.4	0.7
324	Dimethylacetylene	-6.7151E+00	4.2405E-01	-9.8214E-01	-3.3768E+00	434	434	852	852	1.0	0.1
329	3-Methyl-1-butyne	-1.0962E+01	9.9462E+00	-1.0571E+01	4.0170E+00	330	400	834	834	4.3	0.5
327	1-Pentyne	-5.9051E+00	-2.7123E+00	3.7780E+00	-9.0588E+00	301	390	866	866	3.2	0.4
330	1-Hexyne	-1.1230E+01	1.0667E+01	-1.2715E+01	6.9563E+00	254	410	929	929	5.1	1.0
527	2-Hexyne	-5.6510E+00	1.7686E+00	8.2944E-01	-6.5244E+00	331	450	988	988	1.8	0.3
528	3-Hexyne	-5.4448E+00	2.0711E+00	4.2961E-01	-3.9197E+00	306	425	979	979	3.9	0.7
	AROMATICS										
335	Benzene	-7.0200E+00	1.5156E+00	-1.9176E+00	-3.5572E+00	502	502	1012	1012	1.6	0.3
336	Toluene	-7.2827E+00	1.5031E+00	-2.0743E+00	-3.7867E+00	321	440	1065	1065	3.0	0.3
337	Ethylbenzene	-7.5640E+00	1.7919E+00	-2.7040E+00	-2.8573E+00	321	425	1111	1111	0.8	0.1

Table 5A1.4 (Continued)

API ID	COMPOUND NAME	A	B	C	D	TPT	T_{min}	T_{max}	T_c	MAX% ERR	AVE % ERR
339	m-Xylene	-7.6212E+00	1.6059E+00	-2.4451E+00	-3.0594E+00	406	450	1111	1111	3.9	0.2
338	o-Xylene	-7.5579E+00	1.5648E+00	-2.1826E+00	-3.7093E+00	446	446	1135	1135	2.2	0.2
340	p-Xylene	-7.6935E+00	1.8093E+00	-2.5583E+00	-3.0662E+00	516	516	1109	1109	7.5	0.4
341	*n*-Propylbenzene	-8.1015E+00	2.6607E+00	-3.8585E+00	-2.2594E+00	312	425	1149	1149	5.4	0.4
346	1,2,3-Trimelhylbenzene	-7.4913E+00	6.2868E-01	-1.0417E+00	-5.5342E+00	446	515	1196	1196	0.2	0.0
347	1,2,4-Trimethylbenzene	-7.6149E+00	8.8278E-01	-1.5384E+00	-4.7733E+00	413	500	1168	1168	23.7	0.9
344	m-Ethyltoluene	-5.9342E+00	-2.2037E+00	5.9188E-01	-5.9740E+00	320	470	1147	1147	0.4	0.0
343	o-Ethyltoluene	-5.5289E+00	-2.8119E+00	1.2261E+00	-6.4558E+00	346	475	I172	I172	0.4	0.0
345	p-Ethyltoluene	-6.4310E+00	-1.1241E+00	-1.2471E-01	-5.8434E+00	379	515	1152	1152	17.0	1.4
349	*n*-Butylbenzene	-7.8413E+00	1.3055E+00	-2.1437E+00	-5.3415E+00	334	420	1189	1189	5.6	0.7
350	Isobutylbenzene	-8.4004E+00	2.6812E+00	-3.1159E+00	-4.2596E+00	399	515	1170	1170	0.2	0.0
351	sec-Butylbenzene	-4.9441E+00	-4.1279E+00	3.0215E+00	-8.9473E+00	356	530	1196	1196	4.9	0.3
352	tert-Butylbenzene:	-4.7469E+00	-4.5257E+00	3.5334E+00	-9.8554E+00	387	530	1188	1188	0.8	0.1
360	m-Diethylbenzene	-6.3664E+00	-1.5853E+00	2.4398E-01	-6.9613E+00	341	530	1193	1193	1.3	0.1
359	o-Diethylbenzene	-6.3395E+00	-1.4802E+00	5.6585E-02	-6.6393E+00	435	560	1202	1202	0.1	0.0
361	p-Diethylbenzene	-7.7679E+00	9.9952E-01	-1.8941E+00	-5.4073E+00	415	530	1184	1184	0.1	0.0
357	m-Cymene	-8.7809E+00	4.8080E+00	-7.3692E+00	2.0767E+00	377	515	1183	1183	2.7	0.6
356	o-Cymene	-8.8998E+00	5.3860E+00	-8.7555E+00	5.3964E+00	363	460	1192	1192	3.1	0.6
358	p-Cymene	-7.5169E+00	6.5892E-01	-1.1893E+00	-6.2957E+00	369	460	1176	1176	7.6	1.4
364	2-Ethyl-m-xylene	-8.3739E+00	2.5427E+00	-3.7674E+00	-3.2834E+00	462	500	1208	1208	0.6	0.1
367	2-Ethyl-p-xylene	-9.6717E+00	6.2146E+00	-9.2875E+00	4.6701E+00	395	475	1193	1193	3.4	0.8
362	3-Ethyl-o-xylene	-6.2583E+00	-2.0086E+00	6.8240E-01	-7.1221E+00	403	500	1224	1224	0.2	0.1
365	4-Ethyl-m-xylene	-8.9146E+00	4.0730E+00	-6.8716E+00	2.8183E+00	378	470	1197	1197	6.3	0.7
363	4-Ethyl-o-xylene	-7.9716E+00	1.5168E+00	-2.8418E+00	-3.8267E+00	371	470	1201	1201	1.6	0.2
366	5-Ethyl-m-xylene	-6.9990E+00	-1.1790E+00	6.5061E-01	-7.6435E+00	340	455	1179	1179	18.3	1.5
368	1,2,3,5-Tetramethylbenzene	-8.0497E+00	1.4665E+00	-2.5356E+00	-4.5508E+00	449	500	1222	1222	9.6	0.4
370	1,2,4,5-Tetramethylbenzene	-8.3177E+00	1.9813E+00	-3.0463E+00	-4.1731E+00	634	634	1215	1215	0.2	0.0
371	*n*-Pentylbenzene	-8.7573E+00	3.1808E+00	-4.7169E+00	-2.7442E+00	357	560	1224	1224	2.8	0.2
372	*n*-Hexylbenzene	-8.4600E+00	6.7918E-01	-1.4190E+00	-8.1068E+00	382	600	1256	1256	1.8	0.2
541	m-Diisopropylbenzene	-5.4715E+00	-3.3390E+00	3.6774E-01	-4.7440E+00	378	500	1231	1231	0.6	0.1

Table 5A1.4 (Continued)

API ID	COMPOUND NAME	A	B	C	D	TPT	T_{min}	T_{max}	T_c	MAX% ERR	AVE % ERR
542	p-Diisopropylbenzene	-1.3754E+01	1.7938E+01	-2.5589E+01	2.0693E+01	461	600	1240	1240	3.9	0.7
373	*n*-Heptylbenzene	-9.1822E+00	3.1454E+00	-4.8927E+00	-4.5218E+00	405	640	1285	1285	2.0	0.2
374	*n*-Octylbenzene	-1.0776E+01	7.0482E+00	-1.0593E+01	1.7304E+00	427	560	1312	1312	8.0	0.8
384	Styrene	-6.3281E+00	-1.2630E+00	9.9196E-01	-7.1282E+00	437	437	1145	1145	0.6	0.1
	alpha-Methylstyrene	-1.1323E+01	1.2568E+01	-1.9239E+01	2.0119E+01	450	530	1177	1177	7.0	1.5
389	1-Methyl-3-ethenyl-benzene	-5.6636E+00	-3.8811E+00	4.2823E+00	-1.1503E+01	336	575	1183	1183	2.1	0.4
388	1-Methyl-2-ethenyl-benzene	-5.5721E+00	-3.4497E+00	2.3418E+00	-7.4058E+00	368	500	1186	1186	0.4	0.1
390	1-Methyl-4-ethenyl-benzene	-7.5520E+00	1.7146E+00	-3.0985E+00	-2.9725E+00	430	530	1197	1197	1.1	0.3
375	*n*-Nonylbenzene	-1.1122E+01	7.0038E+00	-1.0406E+01	1.1027E+00	448	560	1334	1334	1.4	0.4
376	*n*-Decylbenzene	-1.0549E+01	4.7502E+00	-7.2424E+00	-4.8469E+00	466	600	1355	1355	0.1	0.0
377	*n*-Undecylbenzene	-1.1895E+01	8.0001E+00	-1.2700E+01	4.6027E+00	482	690	1375	1375	1.1	0.2
378	*n*-Dodecylbenzene	-1.0665E+01	3.9860E+00	-7.6855E+00	-1.7721E+00	497	600	1187	1394	9.6	1.8
379	*n*-Tridecylbenzene	-1.1995E+01	6.5968E+00	-1.0188E+01	-5.2923E+00	510	750	1409	1409	2.1	0.4
342	Isopropylbenzene	-7.4655E+00	1.2449E+00	-2.0897E+00	-4.5973E+00	319	410	1136	1136	2.6	0.3
348	1,3,5-Trimethylbenzene	-7.6060E+00	5.3442E-01	-1.0779E+00	-5.7032E+00	411	515	1147	1147	0.6	0.2
422	Ethynylbenzene	NOT APPLICABLE									
385	cis-1-Propenylbenzene	-4.8237E+00	-5.1208E+00	3.3915E+00	-3.8942E+00	381	530	1208	1208	1.9	0.1
386	trans-1-Propenylbenzene	NOT APPLICABLE									
544	m-Divinylbenzene	-2.7274E+00	-1.0970E+01	1.0252E+01	-1.1111E+01	371	545	1246	1246	7.7	1.6
395	2-Phenyl-1-butene	NOT APPLICABLE									
	DIAROMATICS AND OTHER HYDROCARBON RINGS										
383	Cyclohexylbenzene	-9.1251E+00	5.6604E+00	-9.2892E+00	1.4443E+00	504	510	1339	1339	8.1	1.7
184	cis-Decahydronaphthalene	-7.4537E+00	1.3277E+00	-1.2850E+00	-5.9559E+00	414	414	1264	1264	8.0	2.3
185	trans-Decahydronaphthalene	-5.3297E+00	-3.0836E+00	2.4871E+00	-8.0759E+00	437	455	1237	1237	8.2	2.2
446	1,2,3,4-Tetrahydronaphthalene	-7.4138E+00	9.5219E-01	-1.5111E+00	-4.9487E+00	427	427	1296	1296	5.8	1.2
466	Indane	-7.9473E+00	2.5993E+00	-3.3754E+00	-2.5820E+00	399	560	1233	1233	0.9	0.2
463	Indene	-7.3215E+00	4.3264E-01	1.4899E-01	-8.5690E+00	489	489	1237	1237	0.9	1.9
396	Biphenyl	-8.5399E+00	3.7956E+00	-5.8547E+00	-8.3965E-01	616	630	1421	1421	11.5	1.7
427	Naphthalene	-7.6159E+00	1.8626E+00	-2.6125E+00	-3.1447E+00	636	636	1347	1347	17.5	0.8
428	1-Methylnaphthalene	-7.4654E+00	1.3322E+00	-3.4401E+00	-8.8543E-01	437	470	1390	1390	7.1	1.7

Table 5A1.4 (Continued)

API ID	COMPOUND NAME	A	B	C	D	TPT	T_{min}	T_{max}	T_c	MAX% ERR	AVE % ERR
429	2-Methylnaphthalene	-7.6745E+00	1.0179E+00	-1.3791E+00	-5.6038E+00	554	554	1370	1370	7.8	0.6
553	2,6-Dimethylnaphthalene	-7.8198E+00	-2.5419E+00	9.2934E+00	-2.4313E+01	690	690	1399	1399	0.1	0.0
554	2,7-Dimethylnaphthalene	-7.8916E+00	1.0662E+00	-1.8808E+00	-4.9046E+00	664	664	1400	1400	11.7	1.2
430	1-Ethylnaphthalene	-6.7968E+00	-5.5457E-01	-1.2844E+00	-5.4126E+00	467	580	1397	1397	11.1	0.6
436	1-*n*-Butylnaphthalene				NOT APPLICABLE						
474	Anthracene	-8.4533E+00	1.3409E+00	-1.5302E+00	-3.9310E+00	880	880	1571	1571	5.6	0.5
479	Triphenylene	-9.5923E+00	2.4964E+00	-5.1726E+00	-1.8676E+00	848	848	1783	1783	6.1	4.5
480	Benzanthracene	-8.8675E+00	2.3610E+00	-5.7836E+00	-1.8583E+00	780	780	1762	1762	0.1	0.1
482	Naphthacene	-8.8114E+00	2.1305E+00	-4.9584E+00	-5.1349E+00	1134	1134	1777	1777	0.2	0.0
475	Phenanthrene	-1.1662E+01	9.2590E+00	-1.0005E+01	1.2110E+00	670	670	1565	1565	1.0	0.2
476	Pyrene	-7.3955E+00	-1.6482E+00	1.8265E+00	-8.9049E+00	763	763	1685	1685	1.3	0.5
478	Chrysene	-9.2117E+00	2.7463E+00	-6.1751E+00	-1.6216E+00	956	956	1762	1762	0.3	0.1
472	Acenaphthene	-5.8667E+00	-3.2015E+00	1.6783E+00	-5.8469E+00	660	660	1446	1446	0.1	0.0
473	Fluorene	-2.3696E+00	-1.1306E+01	1.0045E+01	-8.1711E+00	698	765	1566	1566	1.7	0.5
183	Bicyclohexyl	-1.1096E+01	9.2231E+00	-1.2163E+01	5.7764E+00	498	535	1309	1309	0.9	0.4
477	Fluoranthene	-1.0694E+01	5.0480E+00	-3.8812E+00	-3.2495E+00	690	690	1629	1629	0.5	0.1
420	cis-1,2-Diphenylethene	-1.6355E+01	2.2016E+01	-2.6080E+01	1.3526E+01	496	540	1411	1411	17.2	5.3
403	1,1-Diphenylethane	-6.8373E-01	-1.7889E+01	1.9724E+01	-2.5417E+01	459	540	1395	1395	1.3	0.4
404	1,2-Diphenylethane	2.1716E+00	-2.2786E+01	1.9828E+01	-1.8348E+01	584	500	1404	1404	1.3	0.2
425	1,3-Diphenylbenzene	-9.5472E+00	3.7483E+00	-5.9589E+00	-2.0600E+00	648	548	1665	1665	1.6	0.3
424	1,2-Diphenylbenzene	-1.1823E+01	1.0865E+01	-1.4519E+01	7.5084E+00	593	710	1604	1604	5.7	0.9
	OTHER AMINES										
746	Pyridine	-6.9178E+00	9.2986E-01	-1.5331E+00	-3.6922E+00	417	425	1116	1116	1.5	0.2
881	Isoquinoline	-6.4830E+00	-7.3169E-01	-4.0328E-02	-4.5232E+00	539	539	1446	1446	2.4	0.3
749	Quinoline	-9.4950E+00	-9.7476E-01	1.5978E+00	-9.3554E+00	465	545	1408	1408	1.9	0.3
750	Dibenzopyrrole	-2.7066E+00	-1.5130E-01	2.2936E+01	-4.7490E+01	932	932	1618	1618	3.4	0.6
751	Acridine	-8.8512E+00	3.4212E+00	-4.8462E+00	-1.8217E+00	690	690	1629	1629	20.2	3.3
	OTHER AMINES										
748	Indole	-7.4931E+00	6.7402E+00	-1.3857E+00	-8.9991E+00	493	505	1422	1422.0	9.8	1.8

Table 5A1.4 (Continued)

API ID	COMPOUND NAME	A	B	C	D	TPT	T_{min}	T_{max}	T_c	MAX% ERR	AVE % ERR
	SULFUR COMPOUNDS										
891	Thiophene	-6.8088E+04	1.0914E+00	-1.1804E+00	-4.4000E+00	423	423	1043	1043	8.4	1.0
892	Tetrahydrothiophene	-6.1636E+00	-4.0400E-01	-9.4974E-02	-4.4263E+00	319	425	1138	1138	4.1	0.3
828	Methyl mercaptan	-6.6009E+00	8.0053E-01	2.1229E-01	-7.4341E+00	270	325	846	846	8.9	3.1
776	Carbonyl sulfide	-6.0631E+00	1.3742E-02	1.2110E+00	-5.6358E+00	242	242	682	682	7.2	1.6
831	Ethyl mercaptan	-7.4669E+00	2.9937E+00	-3.8026E+00	-3.8666E-01	225	300	898	898	6.1	0.4
	OXYGENATED COMPOUNDS										
709	Methanol	-8.6413E+00	1.0671E+00	-2.3184E+00	-1.6780E+00	316	316	923	923	5.9	0.7
710	Ethanol	-8.6857E+00	1.0212E+00	-4.9694E+00	1.8866E+00	286	350	925	925	4.9	0.4
712	Isopropanol	-7.9087E+00	-6.2263E-01	-4.8301E+00	3.8280E-01	334	360	915	915	8.4	1.6
716	tert-Butanol	-7.8116E+00	1.2665E-01	-5.8089E+00	-1.0038E+01	538	538	911	911	11.5	1.4
766	Methyl tert-butyl ether	-7.8925E+00	3.3001E+00	-4.9399E+00	2.2419E-01	296	310	895	895	8.0	1.3
893	tert-Butyl ethyl ether	-6.1886E+00	-1.0802E+00	-9.2815E-01	-2.9318E+00	322	322	925	925	8.7	4.8
865	Diisopropyl ether	-7.2695E+00	4.4887E-01	-9.4746E-01	-5.2803E+00	338	338	900	900	22.7	2.7
767	Methyl tert-pentyl ether	-7.8502E+00	2.8081E+00	-4.5318E+00	-3.2519E+00		285	961	961	1.3	0.4

Figure 5A1.5 – Vapor Pressure of Normal Paraffin Hydrocarbons- High Temperature Range

