

Manual of Petroleum Measurement Standards Chapter 19.4

Evaporative Loss Reference Information and Speciation Methodology

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Evaporative Loss Reference Information and Speciation Methodology

1 Scope

This standard provides methodology to estimate emissions of individual hydrocarbon species using the total emissions of multicomponent hydrocarbon mixtures (such as crude oils and gasoline) estimated from API *MPMS* Chapter 19.1 for fixed-roof tanks, API *MPMS* Chapter 19.2 for floating-roof tanks, API *MPMS* Chapter 19.5 for marine vessels, and other methods used for total hydrocarbon emission estimates. This process is referred to as speciation.

Speciation of emissions from hydrocarbon mixtures accounts for the higher evaporation rate of the more volatile components, resulting in a different composition of the mixture in the vapor phase than in the liquid phase. The methodology presented in this standard assumes that there is sufficient liquid present such that the chemical composition at the liquid surface may be considered to not change as a result of the evaporative loss.

This standard also contains reference information used for estimating emissions in accordance with API *MPMS* Chapter 19.1, API *MPMS* Chapter 19.2, and API *MPMS* Chapter 19.5.

The methodology in this standard applies to:

- a) liquids with vapor pressure that has reached equilibrium with ambient conditions at a true vapor pressure less than the ambient atmospheric pressure (i.e. not boiling);
- b) liquids for which the vapor pressure is known or for which sufficient data are available to determine the vapor pressure;
- c) liquid mixtures where Raoult's Law can be used to describe the vapor phase equilibria.

This methodology does not apply to:

- a) emissions that result from leaks from piping components (e.g. valves, flanges, pumps, connectors);
- b) liquid mixtures where Raoult's Law cannot be used to describe the vapor phase equilibria (e.g. mixtures in which hydrocarbons are dissolved in water, or mixtures of hydrocarbons with alcohols).

2 Normative References

The following referenced documents are indispensable for the application of this document. For dated references, only the edition cited applies. For undated references, the latest edition of the referenced document (including any amendments) applies.

API *Manual of Petroleum Measurement Standards (MPMS)* Chapter 19.1, *Evaporative Loss from Fixed-Roof Tanks*, Fourth Edition, 2012

API *MPMS* Chapter 19.2, *Evaporative Loss from Floating-Roof Tanks*, Third Edition, 2012

API *MPMS* Chapter 19.5, *Atmospheric Hydrocarbon Emissions from Marine Vessel Transfer Operations*, First Edition, September 2009

3 Symbols

The following symbols, units, and source applies to this document.

NOTE Symbols used in [Annex I](#) are listed in [Section I.1](#).

A	vapor pressure constant; units—dimensionless; see Table 1 and Table 2
B	vapor pressure constant; units—°C or °R; see Table 1 and Table 2
C	vapor pressure constant; units—°C or °R; see Table 2
H_i	Henry's law constant for component i ; units—psia; see 7.3.4.2
I	daily total insolation on a horizontal surface; units—Btu/(ft ² day); see Reference [67]
K_i	vapor-liquid equilibrium constant of component i ; units—dimensionless; see 7.2
L_i	emissions of component i ; units—lb; see 5.1.3
L_t	total emissions of all components; units—lb; User
M_i	molecular weight of component i ; units—lb/lb-mole; see Reference [35]
M_L	stock liquid molecular weight; units—lb/lb-mole; see Table 1 and Table 2
M_V	stock vapor molecular weight; units—lb/lb-mole; see Table 1 and Table 2
P_A	atmospheric pressure at the tank site; units—psia; User
P_i	partial pressure of component i in the vapor; units—psia; see 5.1.3
P_i^o	saturated vapor pressure of component i ; units—psia; see 4.3
P_T	total system pressure; units—psia; User
P_V	stock true vapor pressure; units—psia; see 4.2
RVP	stock Reid vapor pressure; units—psi; User
S	stock ASTM D86 distillation slope at 10 volume % evaporated; units—°F/vol. %; see Table 1
T_{LA}	daily average liquid surface temperature; units—°R; see API MPMS Chapters 19.1 and 19.2
T_{MAX}	maximum ambient temperature; units—°F; see Reference [67]
T_{MIN}	minimum ambient temperature; units—°F; see Reference [67]
V	average ambient wind speed at the tank site; units—mi/hr; see Reference [67]
W_i	weight fraction of component i in the liquid; units—dimensionless; see 4.7
W_L	density of stock liquid; units—lb/gal; see Table 1 and Table 2
W_{VC}	density of condensed stock vapor; units—lb/gal; see Table 1
X_i	mole fraction of component i in the liquid; units—dimensionless; see 5.1.3
Y_i	mole fraction of component i in the vapor; units—dimensionless; see 5.1.3
z_i	weight fraction of component i in the vapor; units—dimensionless; see 5.1.3
α	tank surface solar absorptance; units—dimensionless; see Table 6
α_R	tank roof surface solar absorptance; units—dimensionless; see Table 6
α_S	tank shell surface solar absorptance; units—dimensionless; see Table 6

4 Variables

4.1 Meteorological Data

Meteorological data may be used to determine vapor space, liquid bulk, and liquid surface temperatures for storage tanks and can be obtained from local weather records or from historical averages from the National Renewable Energy Laboratory. The data provide 30-year averages for the years 1961 through 1990 ^[67].