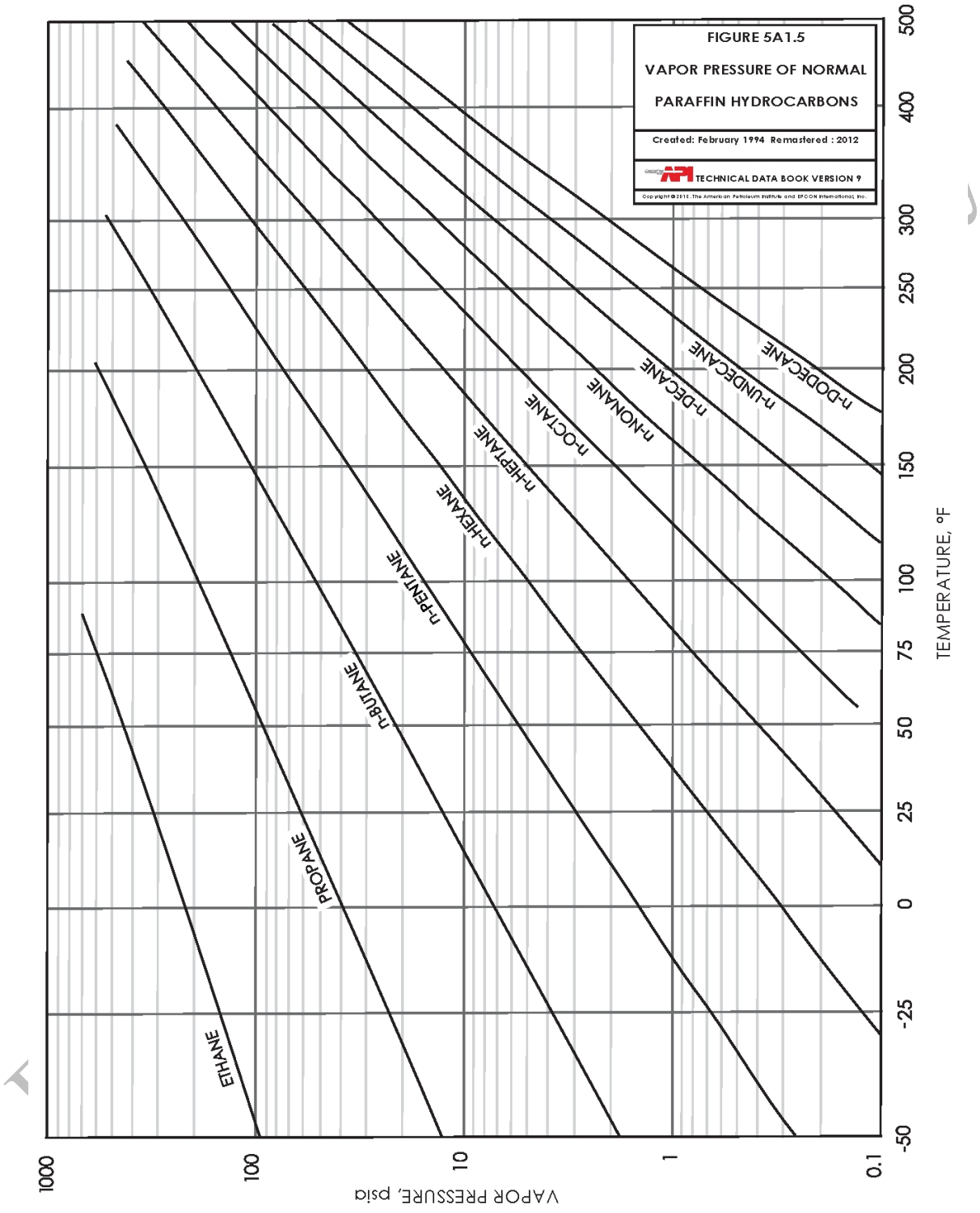


Figure 5A1.6 – Vapor Pressure of Branched Paraffin Hydrocarbons

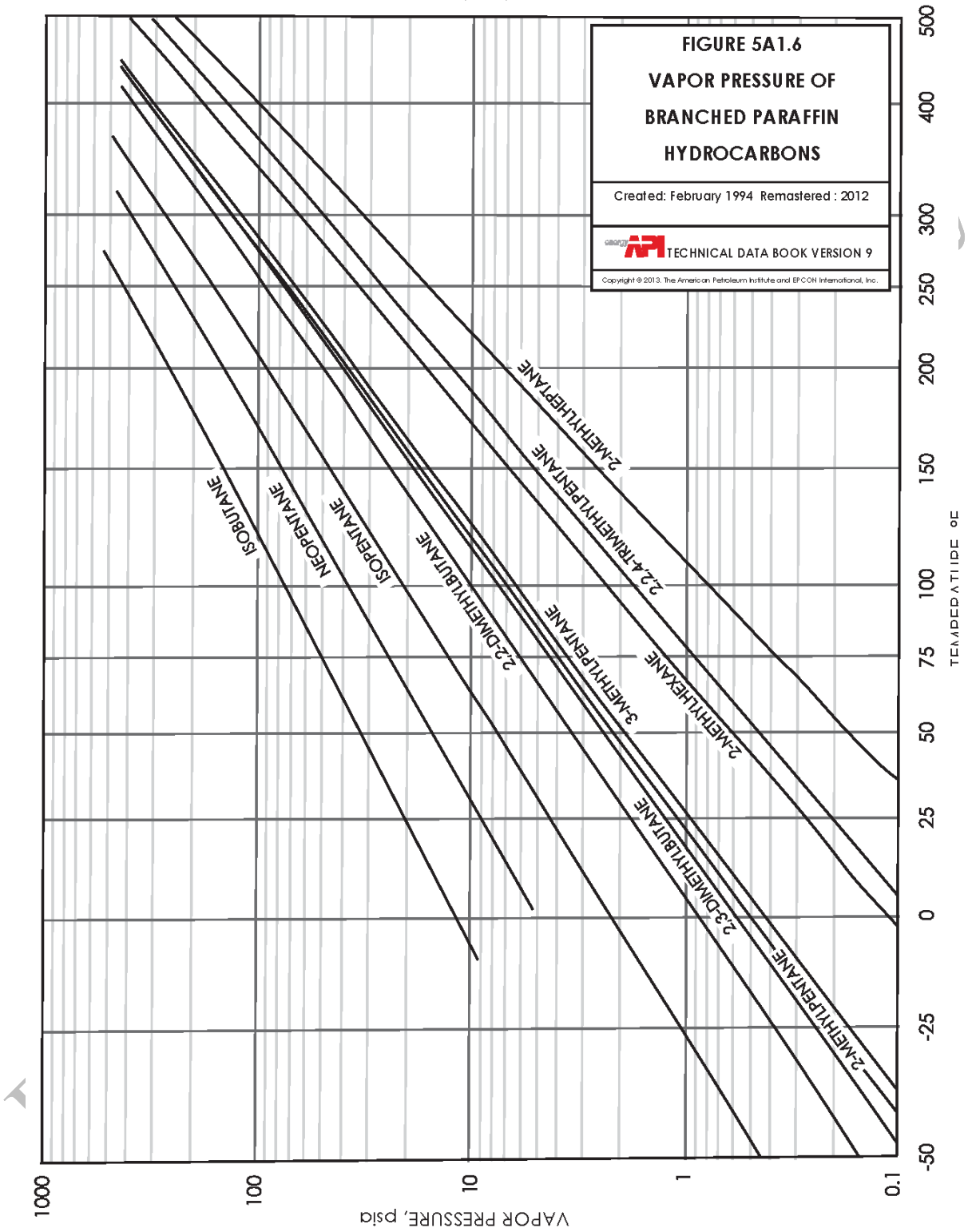


Figure 5A1.7 – Vapor Pressure of Paraffin Hydrocarbons – Low Temperature Range

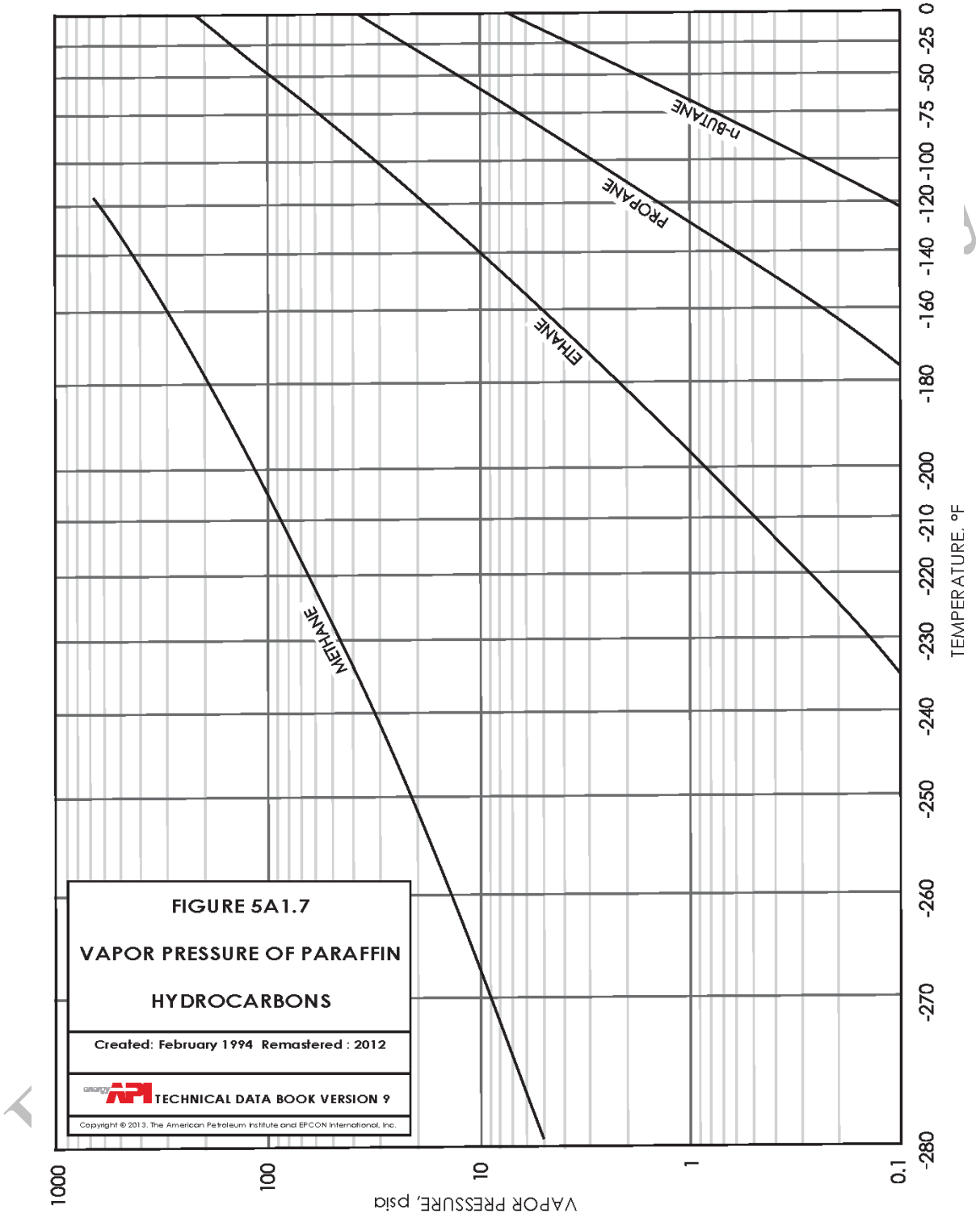


Figure 5A1.8 – Vapor Pressure of Naphthene Hydrocarbons

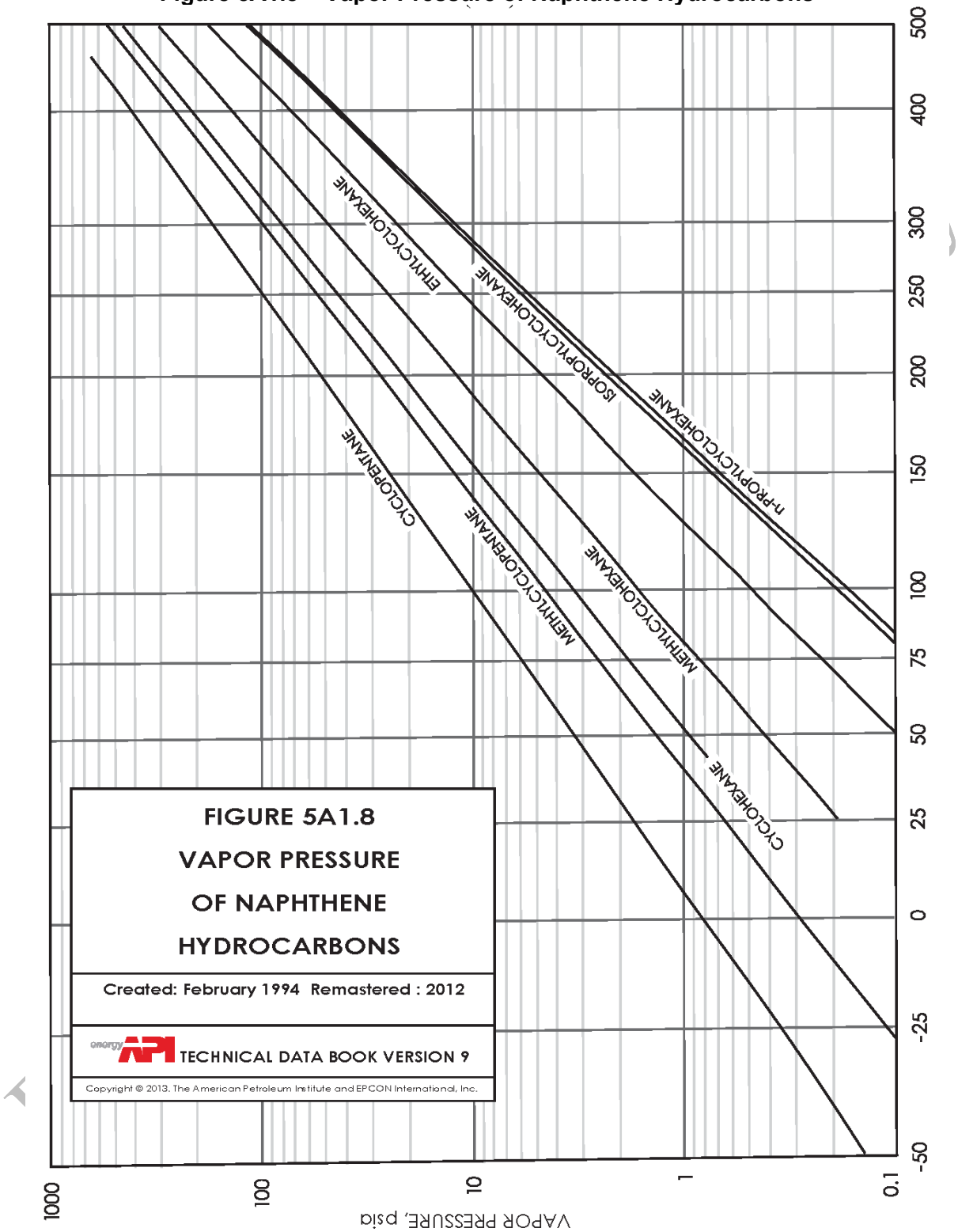


Figure 5A1.9 – Vapor Pressure of Olefin Hydrocarbons

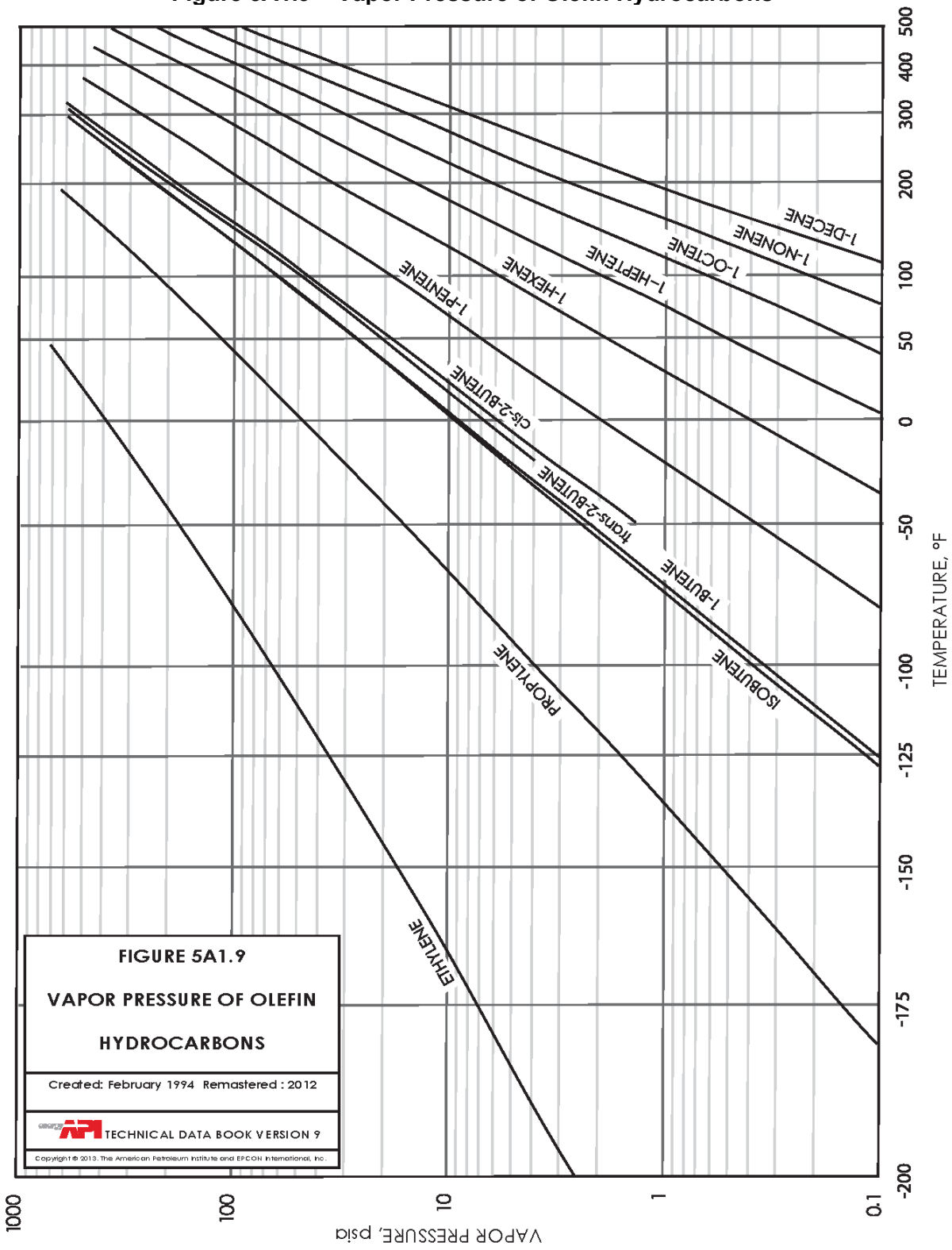


Figure 5A1.10 – Vapor Pressure of Diolefin, Cycloolefin, and Acetylene Hydrocarbons

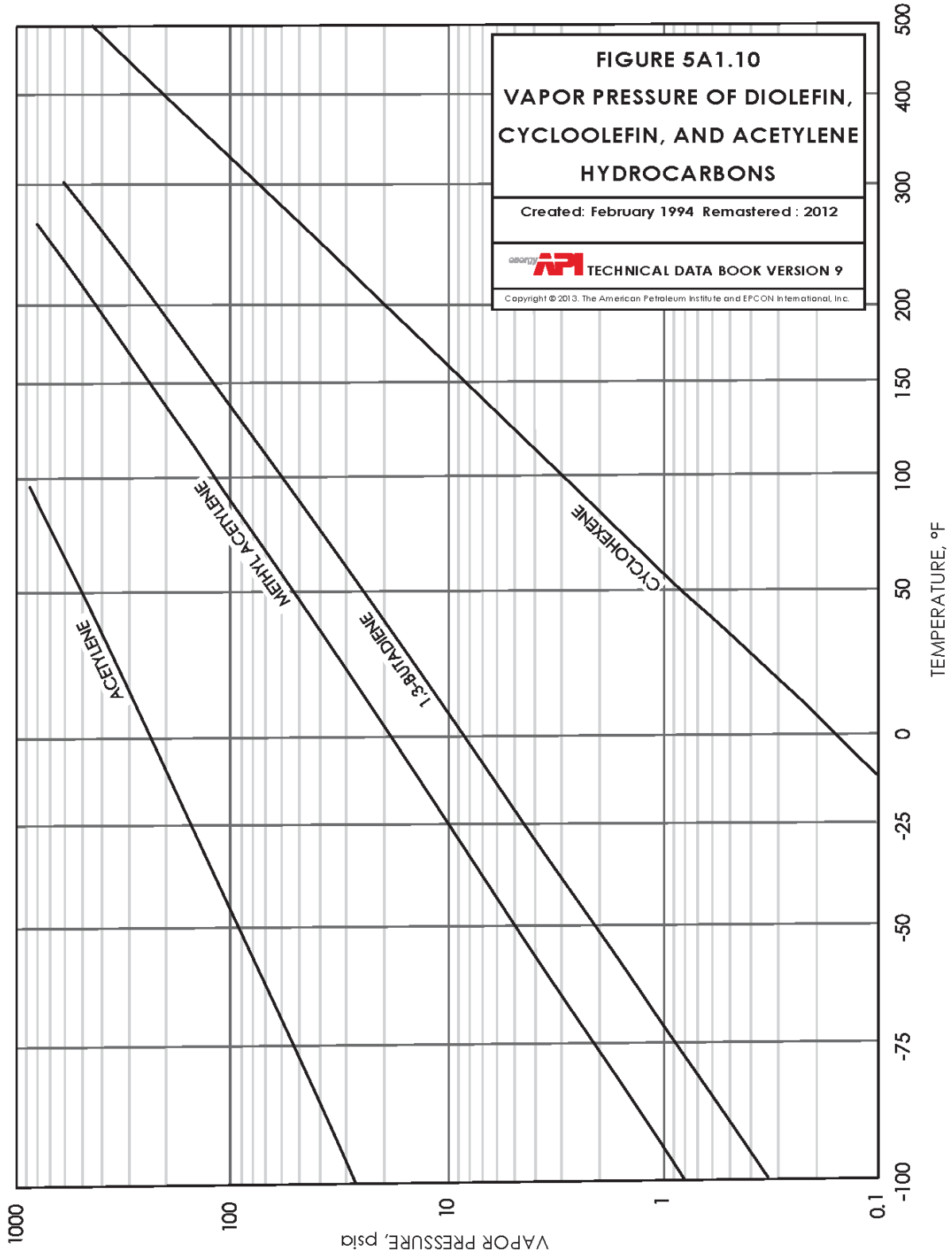


Figure 5A1.11 – Vapor Pressure of Lighter Unsaturated Hydrocarbons

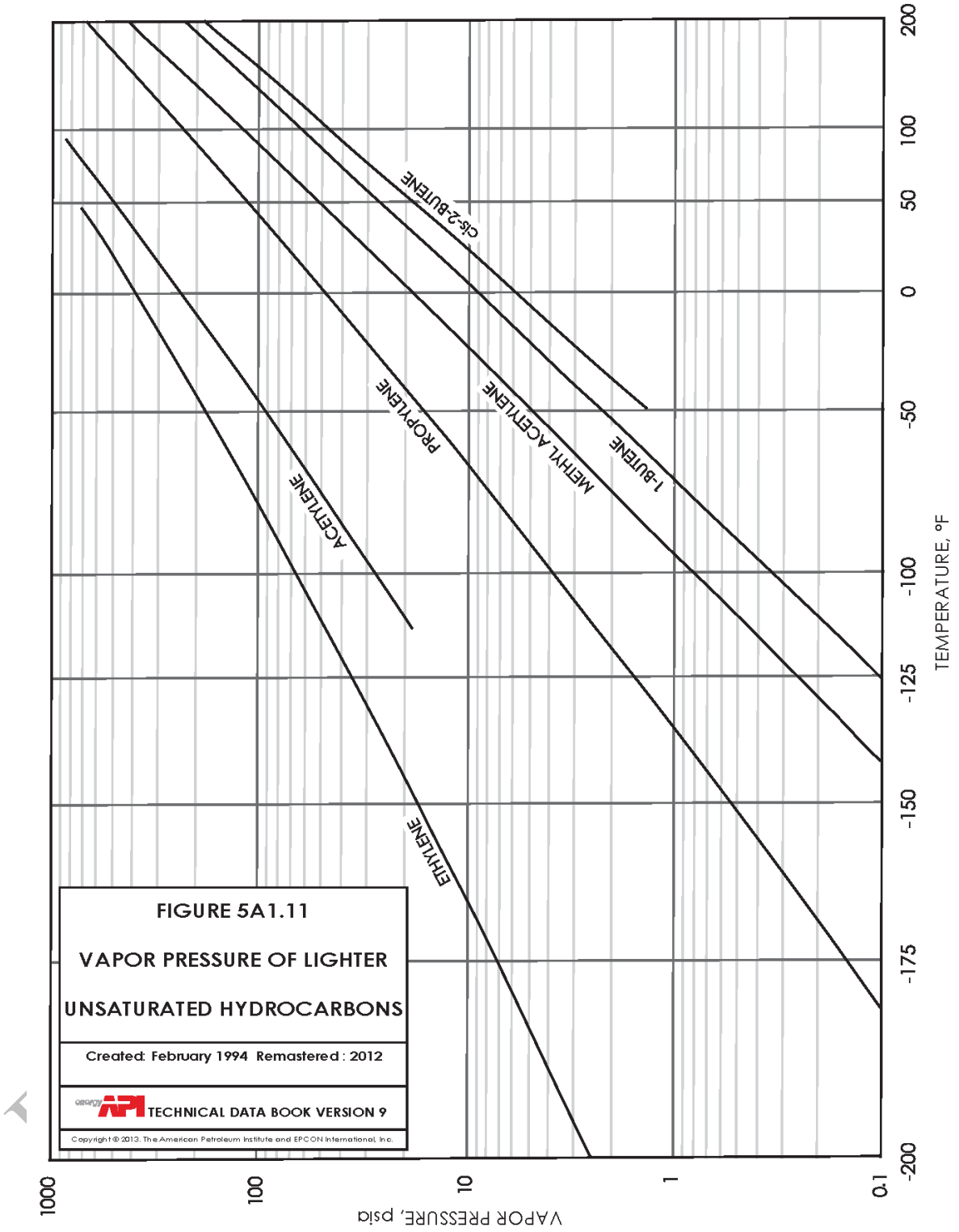


Figure 5A1.12 – Vapor Pressure of Alkylbenzene Hydrocarbons

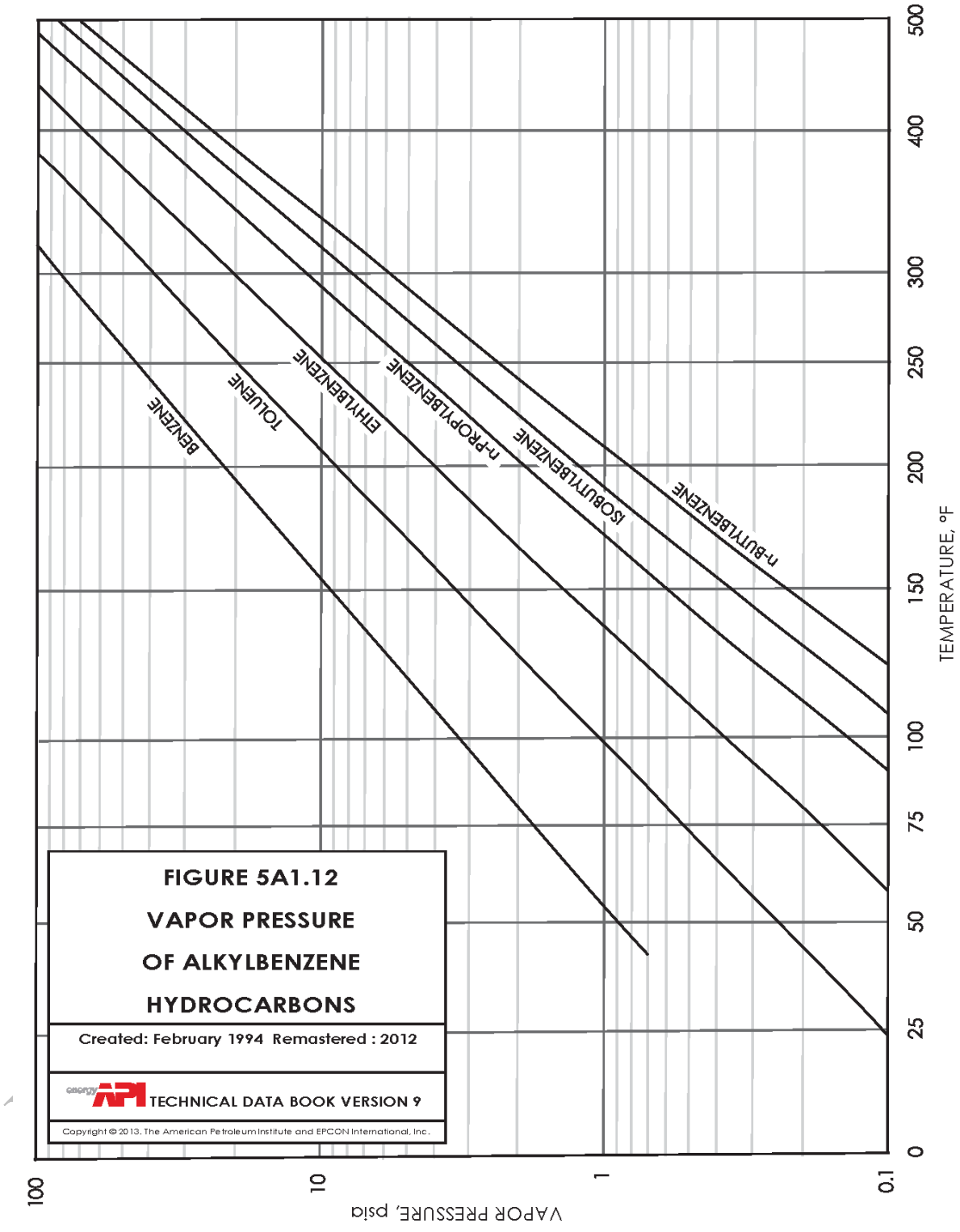


Figure 5A1.13 – Vapor Pressure of Miscellaneous Aromatic Hydrocarbons

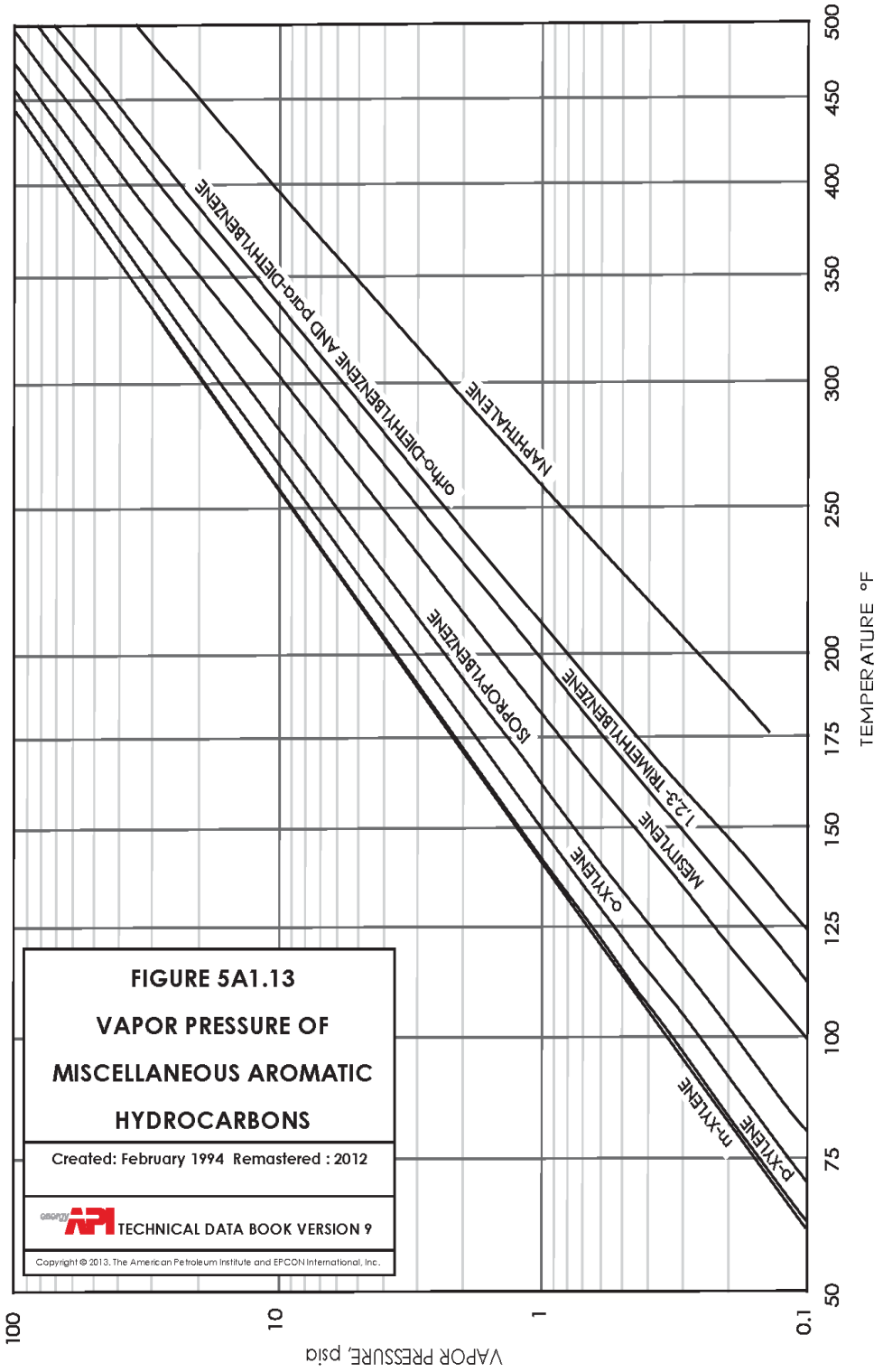


Figure 5A1.14 – Vapor Pressure of Heavy Hydrocarbons

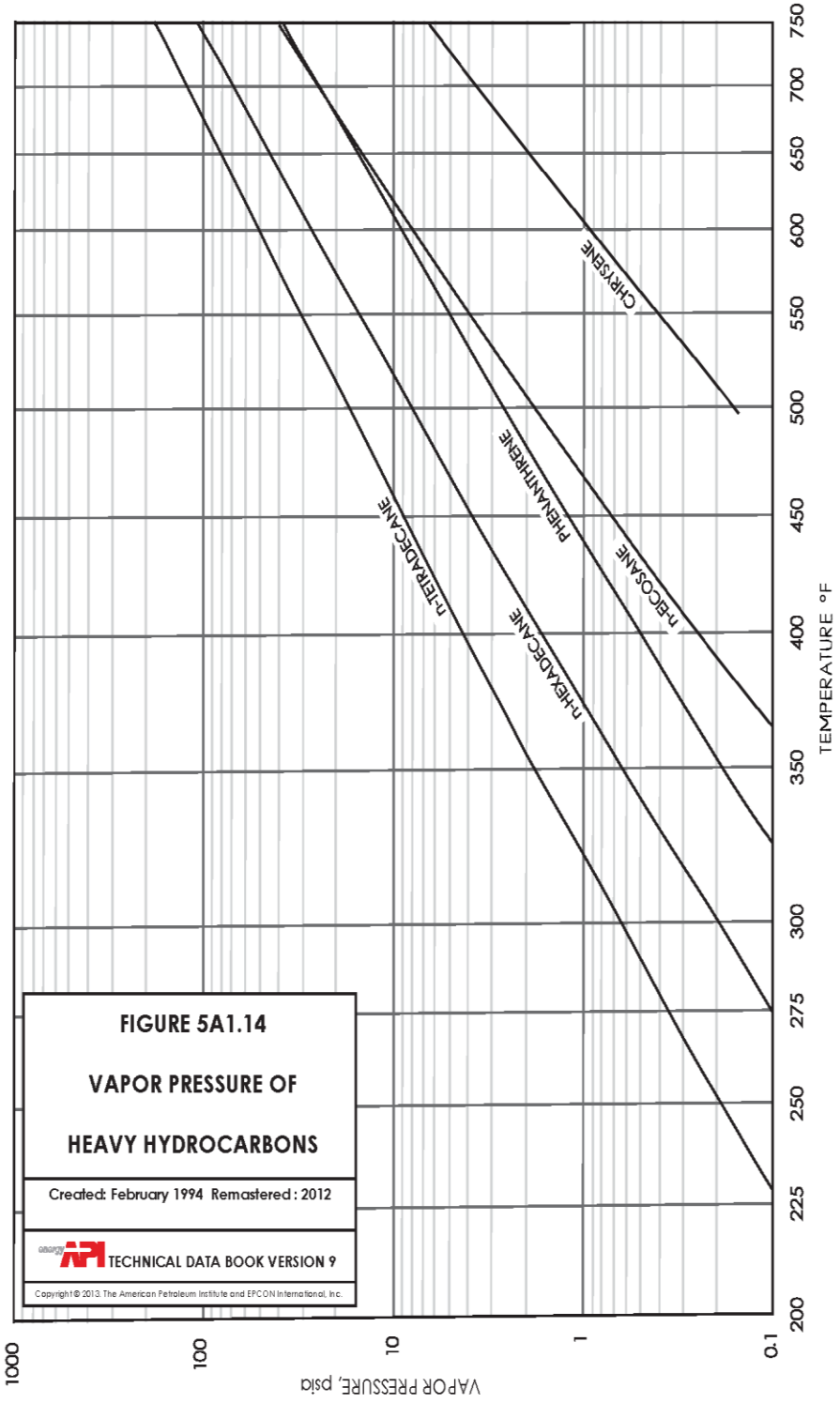
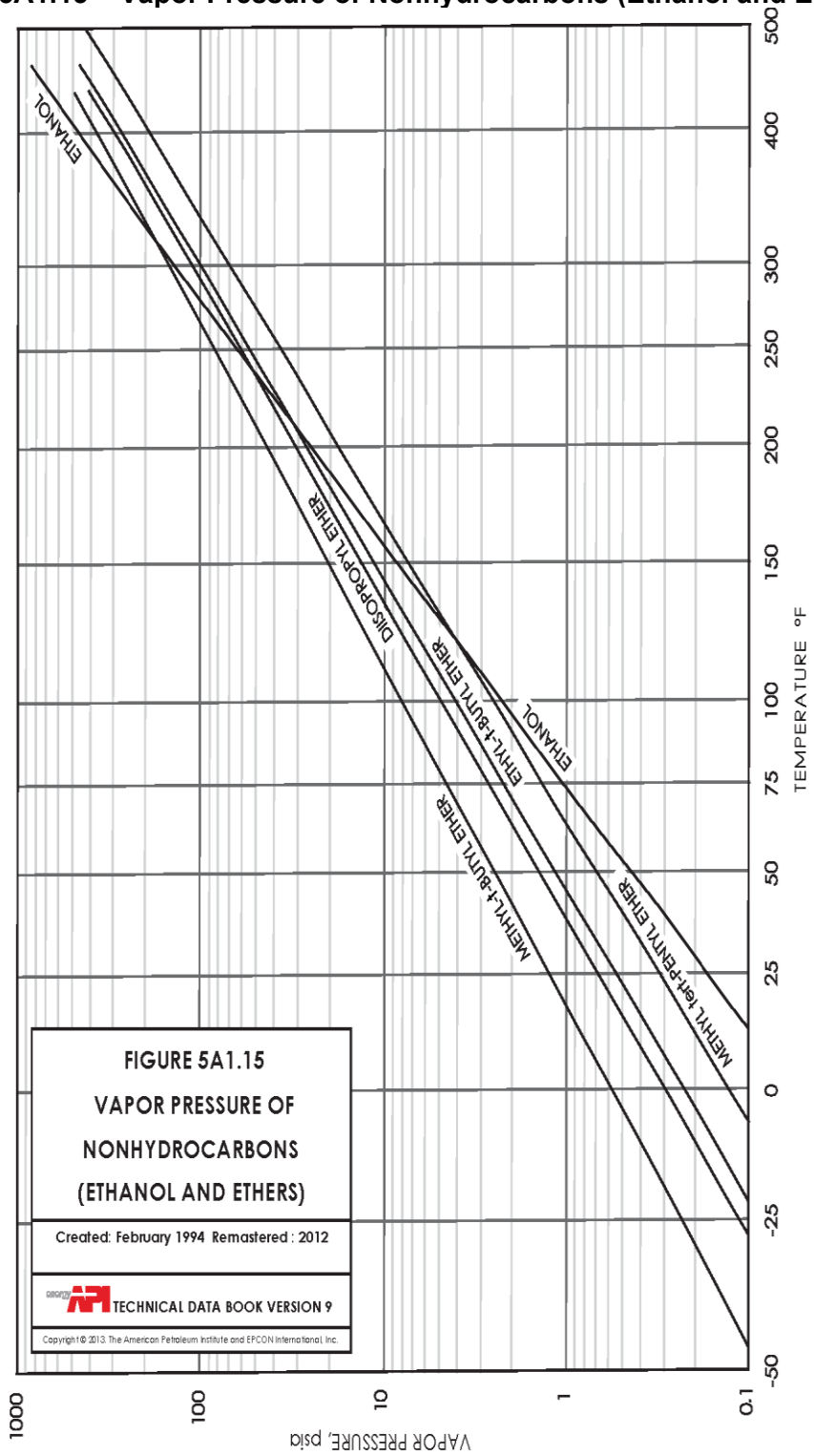


Figure 5A1.15 – Vapor Pressure of Nonhydrocarbons (Ethanol and Ethers)



Comments on Figures 5A1.5 through 5A1.15

Purpose

Experimental vapor pressure data are presented for selected pure hydrocarbons in Figures 5A1.5 through 5A 1.14.