API *MPMS* Chapter 19.1 provides methods for determining tank temperatures for fixed-roof tanks. API *MPMS* Chapter 19.2 provides methods for determining tank temperatures for floating-roof tanks. [Annex I](#) of this standard documents these methods.

4.2 Stock True Vapor Pressure P_v

For storage of pure chemicals, the stock true vapor pressure can be calculated using Antoine's equation, as set forth in [4.3](#).

For selected petroleum liquids, such as gasoline, jet fuels, and No. 2 fuel oil (diesel), the stock true vapor pressure, P_v , can be calculated from Equation (5) using the constants A and B given in [Table 1](#).

For other volatile refined petroleum stocks and crude oils, values for the vapor pressure constants A and B may be calculated as described below, and then the stock true vapor pressure calculated from Equation (5) using the constants A and B thus determined.

- a) For refined petroleum stocks: The vapor pressure constants A and B are calculated from Equation (1) and Equation (2), based on the stock RVP (1 psi to 20 psi) and the slope of the ASTM D86 distillation curve, S , at 10 volume percent evaporated ($^{\circ}\text{F}/\text{vol. } \%$). In the absence of ASTM D86 distillation data on refined petroleum stocks, approximate values of the distillation slope S from [Table 1](#) may be used.

$$A = 15.64 - 1.854 - (0.8742 - 0.328) \text{ in (RVP)} \quad (1)$$

$$B = 8742 - 1042 - (1049 - 179.4) \text{ in (RVP)} \quad (2)$$

The true vapor pressure of refined stocks can also be determined using ASTM D2879 ^[50], particularly for refined stocks that have a vapor pressure below the RVP lower bound of 1 psi. ASTM D2879 allows direct measurement of true vapor pressure at specified temperatures, thereby avoiding any bias or uncertainty that may be associated with the RVP correlations of Equation (1) and Equation (2). Values for the vapor pressure constants A and B may be determined from a regression of the direct measurement data. ASTM D2879 may not be appropriate for mixtures that contain highly volatile components, in that the degassing step of ASTM D2879 may drive these components out of the sample prior to analysis.

- b) For crude oils: The vapor pressure constants A and B are calculated from Equation (3) and Equation (4) based on the RVP (2 psi to 15 psi):

$$A = 12.82 - 0.9672 \text{ in (RVP)} \quad (3)$$

$$B = 7261 - 1216 \text{ in (RVP)} \quad (4)$$

These RVP correlations have a bias that overstates the true vapor pressure of crude oils which are not live at storage conditions, as that term is defined in ASTM D6377 ^[51]. The error is particularly pronounced at the high and low ends of the RVP range and is less significant for mid-grade crude oils. On the other hand, the RVP method of sample collection and preparation may result in the loss of highly volatile components from samples of live crude oil, thereby resulting in an understatement of the true vapor pressure.

For heavy crude oils, the vapor pressure can be determined using the HOST test method described in [Annex E](#).

For crude oils with a vapor pressure between 25 kPa and 180 kPa at 37.8 °C (3.6 psia to 26 psia at 100 °F), true vapor pressure can be determined directly through ASTM D6377 ^[51]. This method allows direct measurement of true vapor pressure over a range of specified temperatures, thereby avoiding any bias or uncertainty that may be associated with the RVP correlations of Equation (3) and Equation (4). Values for the vapor pressure constants A and B may be determined from a regression of the direct measurement data.

The stock true vapor pressure P_v is calculated from the Clausius-Clapeyron equation:

$$P_v = \exp \left[A - \frac{B}{(T_{LA} + 459.7)} \right] \quad (5)$$

This may also be expressed as:

$$P_v = e \left[A - \frac{B}{(T_{LA} + 459.7)} \right] \quad (5)$$

Alternately, if the stock's normal boiling point and API gravity are reliably known, the true vapor pressure can be determined using the Maxwell-Bonnell correlation described in [Annex D](#).