Reliability

The curves reproduce the experimental data from the various sources to within two percent.

Data Sources

The data sources for every compound listed in Chapter 5 are listed below. These sources were used to generate Figures 5A1.5 through 5A1.15 and the correlations in Procedures 5A1.1 and 5A1.3.

Oxygen (70, 274, 320, 361, 332)
Hydrogen (211, 320, 313, 216)
Water (318, 179, 154, 324, 349)
Nitrogen dioxide (211, 171, 313, 145, 268)
Nitric oxide (313, 320, 211, 272)
Nitrous oxide (313, 320, 211, 95)
Ammonia (362, 153, 320, 155, 210, 256, 171, 147)
Chlorine (320, 146, 313)
Hydrogen chloride (320, 171, 155, 210, 350)
Hydrogen sulfide (320, 313, 211, 150, 98)
Carbon monoxide (320, 313, 90, 230, 211, 331, 227)
Carbon dioxide (313, 129, 172, 331)
Sulfur dioxide (313, 331, 211, 320)
Methane (267)
Ethane (152)
Propane (101, 259, 73, 159, 270, 279, 280, 205, 104, 185, 326, 264, 151, 318)
n-Butane (247, 339, 47, 265, 160, 134, 187, 318)
Isobutane (55, 61, 75, 224, 293, 327, 92, 101, 278, 170, 344)
n-Pentane (170, 259, 327, 20, 235, 244, 353, 278, 167, 102, 186)
Isopentane (287, 296, 354)
Neopentane (45, 56, 22, 61, 346, 221)
n-Hexane (109, 148, 195, 162, 176, 304, 311, 318)
2-Methylpentane (318, 353)
3-Methylpentane (353, 318, 104)
2,2-Dimethylbutane (182, 244, 353, 104)
2,3-Dimethylbutane (353, 176, 318, 104)
n-Heptane (195, 243, 304, 93, 138, 175, 213, 301, 354, 220, 104, 318)
2-Methylhexane (169, 220, 318)
3-Methylhexane (138, 220, 318)
2,4-Dimethylpentane (318, 127, 138, 220)
2,2-Dimethylpentane (127, 354, 318)
2,3-Dimethylpentane (318, 127, 138, 19)
3,3-Dimethylpentane (318, 24, 220)
2,2,3-Trimethylbutane (318, 69, 127, 138, 300, 220)
3-Ethylpentane (318, 138, 300, 220)
n-Octane (93, 128, 354, 220, 167)
2,2-Dimethylhexane (318, 354, 220)
2,3-Dimethylhexane (318, 220, 354)
2,4-Dimethylhexane (318, 220, 354)
2,5-Dimethylhexane (318, 220, 354)
3,3-Dimethylhexane (354)
3,4-Dimethylhexane (318, 220, 354)
2-Methylheptane (23, 220, 318)
3-Methylheptane (22, 220, 318)
4-Methylheptane (220, 318)
2,2,4-Trimethylpentane (93, 244, 345, 54, 177, 301, 354, 220, 318)
2,2,3-Trimethylpentane (220, 318)
2,3,3-Trimethylpentane (354, 220, 318)
2,3,4-Trimethylpentane (318, 21, 220)
2,2,3,3-Tetramethylbutane (325, 77)
3-Ethylhexane (318, 354, 220)
2-Methyl-3-ethylpentane (318, 220, 354)
3-Methyl-3-ethylpentane (318, 156, 313, 299)
n-Nonane (86, 138, 354, 318)
2-Methyloctane (318)
3-Methyloctane (318)
4-Methyloctane (318)
2,2-Dimethylheptane (318)
2,6-Dimethylheptane (318)
3,3-Diethylpentane (318)
2,2,5-Trimethylhexane (318)
2,4,4-Trimethylhexane (319)
2,2,3,3-Tetramethylpentane (318, 138)
2,2,3,4-Tetramethylpentane (318, 138)
2,2,4,4-Tetramethylpentane (318, 138)
2,3,3,4-Tetramethylpentane (319, 158)

3-Ethylheptane (318)
2,2-Dimethyl-3-ethylpentane (318)
2,4-Dimethyl-3-ethylpentane (318)
n-Decane (354, 278, 3)
2-Methylnonane (318)
3-Methylnonane (318)
4-Methylnonane (318)
5-Methylnonane (318)
2,2-Dimethyloctane (318, 83)
n-Undecane (318, 80)
n-Dodecane (354, 318)
n-Tridecane (318, 313)
n-Tetradecane (318, 80)
n-Pentadecane (318, 80)
n-Hexadecane (170, 318, 78)
n-Heptadecane (318)
n-Octadecane (318, 331, 207)
n-Nonadecane (318)
n-Eicosane (318, 207)
n-Tetracosane (233, 25)
n-Octacosane (233, 318, 89, 25)
Cyclopentane (318, 46, 340)
Methylcyclopentane (104, 307, 318)
Ethylcyclopentane (104, 313, 307, 318)
1,1-Dimethylcyclopentane (318, 331)
cis-1,2-Dimethylcyclopentane (138, 318)
trans-l,2-Dimethylcyclopentane (138, 318)
cis-1,3-Dimethylcyclopentane (318, 328)
trans-l,3-Dimethylcyclopentane (318)
n-Propylcyclopentane (318)
Isopropylcyclopentane (318, 119, 158)
Cyclohexane (148, 353, 269, 48, 276, 181)
Methylcyclohexane (318, 353, 306, 208)
Ethylcyclohexane (318, 353)
1,1-Dimethylcyclohexane (138, 318)
cis-1,2-Dimethylcyclohexane (353, 318)
trans-l,2-Dimethylcyclohexane (353, 318)
cis-1,3-Dimethylcyclohexane (353, 318)
trans-l,3-Dimethylcyclohexane (353, 318)
cis-1,4-Dimethylcyclohexane (353, 318)
trans-l,4-Dimethylcyclohexane (353, 318)
n-Propylcyclohexane (318, 353)
Isopropylcyclohexane (119, 138)
n-Butylcyclohexane (318)
n-Decylcyclohexane (318, 119)
1-Methyl-l-ethylcyclopentane (252, 318, 113)
Cycloheptane (318, 131)
Cyclooctane (131, 299, 157, 1)
Ethylene (74, 228, 76, 240, 361, 323)
Propylene (85, 126, 229, 140, 270, 191, 279, 334, 173, 323, 299)
1-Butene (164, 224, 57, 44, 61, 191, 279, 310, 170, 193, 255, 350)
cis-2-Butene (61, 291, 134, 335)
trans-2-Butene (61, 134, 335)
Isobutene (191, 262, 283)
1-Pentene (290, 106, 318, 136, 313, 356, 323)
cis-2-Pentene (104, 318, 289)
trans-2-Pentene (104, 318, 289)
2-Methyl-l-butene (318, 290, 363)
2-Methyl-2-butene (318, 191, 290)
3-Methyl-l-butene (318, 289)
1-Hexene (137, 323)
cis-2-Hexene (318, 81)
trans-2-Hexene (318, 81)
cis-3-Hexene (318, 118)
trans-3-Hexene (318, 118)
2-Methyl-l-pentene (318, 81)
2-Methyl-2-pentene (318, 81)
3-Methyl-l-pentene (318, 118)
3-Methyl-*cis*-2-pentene (318, 118)
4-Methyl-l-pentene (318, 81)
4-Methyl-*cis*-2-pentene (318)
4-Methyl-*trans*-2-pentene (318)
2,3-Dimethyl-l-butene (318, 81)
2,3-Dimethyl-2-butene (318, 51, 81, 288)
3,3-Dimethyl-l-butene (318, 122, 51, 299)
2-Ethyl-l-butene (318, 81)
1-Heptene (137, 201, 62, 318)
cis-2-Heptene (318)
trans-2-Heptene (318, 66)
cis-3-Heptene (318)
trans-3-Heptene (318, 66)
2-Methyl-l-hexene (318, 286)
3-Methyl-l-hexene (318)
4-Methyl-l-hexene (318)
2-Ethyl-l-pentene (318)
3-Ethyl-l-pentene (318)
2,3,3-Trimethyl-l-butene (318, 299)
1-Octene (318, 137)
trans-2-Octene (318)
trans-3-Octene (318)
trans-4-Octene (318)
2-Ethyl-l-hexene (318)
2,4,4-Trimethyl-l-pentene (318, 358, 82)
2,4,4-Trimethyl-2-pentene (82, 318)
1-Nonene (318)
1-Decene (318, 137)
1-Undecene (318)
1-Dodecene (318)
1-Tridecene (318)
1-Tetradecene (318)
1 -Pentadecene (321)
1-Hexadecene (318)
1-Heptadecene (323, 2, 158, 284)
1-Octadecene (318)
1-Nonadecene (323)
1-Eicosene (318)
Cyclopentene (331)
Cyclohexene (271, 331)
Cycloheptene (299, 202, 94, 337)
Cyclooctene (94, 202, 135)

Cyclopentadiene (196, 49, 163, 356)
1,3-Butadiene (61, 192, 143, 161, 164, 232, 262, 292, 333, 212, 134, 193, 255, 349)
Isoprene (65, 318)
3-Methyl-l,2-butadiene (318, 104, 251, 299)
1,2-Pentadiene (318, 251)
cis-1,3-Pentadiene (318, 251)
trans-l,3-Pentadiene (318, 251)
1,4-Pentadiene (318)
2,3-Pentadiene (318, 251, 299, 316)
1,3-Cyclohexadiene (226, 197, 120, 308)
2,3-Dimethyl-l,3-butadiene (99, 123)
1,5-Hexadiene (99, 299, 197)
trans, *trans*-2,4-Hexadiene (197, 123)
1,5-Cyclooctadiene (66)
Acetylene (219, 336, 15, 318)
Methylacetylene (318, 246, 330)
Dimethylacetylene (331, 324)
3-Methyl-l-butyne (324)
1-Pentyne (324)
1-Hexyne (149, 157, 324)
2-Hexyne (324)
3-Hexyne (324, 275)
Benzene (60, 312, 364, 360, 6, 322, 7)
Toluene (53, 8, 353, 364, 115, 313, 322)
Ethylbenzene (8, 20, 189, 253, 322, 7)
m-Xylene (263, 138, 175, 8, 322, 7)
o-Xylene (148, 263, 353, 8, 322, 7)
p-Xylene (263, 19, 322, 239, 7, 349)
n-Propylbenzene (136, 353, 322, 199)
Cumene (209, 322, 37)
1,2,3-Trimethylbenzene (318, 65, 322)
1,2,4-Trimethylbenzene (148, 165, 318, 65, 322)
Mesitylene (318, 322)
m-Ethyltoluene (318, 328, 322)
o-Ethyltoluene (318, 328, 322)
p-Ethyltoluene (318, 328, 322, 204, 105)
n-Butylbenzene (318, 331, 199)
Isobutylbenzene (318)
sec-Butylbenzene (318, 271)
tert-Butylbenzene (318, 271)
m-Diethylbenzene (318, 138)
o-Diethylbenzene (318, 138)
p-Diethylbenzene (318)
m-Cymene (318, 37)
o-Cymene (318, 37)
p-Cymene (318, 328, 37)
2-Ethyl-*m*-xylene (132, 318)
2-Ethyl-*p*-xylene (121, 314, 318)
3-Ethyl-*o*-xylene (318)
4-Ethyl-*m*-xylene (121, 314, 318)
4-Ethyl-*o*-xylene (121, 318)
5-Ethyl-*m*-xylene (121, 314. 318)
1,2,3,5-Tetramethylbenzene (318, 64, 302)
1,2,4,5-Tetramethylbenzene (318)
n-Pentylbenzene (318)
n-Hexylbenzene (318)
m-Diisopropylbenzene (113, 223)
p-Diisopropylbenzene (223, 237)
n-Heptylbenzene (318)
n-Octylbenzene (318, 3)
Styrene (67)
alpha-Methylstyrene (313, 319, 236, 338, 342, 50)
m-Methylstyrene (91)
o-Methylstyrene (91, 299)
p-Methylstyrene (91)
n-Nonylbenzene (318, 3)
n-Decylbenzene (318, 79)
n-Undecylbenzene (318)
n-Dodecylbenzene (318, 105, 3, 248, 214, 329)
n-Tridecylbenzene (318)
Ethynylbenzene(111,203,266)
cis-l-Propenylbenzene (319, 222)
trans l-Propenylbenzene (258, 59)
m-Divinylbenzene (313, 114)
2-Phenylbutene-1 (277, 242)
Cyclohexylbenzene (355, 295, 125, 142, 200)
cis-Decahydronaphthalene (32)
trans-Decahydronaphthalene(32)
1,2,3,4-Tetrahydronaphthalene (28, 178, 355, 239, 281, 133, 245)
Indane (315, 112, 13, 166)
Indene (31, 72)
Biphenyl (232, 88, 144, 148, 281)
Naphthalene (318, 4, 80, 96, 97, 130, 139, 174, 241, 343, 27, 107, 27)
1-Methylnaphthalene (148, 237, 355, 207, 348)
2-Methylnaphthalene (80, 39)
2,6-Dimethylnaphthalene (250)
2,7-Dimethylnaphthalene (157, 250)
1-Ethylnaphthalene (318, 113, 190, 198, 234)
1-*n*-Butylnaphthalene (42, 52)
Anthracene (33, 320)
Phenanthrene (29, 250)
Pyrene (170, 303, 328, 318)
Chrysene (170, 108, 30)
Acenaphthene (34)
Fluorene (297, 235)
Bicyclohexyl (271, 347)
Fluoranthene (34)
cis-Stilbene (110, 71, 68, 100, 63, 316, 84, 352, 272)
1,1-Diphenylethane (110, 284)
1,2-Diphenylethane(253)
m-Terphenyl (116)
o-Terphenyl (116)
Pyridine (184, 217, 254, 36)
Isoquinoline (41)
Quinoline (35)
Dibenzopyrrole (171, 313, 65, 282, 235)
Acridine (313, 26, 309)

Indole (40)
Thiophene (318, 313, 65, 271, 16, 238)
Tetrahydrothiophene (271, 168, 318, 16)
Methyl mercaptan (318, 212, 313, 316)
Carbonyl sulfide (211, 273, 209, 313, 180)
Ethyl mercaptan (318, 313, 218, 249, 316)
Methanol (351, 320, 313, 11, 12, 206, 5, 305, 255)
Ethanol (320, 171, 351, 11, 188, 359, 141, 231, 313, 285, 298)
2-propanol (11, 328, 351, 65, 183, 320, 317, 14, 9, 272, 204, 105, 298, 313)
2-Methyl-2-propanol (14, 11, 320, 351, 313, 298)
Methyl *tert*-butyl ether (260, 272, 10, 5, 38, 43, 105, 255, 349)
tert-Butyl ethyl ether (117, 124, 261)
Diisopropyl ether (184, 271, 313, 10, 117)
Methyl *tert*-pentyl ether (272, 87, 257)

Procedure 5A1.16 – Prediction of Vapor Pressures of Pure Hydrocarbons

Discussion

The following equation is useful for predicting the vapor pressures of pure hydrocarbons (and narrow-boiling petroleum fractions) when the critical properties are known or can be estimated. When the critical properties are not available or cannot be accurately estimated, Procedure 5A1.19 is recommended.

$$\ln p_r^* = (\ln p_r^*)^{(0)} + \omega(\ln p_r^*)^{(1)} \; at \; constant \; T_r \qquad (5A1.16\text{-}1)$$

Where:

p_r^* = *reduced vapor pressure* p^*/p_c

p^* = *vapor pressure, in psia*

p_c = *critical pressure, in psia*

$(\ln p_r^*)^{(0)}$ *and* $(\ln p_r^*)^{(1)}$ = *correlation terms that are given in equation, tabular and graphical form*

ω = *acentric factor of hydrocarbon*

T_r = *reduced temperature* T/T_c

T = *temperature, in °R*

T_c = *critical temperature, in °R*

Procedure

Step 1: *Obtain the critical temperature and critical pressure from the pure component properties tables or if not available, estimate values by the procedures of Chapter 4.*

Step 2: *Calculate the reduced temperature.*

Step 3: *Obtain the acentric factor of the hydrocarbon from the pure component properties tables.*

Step 4: *Obtain the correlation terms* $(\ln p_r)^{(0)}$ *and* $(\ln p_r)^{(1)}$ *by either interpolating linearly from Table 5A1.17 or, at a small sacrifice in accuracy, by reading directly from Figure 5A1.18. [Alternately use equations (5A1.16-2) and (5A1.16-3).]*

Step 5: *Calculate the reduced vapor pressure by using equation (5A1.16-1). The vapor pressure is obtained by multiplying the reduced vapor pressure by the critical pressure.*

For computer calculations, the correlation terms that are equivalent to Table 5A1.17 are given by the following equations:

$$(\ln p_r^*)^{(0)} = 5.92714 - 6.09648/T_r - 1.28862 \ln T_r + 0.169347 \, T_r^6 \qquad (5A1.16\text{-}2)$$

$$(\ln p_r^*)^{(1)} = 15.2518 - 15.6875/T_r - 13.4721 \ln T_r + 0.43577 \, T_r^6 \qquad (5A1.16\text{-}3)$$

Comments on Procedure 5A1.16

Purpose

Procedure 5A1.16 is presented as the best method for predicting the vapor pressure of a pure hydrocarbon which is not treated directly in Procedures 5A1.1 or 5A1.3 or Figures 5A1.5 through 5A1.14. Critical conditions and acentric factor are required. The method can also be applied to narrow-boiling petroleum fractions. In the absence of critical data, use Procedure 5A1.19.

Limitations

Equation (5A1.16-1) is valid only for nonpolar substances. The method is restricted to reduced temperatures greater than 0.30 but below the critical point. This methods is not accurate below the freezing point.

Reliability

Equation (5A1.16-1) reproduces experimental data for pure hydrocarbons to within an average error of 3.5 percent when the critical properties are known. The method is most reliable for reduced temperatures between 0.5 and 0.95. When the critical properties and the acentric factor are estimated, the errors will be larger. The method has not been tested with petroleum fraction data.

Literature Sources

This procedure is based on the vapor pressure equations of Lee, B.I. and Kesler, M.G., *AIChE J.,* **21** 510 (1975).

Example

Predict the vapor pressure of 1-butene at 208.4 °F.

From the pure component properties tables, the critical temperature is 295.4 °F and the critical pressure is 583.1 psia. The reduced temperature is

$$\frac{208.4 + 459.7}{295.4 + 459.7} = 0.8847$$

From the pure component properties tables, the acentric factor is 0.1845. By linear interpolation from Table 5A1.17:

$$-(ln\, p_r^*)^{(0)} = 0.7250 \; and \; -(ln\, p_r^*)^{(1)} = 0.6213$$

Using equation (5A1.16-1):

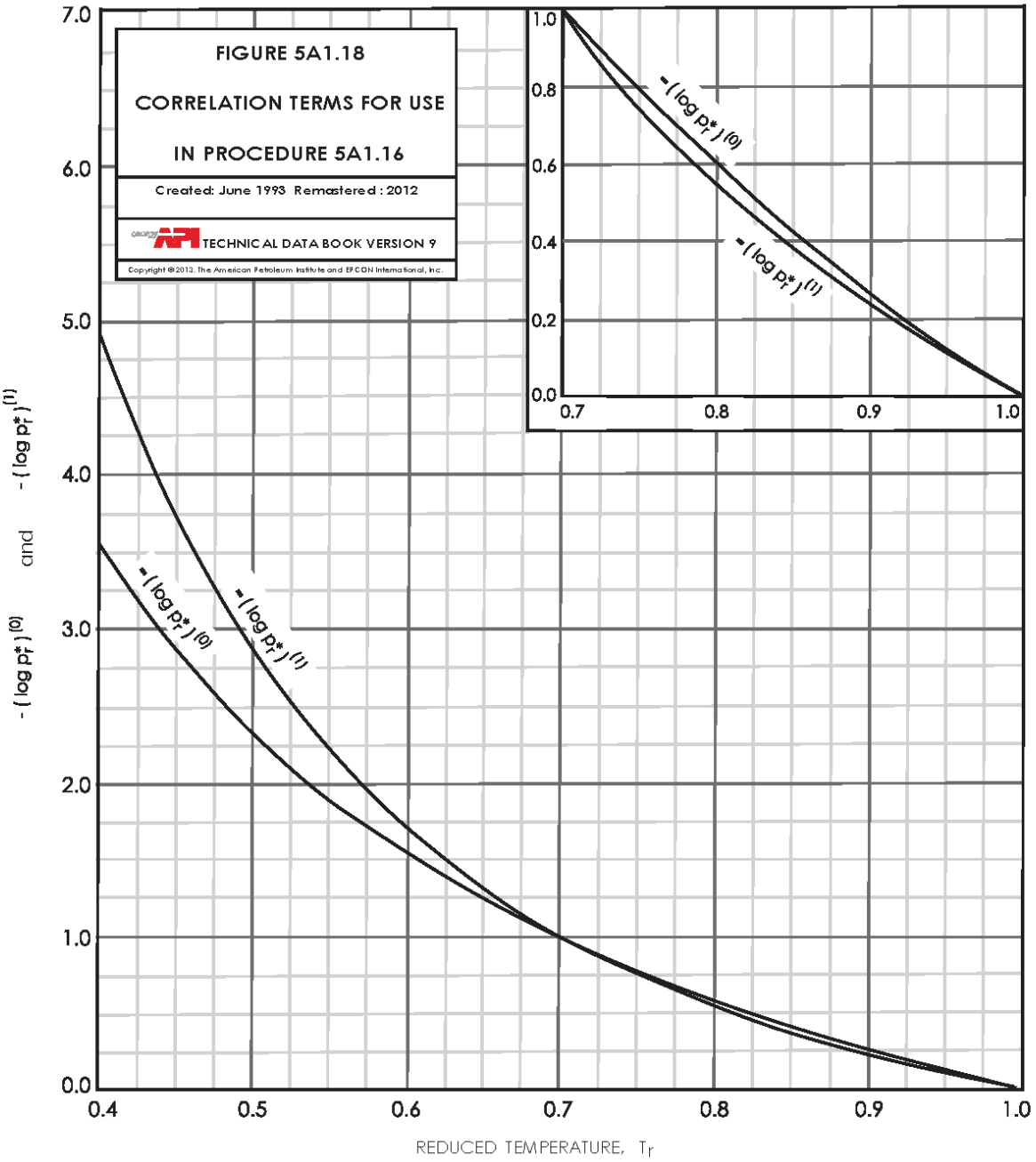
*ln p_r**	=	*– 0.7250 + 0.1845 (– 0.6213) = – 0.8397*
*p_r**	=	*0.4319*
*p**	=	*0.4319 (583.1) = 251.8 psia*

The experimental value is 250 psia.

Table 5A1.17 – Correlation Terms for Use in Procedure 5A1.16

T_r	$-(\ln p_r^*)^{(0)}$	$-(\ln p_r^*)^{(1)}$
1.00	0.000	0.000
0.98	0.118	0.098
0.96	0.238	0.198
0.94	0.362	0.303
0.92	0.489	0.412
0.90	0.621	0.528
0.88	0.757	0.650
0.86	0.899	0.781
0.84	1.046	0.922
0.82	1.200	1 .073
0.80	1.362	1.237
0.78	1.531	1.415
0.76	1.708	1.608
0.74	1.896	1.819
0.72	2.093	2.050
0.70	2.303	2.303
0.68	2.525	2.579
0.66	2.761	2.883
0.64	3.012	3.218
0.62	3.280	3.586
0.60	3.568	3.992
0.58	3.876	4.440
0.56	4.207	4.937
0.54	4.564	5.487
0.52	4.951	6.098
0. 50	5.370	6.778
0.48	5.826	7.537
0.46	6.324	8.386
0.44	6.869	9.338
0.42	7.470	10.410
0.40	8.133	11.621
0.38	8.869	12.995
0.36	9.691	14.560
0.34	10.613	16.354
0.32	11.656	18.421
0.30	12.843	20.820

Figure 5A1.18 – Correlation Terms for Use in Procedure 5A1.16



Procedure 5A1.19 – Prediction of Vapor Pressures of Pure Hydrocarbons and Narrow-Boiling Petroleum Fractions

Discussion

This procedure was last updated in 1994. Figures 5A1.20 and 5A1.21 are useful for predicting the vapor pressures of pure hydrocarbons and narrow-boiling petroleum fractions when the critical properties or the acentric factors are not known and cannot be estimated. When these properties are available, Procedure 5A1.16 is recommended.

Procedure

Step 1: *Obtain the normal boiling point of the hydrocarbon from the pure component properties tables and the Watson K from Chapter 2.*

Step 2: *Read a vapor pressure from Figure 5A1.20 using $t_b = t'_b$, where t_b is the normal boiling point and t'_b is the normal boiling point corrected to K = 12 (both in degrees Fahrenheit). For naphthenes, olefins, acetylenes and low- molecular-weight (<C_5) paraffins, it is not generally beneficial to apply the Watson K correction, so the procedure is complete. For other hydrocarbons, proceed to Step 3.*

Step 3: *Using the vapor pressure from Step 2, obtain a K-correction from Figure 5A1.21. Subtract this Δt (corrected with f multiplier for superatmospheric pressures) from the true normal boiling point to get the corrected normal boiling point, t'_b.*

Step 4: *Repeat Steps 2 and 3 until the pressure used to estimate the K-correction in Step 3 agrees within desired limits with the value predicted in Step 2. In each repetition, the t'_b from Step 3 is used in Step 2.*

Note: *To estimate a normal boiling point from a known vapor pressure, simply determine the t'b from Figure 5A1.20 and add the K-correction from Figure 5A1.21. No trial-and-error approach is necessary.*

This procedure may also be used with a digital computer. Figure 5A1.20 was generated from the following equation:

$$\log p^* = \frac{3000.538\,X - 6.761560}{43X - 0.987672} \quad for\ X > 0.0022\ (p^* < 2\ mm\ Hg) \qquad (5A1.19\text{-}1)$$

$$\log p^* = \frac{2663.129\,X - 5.994296}{95.76X - 0.972546} \quad for\ 0.0013 \le X \le 0.0022\ (2\ mm\ Hg \le p^* \le 760\ mm\ Hg) \qquad (5A1.19\text{-}2)$$

$$\log p^* = \frac{2770.085\,X - 6.412631}{36\,X - 0.989679} \quad for\ X, 0.0013\ (p^* > 760\ mm\ Hg) \qquad (5A1.19\text{-}3)$$

Where:

*p** = *vapor pressure, in mm Hg.*

$$X = \frac{\frac{T'_b}{T} - 0.0002867(T'_b)}{748.1 - 0.2145(T'_b)} \qquad \textit{(5A1.19-4)}$$

Where:

T'_b = *normal boiling point, in °R*

T = *absolute temperature, in °R*

Figure 5A1.21 was generated from the following two equations:

$$\Delta T = T_b - T'_b = 2.5f(K - 12)\, log\frac{p^*}{760} \qquad \textit{(5A1.19-5)}$$

Where:

T_b = *normal boiling point, in °R*

f = *correction factor. For all subatmospheric vapor pressures and for all substances having normal boiling points greater than 400 °F, f = 1. For substances having normal boiling points less than 200 °F, f = 0. For superatmospheric vapor pressures of substances having normal boiling points between 200 °F and 400 °F, f is given by:*

$$f = \frac{T_b - 659.7}{200} \qquad \textit{(5A1.19-6)}$$

K = *Watson characterization factor.*

Comments on Procedure 5A1.19

Purpose

Procedure 5A1.19 is presented as an alternate method of predicting the vapor pressure of pure hydrocarbons or narrow-boiling hydrocarbon mixtures. It is recommended for pure hydrocarbons only when Procedure 5A1.16 cannot be applied because critical properties or acentric factors are not available. The normal boiling point and Watson K are required inputs to this method.

Limitations

This procedure is limited to pure hydrocarbons and narrow-boiling range petroleum fractions, i.e., those having less than 50 °F differences in a true-boiling point (TBP) distillation. Appropriate procedures in Chapter 8 are recommended for wide-boiling range fractions.

Reliability

Figures 5A1.20 reproduces experimental data for pure hydrocarbons to within an average error of eight percent for $p^* > 1$ mm Hg and 30 percent for p^* between 10^{-6} and 1 mm Hg. For $p^* < 10^{-6}$ mm Hg no experimental data are available and the reliability for the method is unknown. The method is most reliable for vapor pressures near atmospheric pressure. The method has not been tested with petroleum fraction data.

Literature Sources

Figures 5A1.20a-e and 5A1.21 and equations (5A1.19-4) and (5A1.19.5) were adapted from Maxwell and Bonnell, *Vapor Pressure Charts for Petroleum Engineers,* Esso Research and Engineering Company, Linden, N.J. (1955). Equations (5A1.19-1) through (5A1.19-3) were provided by Exxon Research and Engineering Company in 1977. Figure 5A1.20f is from Beerbower, A. and Zudkevitch, D.,"Predicting the Evaporation Behavior of Lubricants in Space Environment," Preprints, Divisions of Petroleum Chemistry, American Chemical Society, Los Angeles Meeting, **8**(2) C-99 (April 1963).

Examples

A. Calculate the vapor pressure of 1,2,3,4-tetrahydronaphthalene (tetralin) at 302 °F.

From the pure component properties tables, the boiling point is 405.7 °F, and from Chapter 2, the Watson *K* is 9.78.

For the first trial, assume $t'_b = t_b = 405.7$ °F. Using this t'_b and the desired temperature, 302 °F, the first estimate of the vapor pressure is read from figure 5A1.20a as 0.20 atm. This vapor pressure (152 mm Hg) and a Watson *K* of 9.78 are used in Figure 5A1.21 to estimate the Watson *K* - correction, $\Delta t = 4.0$ °F. The t'_b for the second trial is $t_b - (t_b - t'_b) = 405.7 - 4.0 = 401.7$ °F.

Using the new t'_b, the second trial vapor pressure is 0.21 atm (160 mm Hg) from Figure 5A1.20a. From Figure 5A1.21, the new Watson *K*-correction is 3.9 °F; thus, the third trial t'_b is 405.7 – 3.9 = 401.8 °F.

With $t'_b = 401.8$ °F, the estimated vapor pressure for the third trial is read from Figure 5A1.20a as 0.21 atm. This value is identical with the second trial vapor pressure; thus, the trial-and- error solution is satisfied.

The estimated vapor pressure, 3.1 psia, agrees well with an experimental value of 3.13 psia.

B. A petroleum fraction exhibits the following TBP distillation curve at 10 mm Hg:

Distillation, percent by volume	10	30	50	70	90
Temperature, °F	350	380	425	500	600

Estimate the average normal boiling point of the 10 to 30 percent portion (the Watson *K* is 12.5) of the fraction.

The average boiling point at 10 mm Hg is 365 °F. From 5A1.20b, t'_b = 628 °F. From Figure 5A1.21, $t_b - t'_b$ = –2.4 °F.

Therefore, the average normal boiling point = t_b - ($t_b - t'_b$) = 628 – 2.4= 628 °F.

Figure 5A1.20a – Vapor Pressure of Pure Hydrocarbons and Narrow Boiling Range Petroleum Fractions

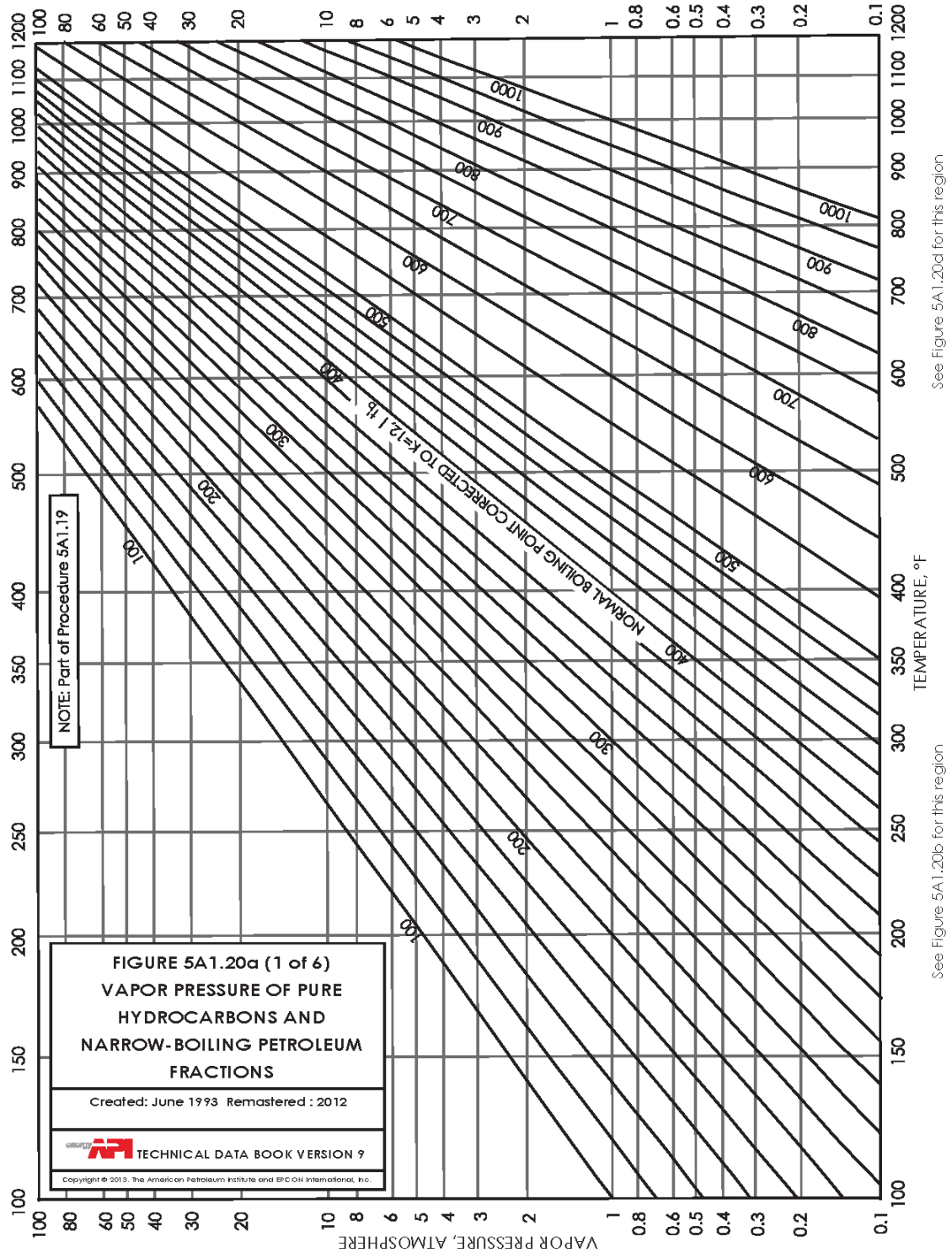


Figure 5A1.20b – Vapor Pressure of Pure Hydrocarbons and Narrow Boiling Range Petroleum Fractions

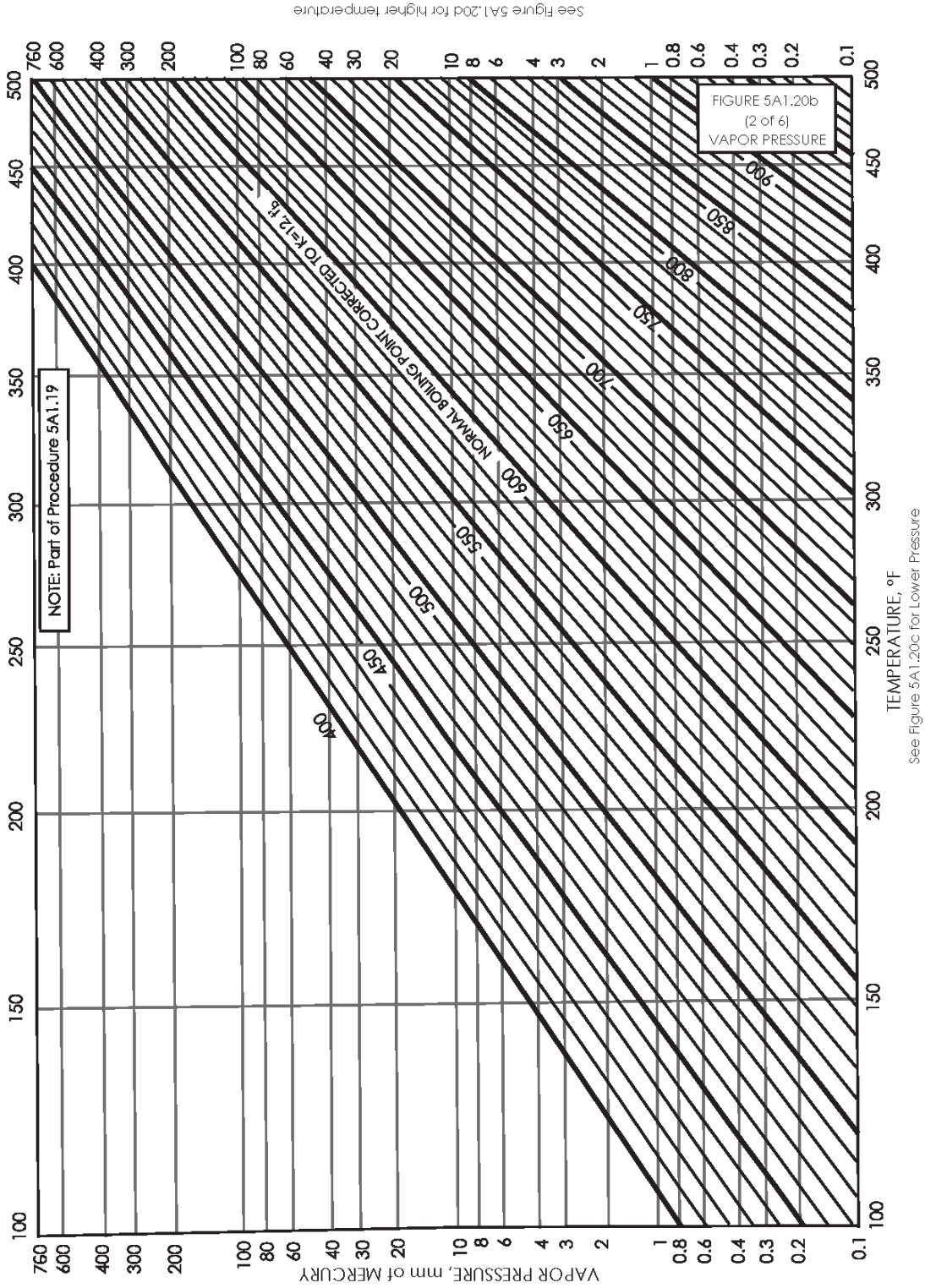


Figure 5A1.20c – Vapor Pressure of Pure Hydrocarbons and Narrow Boiling Range Petroleum Fractions

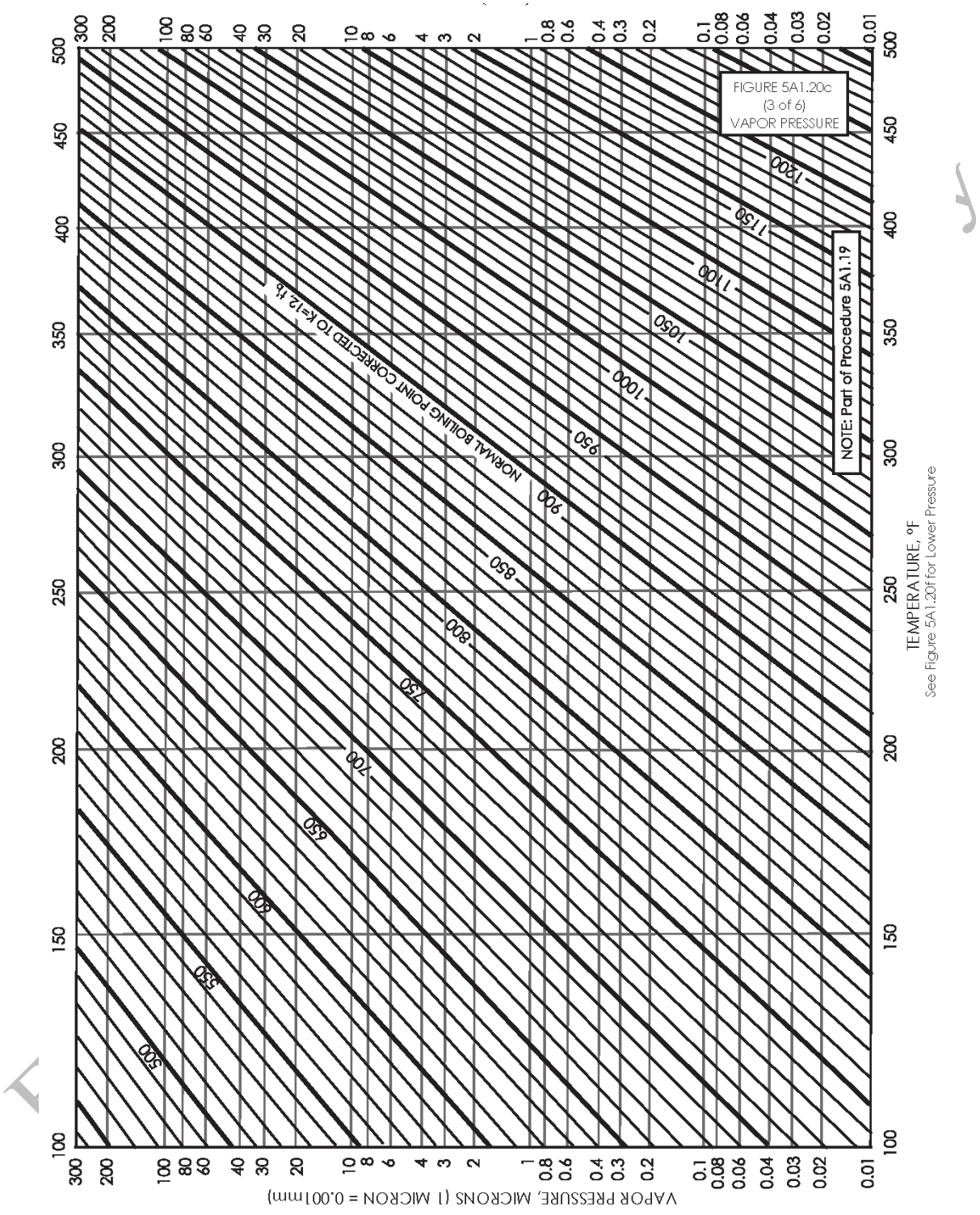


Figure 5A1.20d – Vapor Pressure of Pure Hydrocarbons and Narrow Boiling Range Petroleum Fractions

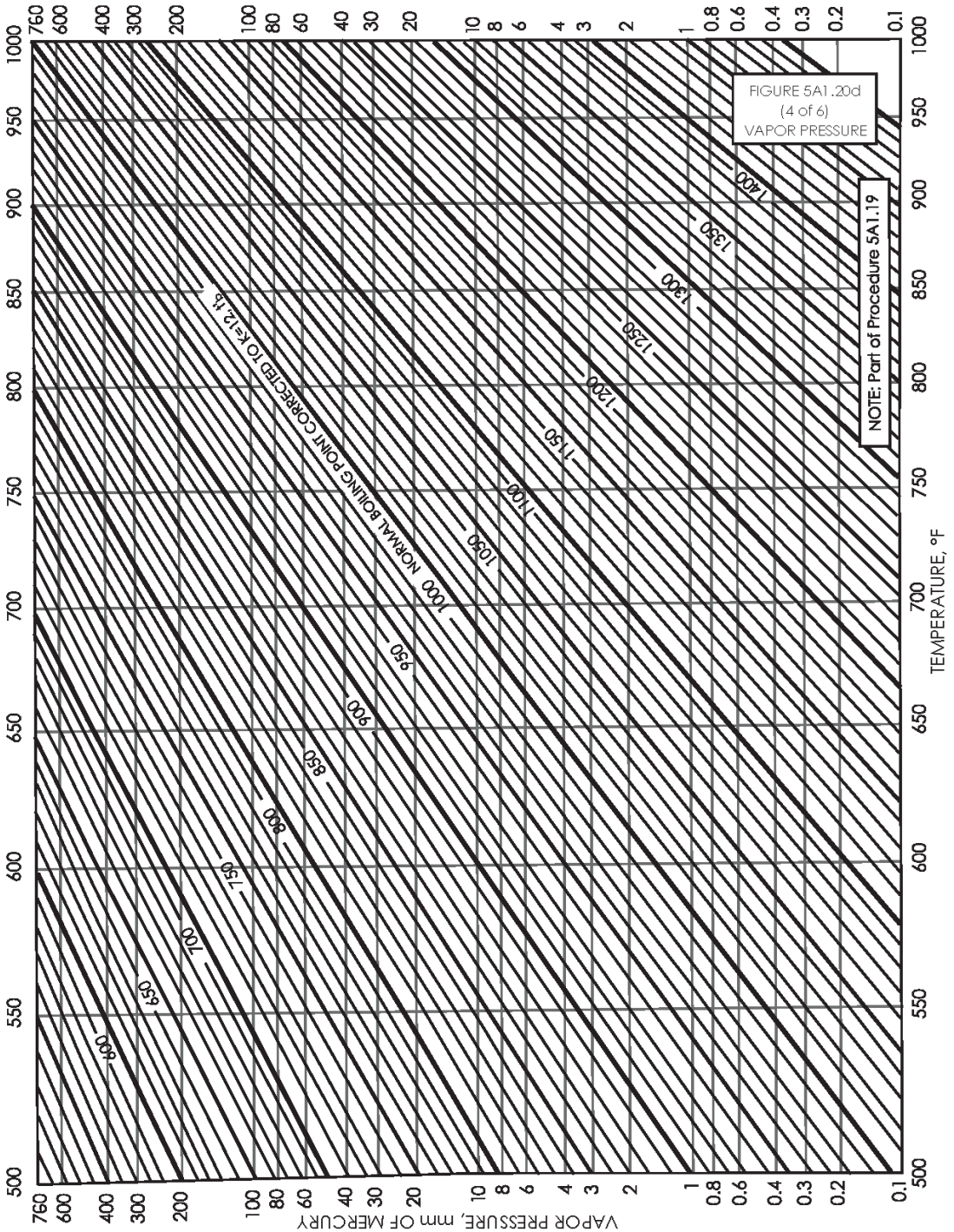


Figure 5A1.20e – Vapor Pressure of Pure Hydrocarbons and Narrow Boiling Range Petroleum Fractions

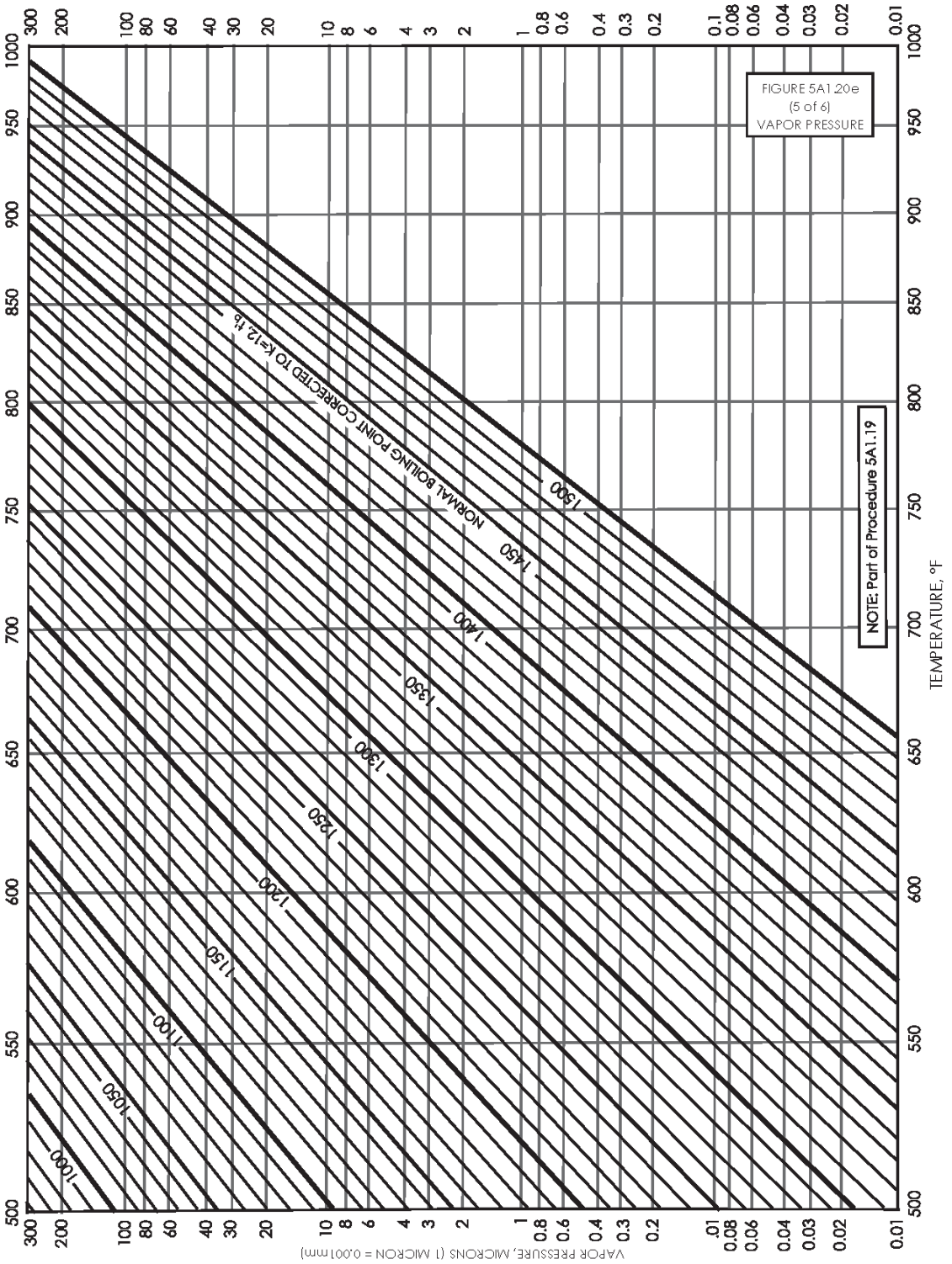


Figure 5A1.20f – Vapor Pressure of Pure Hydrocarbons and Narrow Boiling Range Petroleum Fractions

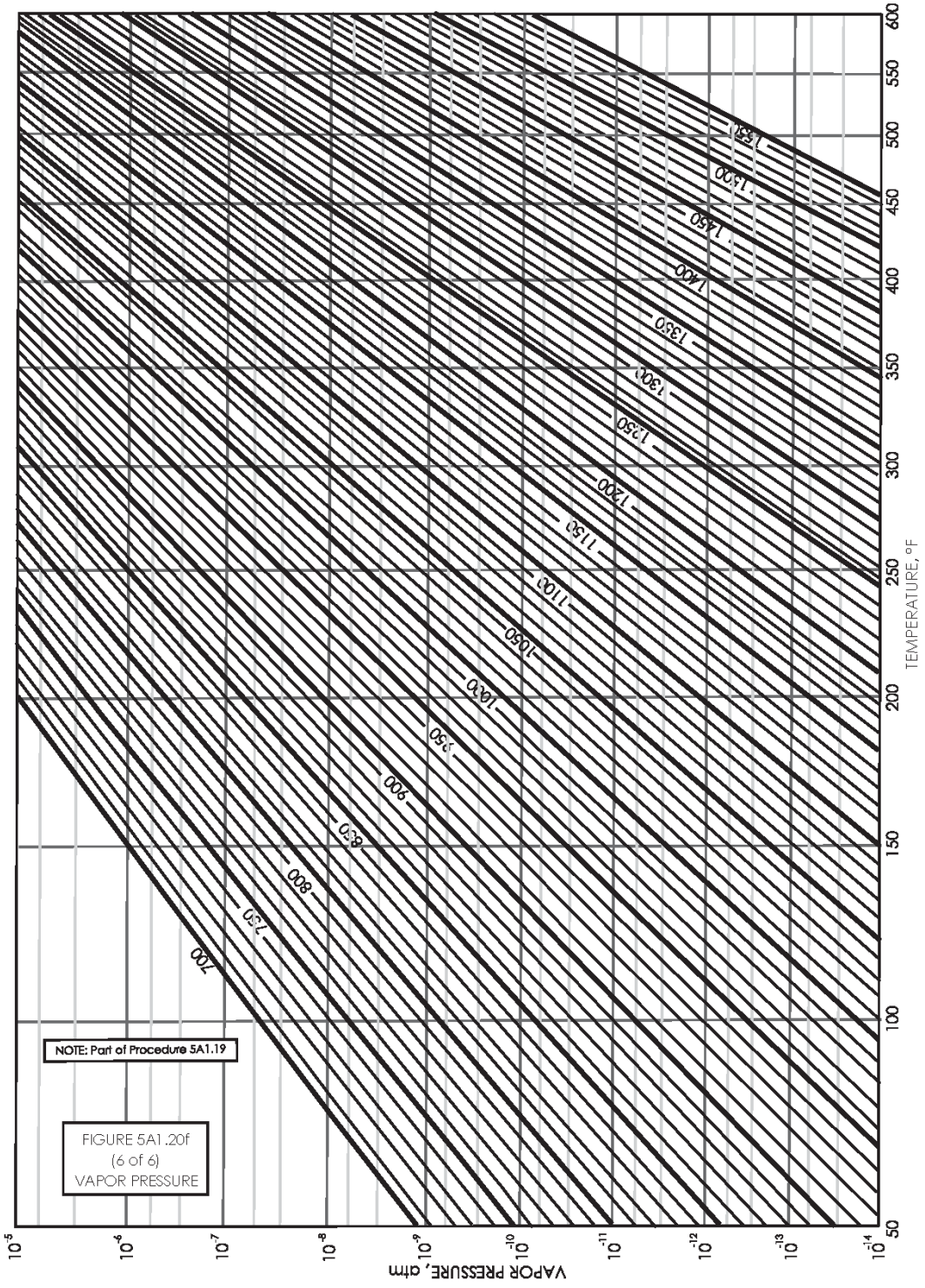
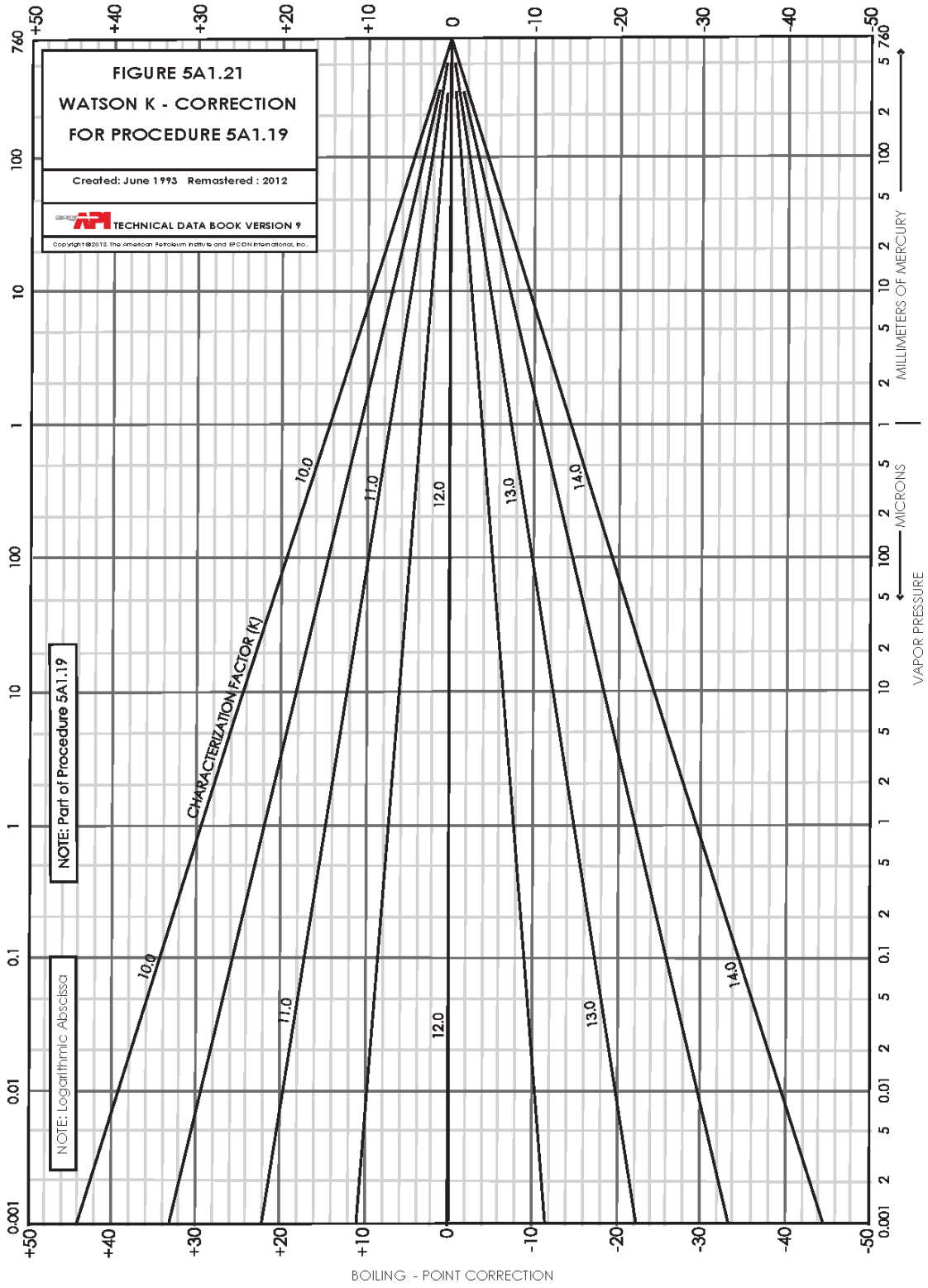
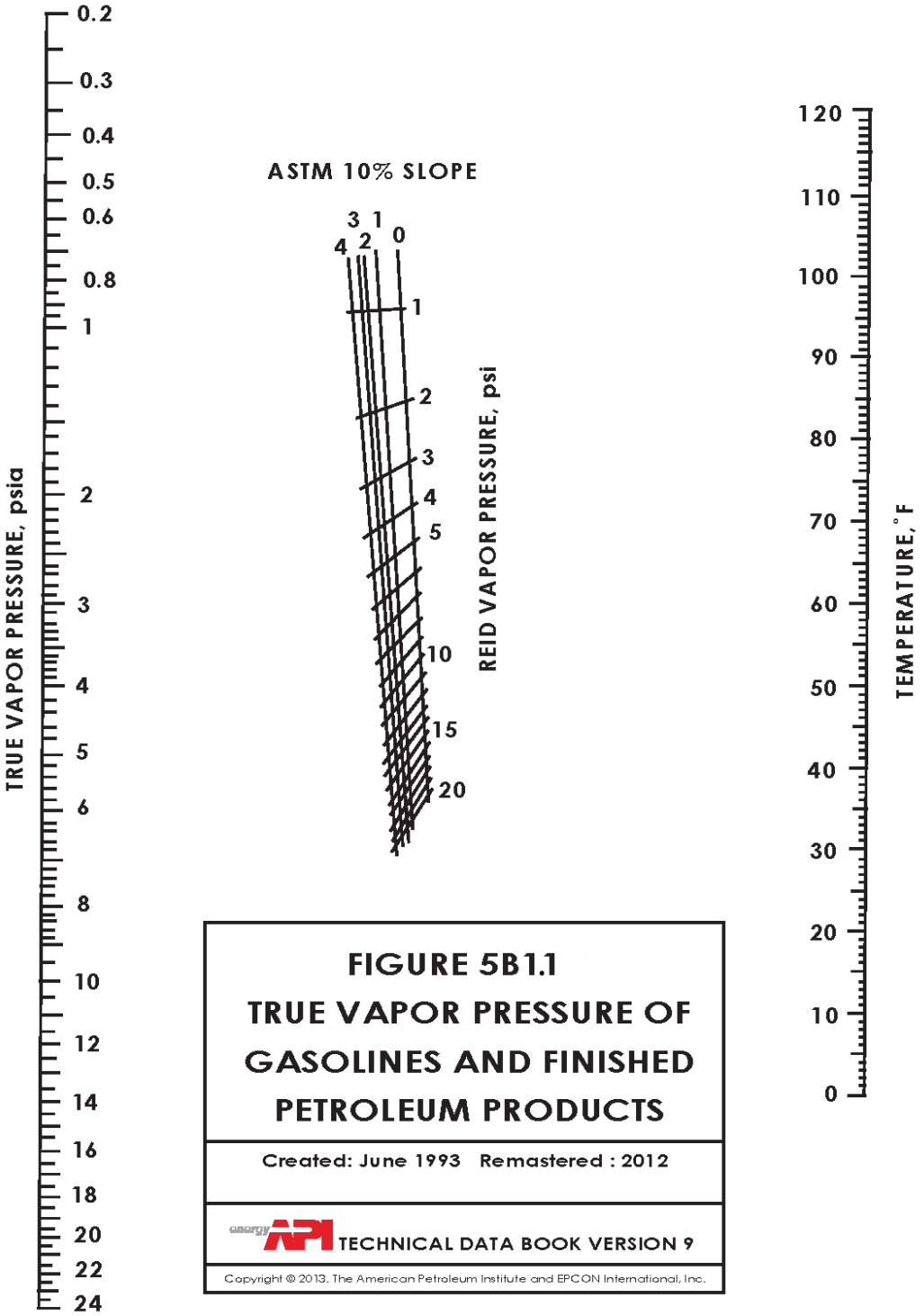


Figure 5A1.21 – Watson K – Correction for Procedure 5A1.19



5B Reid Vapor Pressure and True Vapor Pressure

Figure 5B1.1 – True Vapor Pressure of Gasolines and Finished Petroleum Products



Comments on Figure 5B1.1

Purpose

Figure 5B1.1 is useful for estimating the true vapor pressure (TVP) of a gasoline or a finished petroleum product at normal storage temperatures. Figure 5B1.2 is recommended for estimating the true vapor pressure of crude oils.

Reliability

No estimate of the reliability of this figure is available.

Notation

Slope = slope of the ASTM D86 distillation curve at ten percent by volume distilled = $\frac{T_{15}-T_5}{10}$, in °F/ % distilled.

Special Comments

In the absence of distillation data, these approximate values of the ASTM ten percent slope may be used:

Motor gasoline	3	Light naphtha (9 to 14 psi RVP)	3.5
Aviation gasoline	2	Naphtha (2 to 8 psi RVP)	2.5

The following equation can be used instead of Figure 5B1.1:

$$TVP = exp\Big[A + B\sqrt{S} + C\,ln(RVP) + D\sqrt{S}\,ln(RVP) + P \times RVP + \big(E + G\sqrt{S} + H\sqrt{S}\,ln(RVP) + O \times RVP\big) \times T + \big[ZI + ZJ\sqrt{S} + ZK\,ln(RVP) + ZL\sqrt{S}\,ln(RVP) + ZM \times RVP + ZN(RVP)^2\big] \times \left(\frac{1}{T}\right)\Big] \quad (5B1.1.\text{-}1)$$

Where:

T	=	*temperature, in °R*
S	=	*ASTM 10%* $\frac{°F}{\%\ distilled}$
RVP	=	*Reid vapor pressure, in psi*
A	=	*21.36512862*
B	=	*–6.7769666*
C	=	*–0.93213944*
D	=	*1.42680425*
E	=	*–0.00568374*
G	=	*0.00477103*
H	=	*–0.00106045*

ZI	=	*–10177.78660360*
ZJ	=	*2306.00561642*
ZK	=	*1097.68947465*
ZL	=	*–463.19014182*
ZM	=	*65.61239475*
ZN	=	*0.13751932*
O	=	*0.00030246*
P	=	*–0.29459386*

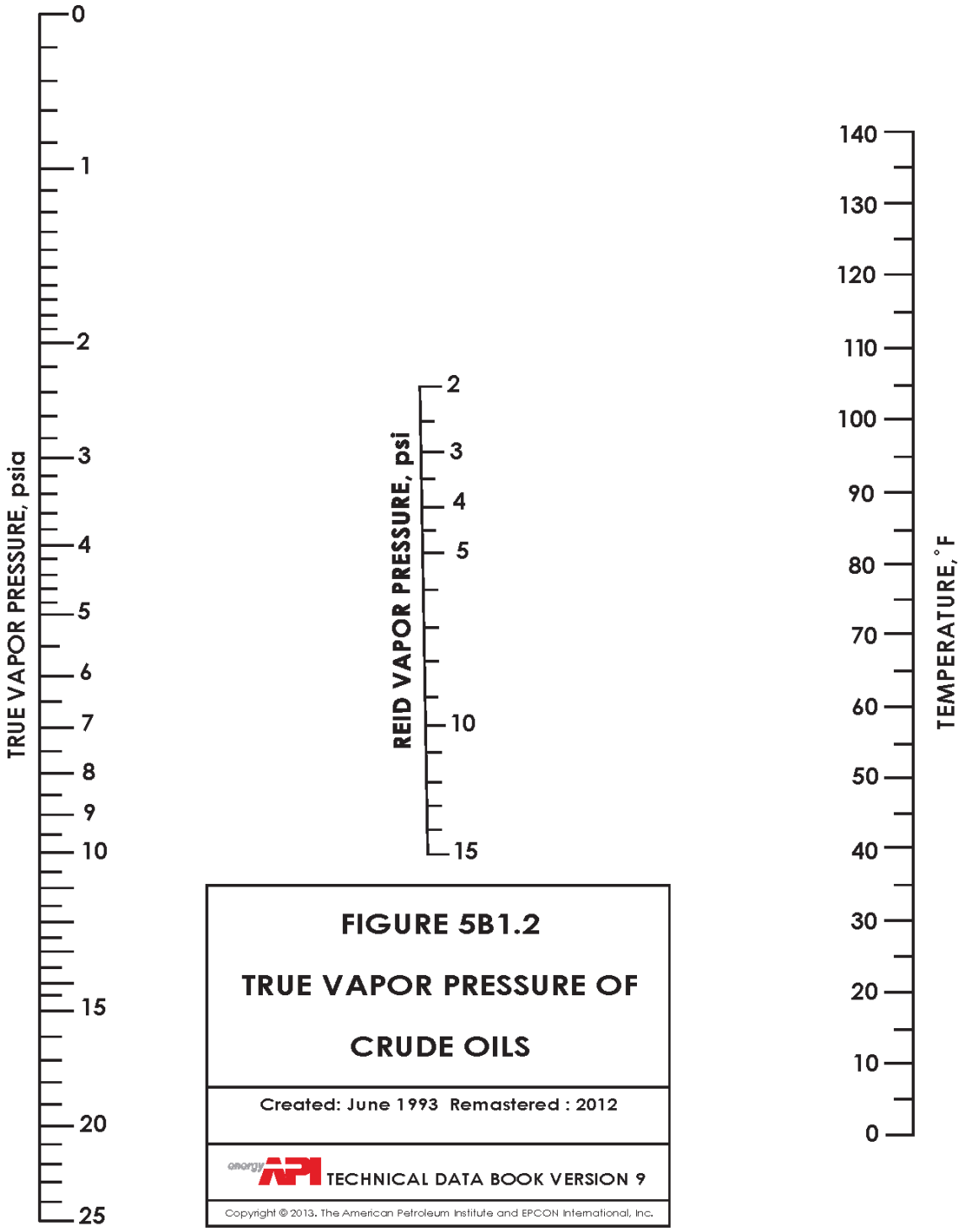
Literature Source

The figure is given in *API Bull. 2513*: *Evaporative Loss in the Petroleum Industry-Causes and Control*, American Petroleum Institute, New York (1959, Reaffirmed 1973). The equations were derived in API Publication 2517: Evaporative Loss from External Floating Roof Tanks" Third edition, 1989.

Example

Estimate the TVP at 70 °F of naphtha having a ten percent ASTM slope of 3.5 and a Reid vapor pressure (RVP) of 11 psi. Locate the point on the grid of Figure 5B1.1 corresponding to a slope of 3.5 and RVP of 11 psi. A straight line extended from the 70 °F point on the temperature scale through this grid point intersects the TVP scale at 6.9 psia.

Figure 5B1.2 – True Vapor Pressure of Crude Oils



Comments on Figure 5B1.2

Purpose

Figure 5B1.2 is useful for estimating the true vapor pressure (TVP) of a crude oil at normal storage temperatures. Figure 5B1.1 is recommended for estimating the true vapor pressures of gasolines and finished products.

Reliability

No estimate of the reliability of this figure is available.

Special Comments

The following equation can be used instead of Figure 5B1.2.

$$ln(TVP) = A + B\,ln(RVP) + C(RVP) + DT + \frac{(E + F\,ln(RVP) + G(RVP)^4)}{T} \qquad (5B1.2\text{-}1)$$

Where:

T	=	*Temperature, in °R*
RVP	=	*Reid vapor pressure, in psi*
TVP	=	*True vapor pressure, in psi*
A	=	*7.78511307*
B	=	*–1.08100387*
C	=	*0.05319502*
D	=	*0.00451316*
E	=	*–5756.85623050*
F	=	*1104.41248797*
G	=	*–0.00068023*

Applicable Ranges:

0 °F < *T* (°F) < 140 °F and 2 psi < *RVP* < 15 psi

Literature Source

The figure was given in API Bull. 2513: *Evaporation Loss in the Petroleum Industry-Causes and Control,* American Petroleum Institute, New York (1959, Reaffirmed 1973). Also API Publication 2517, Third Edition, February 1989.

Example

Estimate the *TVP* at 70 °F of a crude oil having an *RVP* of 6 psi. A straight line on the Figure 5B1.2 connecting the 70 °F point on the temperature scale and the 6 psi *RVP* point intersects the *TVP* scale at 4.2 psia.

Procedure 5B1.3 – Blending Method for Reid Vapor Pressure

Discussion

This procedure was last updated in 1999. This procedure estimates the Reid vapor pressure for a blend of pure components and/or petroleum fractions. The Reid vapor pressure of each stream and the molar blending ratio are required for this method. The Reid vapor pressure of the blend is estimated from:

$$RVP_b = \left(\sum_i v_i RVP_i^{\alpha} \right)^{1/\alpha} \qquad (5B1.3\text{-}1)$$

Where:

RVP_b	=	*Reid vapor pressure of the blend, in psi*
α	=	*1.2*
v_i	=	*volume fraction of stream i*
RVP_i	=	*Reid vapor pressure of stream i, in psi*

For a pure component, RVP_i is taken as the pure component true vapor pressure at 100 °F.

This procedure is not recommended for widely dissimilar components or streams.

Procedure

Step 1: *Obtain the vapor pressure of pure components at 100 °F from the pure component properties tables or the Reid vapor pressure of any stream.*

Step 2: *Calculate the Reid vapor pressure of the blend from Equation (5B1.3-1).*

Comments on Procedure 5B1.3

Purpose

This procedure is used to estimate the Reid vapor pressure of a blend of components with known Reid vapor pressures, as defined in ASTM Procedure D323-94.

Limitations

This method is limited to pure components and petroleum fractions. It is not recommended for widely dissimilar blends.

Reliability

This procedure has not been extensively tested. For applicable systems, the method is on average accurate to within 1 psi. Higher errors can be expected for mixtures of unlike components.

Example

Estimate the Reid vapor pressure of a blend that contains 7.56 gallons of tert-butyl ethyl ether and 92.44 gallons of isopentane.

Step 1: From the pure component properties tables, obtain needed data.

Step 2: Calculate the Reid vapor pressure of the blend using equation (5B1.3-1).

$$RVP_b = (0.0756(4.1478)^{1.2} + 0.9244(20.4643)^{1.2})^{1/1.2}$$

$$RVP_b = 19.2 \text{ psi}$$

An experimental Reid vapor pressure for this blend is 19.0 psi.

Procedure 5B1.4 – Prediction of Reid Vapor Pressure

Discussion

This procedure was last updated in 1999.This procedure predicts the Reid vapor pressure of a fully defined mixture by simulating ASTM Procedure D323-94. If it is necessary to simulate a partially undefined mixture such as a petroleum fraction or a crude oil, please see the special comments for this procedure.

The method calculates the Reid vapor pressure of the liquid sample in two steps. First, the chilled sample is saturated with air. Then, one part of the sample is mixed with four parts by volume of air at 100 °F and atmospheric pressure. This mixture is then flashed at 100 °F and a constant total volume. The calculated flash pressure is then corrected to obtain the Reid vapor pressure.

Procedure

Step 1: *The input to this procedure is a liquid sample of known molar composition. For each component of the input, and for oxygen and nitrogen, obtain the molecular weight, critical temperature, critical pressure, acentric factor, Z_{RA} (a constant from Table 6A1.2), and the S_2 term from Table 8D1.3.*

Step 2: *Saturate the sample with air using Procedure 8D1.1. The flash is conducted at 33 °F and 14.696 psia. The feed to the flash is 98 mole % sample and 2% bone dry air. The liquid from this flash is used for the remainder of the simulation.*

Step 3: *Use Procedure 6A2.1 to calculate the liquid density of the liquid product from Step 2 in units of pound moles per cubic foot.*

Step 4: *One cubic foot of the sample is fed to the second flash. Multiply the liquid density by one cubic foot to obtain the total pound moles that will be fed to the second flash. The pound moles of each individual component are obtained by multiplying the total pound moles by the liquid mole fractions from the first flash.*

Step 5: *Calculate the pound moles of air needed for a 4 to 1 vapor to liquid ratio at the start of the second flash. The air is fed to the flash at 100 °F and 14.696 psia. From the ideal gas law, 0.0079 pound moles of nitrogen and 0.0021 pound moles of oxygen are required.*

Step 6: *Sum the pound moles of both the liquid sample from Step 4 and the vapor from Step 5 to obtain the total pound moles in the mixed feed. The mole fraction of each component in the feed is obtained by dividing the pound moles of the component by the total pound moles.*

Step 7: *Flash the mixed feed at 100 °F and a constant volume of 5 ft^3 using Procedure 8D1.1. Iterate on the pressure until the volumes of the two phases sums to 5 ft^3. The volumes of the phases are found with a material balance calculation and appropriate density equation. For the vapor phase, calculate the density from the gas law with a compressibility factor from the flash calculation. Procedure 6A2.1 is recommended for determining the liquid density.*

Step 8: *Subtract 14.696 psi from the flash pressure. The resulting value is the predicted Reid vapor pressure.*

Comments on Procedure 5B1.4

Purpose

This procedure is used to simulate ASTM Reid vapor pressure experimental procedures.

Limitations

The Reid vapor pressure experiments are highly sensitive to the presence of trapped gases and light hydrocarbons. If gases or paraffins with a carbon number less than seven are present in the mixture, reliable predictions are only possible if the mole fractions of these light components are accurately measured.

This method does not account for water in the atmosphere because the experimental procedure does not require any correction for moisture or any record of the moisture content of the air. Further, calculations made while creating this method demonstrated that the presence of water had negligible impact on the predicted Reid vapor pressure.

Reliability

For defined mixtures, the method reproduces experimental data to an average deviation of 0.6 psi. For petroleum fractions and whole crude oils, the average deviation from experimental data is 0.8 psi.

Example A

Simulate the Reid experiment for a mixture that is 93.57 mole % isopentane and 6.43 mole % ethyl- tert-butyl ether (ETBE). The required parameters for isopentane, ETBE, nitrogen, and oxygen are listed below.

	Molecular Weight	T_c (°F)	P_c (psia)	Acentric Factor	Z_{RA}	S_2
Isopentane	72.15	369.10	490.38	0.2275	0.2718	–0.003898
ETBE	102.18	465.53	440.92	0.2957	0.2726	0.046280
Oxygen	32.00	–181.43	731.44	0.0222	0.2890	0.0
Nitrogen	28.01	–232.51	493.14	0.0377	0.2893	–0.011 016

Use Procedure 8D1.1 to perform a flash calculation at 33 °F and 14.7 psia of the sample saturated with 2 mole% air.

Component	Mole Fraction Feed	Mole Fraction Liquid
Isopentane	0.9170	0.9338
ETBE	0.0630	0.0648
Oxygen	0.0042	0.0005
Nitrogen	0.0158	0.0009

From Procedure 6A2.1, the liquid density of the saturated sample is 0.5483 lb-mole/ft^3.

One cubic foot that contains 0.5483 pound mole of sample will be fed to the second flash calculation. To determine the pound moles of each component, multiply by liquid mole fractions from first flash calculation.

Component	Pound Moles
Isopentane	0.5120
ETBE	0.0355
Oxygen	0.0003
Nitrogen	0.0005

Add 0.0077 pound mole of nitrogen and 0.0021 pound mole of oxygen to the feed. Calculate the mole fraction of each component in the feed.

Component	Pound Moles	Mole Fraction
Isopentane	0.5120	0.9174
ETBE	0.0355	0.0636
Oxygen	0.0024	0.0043
Nitrogen	0.0082	0.0147
Total	**0.5581**	

Using procedure 8D1.1, perform a flash calculation on this feed at 100 °F and a constant volume of 5 ft^3. The flash pressure is found to be 33.8 psia by iteration. Subtracting atmosphere pressure from the flash pressure yields the predicted Reid vapor pressure of 19.1 psi. The experimental value for this system from Wiltec Research Co. is 19.0 psi.

Special Comments

This procedure requires a fully defined mixture as a feed stream. However, for petroleum fractions and whole crude oils, it is expensive to fully define the mixture. Therefore, it is possible to treat the components of a complex mixture as a blend of real pure components and a pseudocomponent.

Accurate predictions are only possible if the light components, trapped gases and paraffins up to a carbon number of 6, are treated as real components. The heavy residual can then be treated as a single pseudocomponent created from distillation data. The following steps are recommended for generating the pseudocomponent. This procedure will require the specific gravity of the sample and the true boiling distillation that can be estimated from a D86 distillation. It is also necessary to know the volume percentage of the entire light end. This percentage will be called the break volume. In other words, the break volume is the point at which the distillation goes from defined components to the pseudocomponents.

Step 1: *Calculate the volume average boiling point (VABP) using Equation 2.0-3.*

Step 2: *Use Procedure 2B1.1 to calculate the mean average boiling point (MeABP).*

Step 3: *Calculate the sample's Watson K from Equation 2-0.8.*

Step 4: *Determine the volume percent at which one half of the residual is distilled. The calculation is accomplished by taking the average of the break volume and 100%. The result is called the residual's midpoint volume.*

Step 5: *Interpolate from the true boiling point data to find the true boiling temperature at which the residual's midpoint volume will occur. This temperature is assumed to be the residual's mean average boiling point.*

Step 6: *Assume that the Watson K is constant for the entire sample. Calculate a specific gravity for the residuals from the definition of the Watson K.*

Step 7: Characterize the pseudocomponent using

Critical Temperature	*Procedure 4D3.1*
Critical Pressure	*Procedure 4D4.1*
Acentric Factor	*Procedure 2B3.1*
Molecular Weight	*Procedure 2B2.1*

The Z_{RA} parameter can be obtained from Procedure 6A1.1 using the calculated specific gravity. The S_2 parameter is set equal to zero for pseudocomponents.

Example B

Create a heavy residual pseudocomponent for a crude oil given the following data.

Volume % distilled	10	30	50	70	90
True Boiling Temperature (°F)	170.6	350.6	540.5	760.8	1141.3

The specific gravity is 0.8445. The light end is known to be 8.86 vol. % (the break volume) of the sample.

Calculate the volume average boiling point:

$$VABP = (170.6 + 350.6 + 540.5 + 760.8 + 1141.3)/5 = 592.8\ °F$$

From Procedure 2B1.1, the mean average boiling point is 587.4 F. The Watson *K* is 12.02.

From the break volume of 8.86%, the residual midpoint is calculated as:

$$\frac{8.86\% + 100\%}{2} = 54.43\%$$

Interpolating with the distillation data gives a mean average boiling point for the residual of 589.3 F. The specific gravity of the residual is calculated as:

$$SG = \frac{(589.3 + 459.67)^{1/3}}{12.02} = 0.8453$$

The pseudocomponent is then characterized as:

Critical Temperature (4D3.1)	*920.0 °F*
Critical Pressure (4D4.1)	*220.4 psia*
Acentric Factor (2B3.1)	*0.6488*
Molecular Weight (2B2.1)	*248.0*
Z_{RA} (6A2.13)	*0.2419*

For whole crude oils, if the atmospheric residuum of a crude oil is not known, the physical properties of the atmospheric residuum of another crude oil may be substituted with little additional loss of accuracy. It is therefore possible to predict the Reid vapor pressure of a crude

oil from the light end compositions and a reference heavy residual. This approach is not recommended for light or narrow boiling fractions.

Procedure 5B1.5 – Prediction of ASTM D6377 Test Method for Determination of Vapor Pressure of Crude Oil: VPCRx (Expansion Method)

Discussion

This procedure was last updated in 2026. This procedure predicts the vapor pressure of a fully defined mixture by simulating ASTM Procedure D6377. If it is necessary to simulate a partially undefined mixture such as a petroleum fraction or a crude oil, please see the special comments for this procedure. D6377 allows specification of both a temperature series and a V/L series. The mixture is flashed at the specified temperature and initial pressure guess. The V/L is then calculated and the flash pressure adjusted until the specified V/L is obtained.

Procedure

Step 1: *The input to this procedure is a liquid sample of known molar composition. For each component of the input obtain the molecular weight, critical temperature, critical pressure, acentric factor, Z_{RA} (a constant from Table 6A1.2), and the S_2 term from Table 8D1.3.*

Step 2: *Determine the bubble point pressure at the specified temperature using Procedure 8D1.1.*

Step 3: *Flash the feed at the specified temperature at an initial pressure guess which is below the bubble point pressure using Procedure 8D1.6. A reasonable first guess is 80% of the bubble pressure.*

Step 4: *Calculate the vapor molar density from the gas law with the vapor phase compressibility factor determined during the last step of the flash calculation. Calculate the liquid molar density according to Procedure 6A2.1. Calculate the vapor volume by dividing the lbmoles vapor by the vapor molar density and the liquid volume by dividing the lbmoles liquid by the liquid molar density.*
Calculate the vapor to liquid volume ratio, V/L

Step 5: *Repeat step 4 and adjust the pressure until the desired V/L ratio is obtained. If V/L is below the target, lower the pressure further (e.g. 80% of previous guess). If V/L is above the target, raise the pressure (e.g. half-way between two guesses that bracket the desired V/L value, note that at the bubble point V/L = 0).*

Purpose

This procedure is used to simulate the ASTM D6377 Test Method for Determination of Vapor Pressure of Crude Oil: VPCRx (Expansion Method).

Limitations

True vapor pressure measurements and calculations are highly sensitive to the quantity of light gases and hydrocarbons present. The mole fractions of light gases and hydrocarbons with less than seven carbons greatly influence the accuracy of these predictions.

Reliability

The largest source of error in the method is the accuracy of the lights in the measured composition.

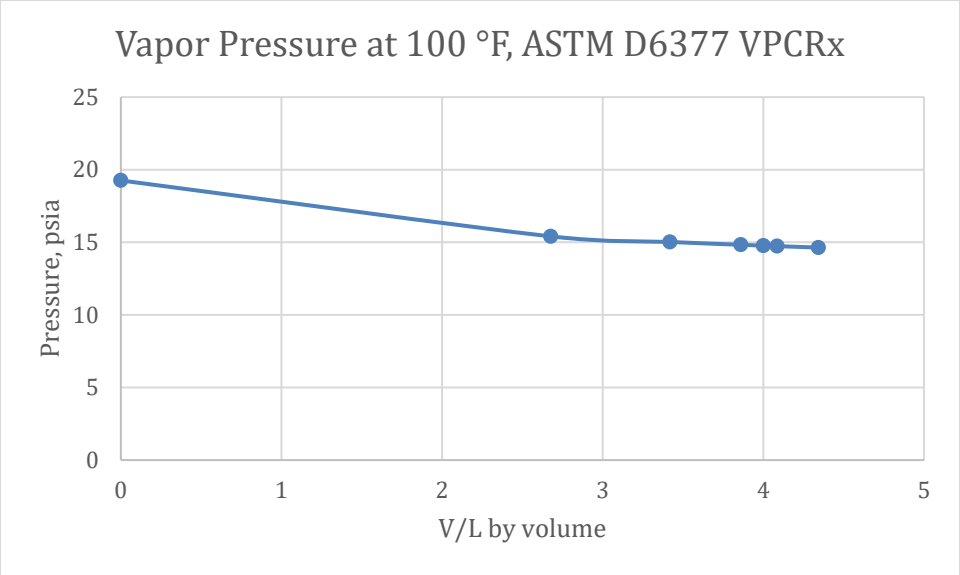
Example A

Simulate the vapor pressure of the mixture given below at 100 °F and V/L ratios of 0 (bubble point) and 4. The C7+ fraction is characterized as pentadecane. The required parameters are listed in the following table:

Component	Mole %	MW	Tc (°F)	Pc (psia)	w	Z_{RA}	S_2
Methane	0.134	16.042	-116.7	667.03	0.01155	0.2896	-0.01222
Ethane	0.358	30.069	89.906	706.62	0.09949	0.281	-0.01242
Propane	1.221	44.096	206.02	616.12	0.15229	0.2766	-0.00379
Isobutane	3.706	58.122	274.37	527.94	0.18352	0.2752	0.00301
n-Butane	3.706	58.122	305.55	550.56	0.20016	0.273	0.006209
Neopentane	0.299	72.149	321.17	463.54	0.19566	0.2718	0.000695
Isopentane	13.435	72.149	369.05	490.23	0.22788	0.2716	-0.00535
n-Pentane	14.928	72.149	385.79	488.78	0.25151	0.2686	-0.00636
Isohexane	24.999	86.175	436.19	440.91	0.27915	0.2689	-0.0039
n-Hexane	16.125	86.175	454.01	438.74	0.30126	0.2645	-0.00746
n-Pentadecane	21.090	212.415	814.73	214.66	0.68632	0.2384	-0.03363

Using procedure 8D1.1, perform a flash calculation on this feed at 100 °F and the specified volumetric V/L. The liquid density of the saturated sample is calculated using Procedure 6A2.1 and the vapor density is from the SRK calculation. The iteration history is given below along with a graph of pressure versus V/L.

Pressure	V/L	Density, lbmol/ft3		V/L	Next	
psia	molar	Liquid	Vapor	volume	Pressure	Method
19.26	0	0.3792	3.29E-03	0.00	15.408	80% of value
15.408	1.87E-02	0.3771	2.63E-03	2.68	12.326	80% of value
12.326	9.28E-02	0.3694	2.10E-03	16.31	13.867	Bisection of bounding values
13.867	4.37E-02	0.3744	2.37E-03	6.91	14.638	Bisection of bounding values
14.638	2.89E-02	0.3760	2.50E-03	4.34	15.023	Bisection of bounding values
15.023	2.33E-02	0.3765	2.57E-03	3.42	14.830	Bisection of bounding values
14.830	2.60E-02	0.3763	2.54E-03	3.86	14.734	Bisection of bounding values
14.734	2.73E-02	0.3760	2.51E-03	4.09	14.771	Secant Guess of bounding values
14.771	2.69E-02	0.3764	2.53E-03	4.00		



The calculated bubble point at 100 °F is 19.26 psia, with a liquid density of 0.3792 lbmol/ft3 and an equilibrium vapor density of 0.00329 lbmol/ft3.

Special Comments

This procedure requires a fully defined mixture as a feed stream. However, for petroleum fractions and whole crude oils, it is possible to treat the components of the complex mixture as a blend of pure components and pseudocomponents. The most accurate predictions are realized when the light gases and hydrocarbons up to a carbon number of 6 are treated as pure components. The residual can then be treated as either a single pseudocomponent or as a distribution of pseudocomponents created from distillation data. The following steps are recommended to generate the pseudocomponents. This procedure will require the specific gravity of the sample and the true boiling distillation which can be estimated from D86 distillation data. The volume percentage of the entire light end is also required. This percentage will be called the break volume. In other words, the break volume is the point at which the distillation goes from defined components to the pseudocomponents.

Step 1: *Calculate the volume average boiling point (VABP) using Equation 2.0-3.*

Step 2: *Use Procedure 2B1.1 to calculate the mean average boiling point (MeABP).*

Step 3: *Calculate the sample's Watson K from Equation 2-0.8.*

Step 4: *Determine the volume percent at which one half of the residual is distilled. The calculation is accomplished by taking the average of the break volume and 100%. The result is called the residual's midpoint volume.*

Step 5: *Interpolate from the true boiling point data to find the true boiling temperature at which the residual's midpoint volume will occur. This temperature is assumed to be the residual's mean average boiling point.*

Step 6: *Assume that the Watson K is constant for the entire sample. Calculate a specific gravity for the residuals from the definition of the Watson K.*

Step 7: *Characterize the pseudocomponent using the following:*
Critical Temperature Procedure 4D3.1
Critical Pressure Procedure 4D4.1

Acentric Factor Procedure 2B3.1
Molecular Weight Procedure 2B2.1
The Z_{RA} parameter using equation 6A2.3-1 and specific gravity.
The S_2 parameter is zero for pseudocomponents.

Example B

Simulate the vapor pressure of the mixture given below at 100 °F and V/L ratios of 0 (bubble point), and 4.

Create a heavy residual pseudocomponent for a crude oil given the following data.

Volume % Distilled	TBP, °F
10	170.6
30	350.6
50	540.5
70	760.8
90	1141.3

The specific gravity is 0.8445. The light end is known to be 8.86 vol. % (the break volume) of the sample. Calculate the volume average boiling point.

$$VABP = \frac{(170.6 + 350.6 + 540.5 + 760.8 + 1141.3)}{5} = 592.8\ °\text{F}$$

From Procedure 2B1.1, the mean average boiling point is 587.4 F. The Watson K is 12.02.

From the break volume of 8.86%, the residual midpoint is calculated as:

$$\frac{8.86\% + 100\%}{2} = 54.43\%$$

Interpolating with the distillation data gives a mean average boiling point for the residual of 589.3 F. The specific gravity of the residual is calculated as:

$$SG = \frac{(589.3 + 459.67)^{\frac{1}{3}}}{12.02} = 0.8453$$

The pseudocomponent is then characterized as:

Critical Temperature (4D3.1) = 920.0 °F

Critical Pressure (4D4.1) = 220.4 psia

Acentric Factor (2B3.1) = 0.6488

Molecular Weight (2B2.1) = 248.0

Z_{RA} (6A2.13) = 0.2419

This approach is not recommended for light or narrow boiling fractions.

The composition including the lights is given in the following table:

Component	Mole %
Methane	0.5
Ethane	19.8
Propane	50
Isobutane	5
n-Butane	5
n-Pentane	9.7
n-Hexane	10
Pseudo 589.3 °F, 0.8453 sg	100

Using procedure 8D1.1, perform a flash calculation on this feed at 100 °F and the specified volumetric V/L. The liquid density of the saturated sample is calculated using Procedure 6A2.1 and the vapor density is from the SRK calculation. The iteration history is given below.

Pressure	V/L	Density, lbmol/ft3		V/L	Next	
psia	molar	Liquid	Vapor	volume	Pressure	Method
18.65	0	0.2194	3.13E-03	0.00	14.92	80% of value
14.92	9.16E-03	0.2183	2.52E-03	0.79	11.936	80% of value
11.936	1.87E-02	0.2172	2.00E-03	2.03	9.549	80% of value
9.549	2.78E-02	0.2162	1.60E-03	3.75	9.071	95% of value
9.071	2.97E-02	0.2159	1.52E-03	4.23	9.310	Bisection of bounding values
9.310	2.87E-02	0.2161	1.57E-03	3.95	9.191	Bisection of bounding values
9.191	2.92E-02	0.2160	1.54E-03	4.09	9.269	Secant Guess of bounding values
9.269	2.89E-02	0.2161	1.56E-03	4.00		

The calculated bubble point at 100 °F is 18.65 psia, with a liquid density of 0.2194 lbmol/ft3 and an equilibrium vapor density of 0.00313 lbmol/ft3. For V/L = 4 at 100 °F the pressure is 9.269 psia.

Example C

Simulate the vapor pressure of the Bakken mixture given below at 100 °F and V/L ratios of 0 (bubble point), and 4. The lights are characterized as pure components through n-heptane. Above n-heptane the heavies are characterized as pseudocomponents. The composition is listed in the following table and the pseudocomponents are characterized:

Component	Mass Fraction
Methane	0.000E+00
Ethane	3.000E-04
Propane	9.100E-03
i-Butane	5.700E-03
n-Butane	2.710E-02
Neopentane	2.000E-04
i-Pentane	1.540E-02
n-Pentane	2.720E-02
2.2-Dimethylbutane	9.000E-04
Cyclopentane	3.400E-03
2-Methylpentane	2.100E-02
n-Hexane	2.050E-02
Methylcyclopentane	1.760E-02
2,4-Dimethylpentane	1.300E-03
Benzene	1.100E-03
Cyclohexane	4.800E-03
1.1-Dimethylcyclopentane	3.250E-02
3-Methylhexane	1.710E-02
n-Heptane	1.800E-02
Pseudo260*	4.413E-02
Pseudo288*	4.726E-02
Pseudo316*	4.708E-02
Pseudo343*	4.636E-02
Pseudo371*	3.688E-02
Pseudo399*	3.729E-02
Pseudo427*	3.734E-02
Pseudo454*	3.524E-02
Pseudo482*	3.518E-02
Pseudo510*	3.416E-02
Pseudo537*	3.119E-02
Pseudo565*	3.175E-02
Pseudo593*	3.085E-02
Pseudo620*	2.815E-02
Pseudo648*	2.601E-02
Pseudo701*	6.888E-02
Pseudo798*	6.083E-02
Pseudo884*	4.161E-02
Pseudo1026*	5.657E-02

Pseudo	NBP (°F)	MW	60 F Density (lb/ft3)
Pseudo260*	260.18	101.18	48.57
Pseudo288*	287.97	107.69	49.20
Pseudo316*	316.28	115.34	49.72
Pseudo343*	342.81	123.06	50.30
Pseudo371*	371.49	132.33	50.86
Pseudo399*	399.28	141.44	51.43
Pseudo427*	426.89	151.02	51.98
Pseudo454*	454.45	161.19	52.51
Pseudo482*	482.32	171.96	53.04
Pseudo510*	509.58	183.02	53.55
Pseudo537*	537.34	194.83	54.04
Pseudo565*	565.32	207.24	54.55
Pseudo593*	592.61	219.77	55.03
Pseudo620*	620.23	232.76	55.50
Pseudo648*	647.90	245.96	55.96
Pseudo701*	700.87	271.12	56.84
Pseudo798*	797.77	322.55	58.33
Pseudo884*	883.74	376.84	59.68
Pseudo1026*	1025.86	455.08	61.57

Following the steps described in Procedure 5B1.5 and Examples A and B the following results are calculated.

Pressure	V/L	Density, lbmol/ft3		V/L	Next	
psia	molar	Liquid	Vapor	volume	Pressure	Method
13.609	0	0.348272	2.31E-03	0.00	10.887	80% of value
10.887	2.52E-02	0.344845	1.84E-03	4.85	12.248	Bisection of bounding values
12.248	1.13E-02	0.346717	2.08E-03	1.92	11.568	Bisection of bounding values
11.568	1.80E-02	0.345821	1.96E-03	3.23	11.228	Bisection of bounding values
11.228	2.15E-02	0.345343	1.90E-03	4.00		

The calculated bubble point at 100 °F is 13.61 psia, with a liquid density of 0.3483 lbmol/ft3 and an equilibrium vapor density of 0.00231 lbmol/ft3.

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