Table 1—Typical Properties of Selected Petroleum Liquids

Petroleum Liquid Mixture	Vapor Molecular Weight ^a	Liquid Molecular Weight ^b	Condensed Vapor Density (at 60 °F) ^c (see Note 1)	Liquid Density ^a (see Note 2)	ASTM D86 Distillation Slope ^d	Vapor Pressure Equation Constants ^e		True Vapor Pressure (at 60 °F) (see Note 3)
	M_v	M_L	W_{vc}	W_L	S	A	B	P_v
	lb/lb-mole	lb/lb-mole	lb/gal	lb/gal	°F/vol %	dimensionless	°R	psia
Midcontinent Crude Oil	50	207	4.5	7.1	—	Equation (3)	Equation (4)	—
Refined Petroleum Stocks	—	—	—	—	—	Equation (1)	Equation (2)	—
Motor Gasoline RVP 13	62	92	4.9	5.6	3.0	11.644	5043.6	7.0
Motor Gasoline RVP 10	66	92	5.1	5.6	3.0	11.724	5237.3	5.2
Motor Gasoline RVP 7	68	92	5.2	5.6	3.0	11.833	5500.6	3.5
Light Naphtha RVP 9–14	—	—	—	—	3.5	—	—	—
Naphtha RVP 2–8	—	—	—	—	2.5	—	—	—
Aviation Gasoline	—	—	—	—	2.0	—	—	—
Jet Naphtha (JP-4)	80	120	5.4	6.4	—	11.368	5784.3	1.3
Jet Kerosene (Jet A)	130	162	6.1	7.0	—	12.390	8933.0	0.008
No. 2 Fuel Oil (Diesel)	130	188	6.1	7.1	—	12.101	8907.0	0.006
No. 6 Fuel Oil	130	387	6.4	7.9	—	10.781	8933.0	0.002
Vacuum Residual Oil ^f	190	387	6.4	7.9	—	10.104	10,475.5	0.00004

NOTE 1 Condensed vapor density is not used to estimate or speciate emissions but is used to convert pounds of emissions to equivalent gallons. This may have application to inventory reconciliation but is typically not needed for reporting emissions. For multicomponent petroleum liquids, the condensed vapor density, W_{vc} , is less than the stock liquid density, W_L . If the condensed vapor density is unknown, it may be estimated from the following equation ^e (which was developed primarily for gasoline stocks): $W_{vc} = 0.08 M_v$

NOTE 2 Liquid density is not used to speciate emissions, but it is a required property for estimating working (clingage) loss from a floating-roof tank.

NOTE 3 True vapor pressure is calculated from Equation (5).

- ^a U.S. EPA Report AP-42, Fifth Edition, November 2006 ^[15], Table 7.1-2.
- ^b Liquid molecular weights from “Memorandum from Patrick B. Murphy, Radian/RTP to James F. Durham, EPA/CPB Concerning Petroleum Refinery Liquid HAP and Properties Data, August 10, 1993,” as adopted in versions 3.1 and 4.0 of EPA’s TANKS software.
- ^c API *MPMS* Chapter 19.1, Third Edition ^[3], 19.1.2.2.2.13.
- ^d API 2518 June 1962 ^[47], Figure 1.
- ^e For motor gasolines, see API 2519, Third Edition, Figure 4; for crude oil, see API 2519, Third Edition, Figure 5; for Jet Naphtha, Jet Kerosene, and No. 2 Fuel Oil, see Barnett and Hibbard ^[39]; for No. 6 Fuel Oil, see [Annex G](#).
- ^f Properties given for Vacuum Residual Oil are those given for Residual Fuel Oil No. 6 in API *MPMS* Chapter 19.4, Second Edition ^[41], Table 1.

4.3 Component Saturated Vapor Pressure P_i^o

A component's saturated vapor pressure, P_i^o , can be calculated using Antoine's equation:

$$P_i^o = 0.019337 \log^{-1} \left[A - \frac{B}{(T_{LA} - 32) 5/9 + C} \right] \quad (6)$$

This may also be expressed as:

$$P_i^o = (0.019337) 10 \left[A - \frac{B}{(T_{LA} - 32) 5/9 + C} \right] \quad (6)$$

where

P_i^o is the vapor pressure, at temperature T_{LA} , of component i (psia),

T_{LA} is the stock liquid surface temperature (°F), and

A, B, C are Antoine constants. The Antoine constants A , B , and C for selected petrochemicals are given in [Table 2](#). Antoine's equation is discussed further in [Annex B](#). The units conversion term, 0.019337, has units of (psia/mmHg).

If Antoine constants for a particular component are not available, the vapor pressure may be found from published values of vapor pressure at given increments of temperature ^[22, 23]. For estimating vapor pressure at a particular temperature T that is not listed, the following relationship should be used:

$$\log P_i^o = \log P_1 + \left[\frac{\frac{1}{T} - \frac{1}{T_1}}{\frac{1}{T_2} - \frac{1}{T_1}} \right] \log \frac{P_2}{P_1} \quad (7)$$

where

P_1 vapor pressure at temperature T_1 , and

P_2 vapor pressure at temperature T_2 .

This is the equation of the line through the points $(1/T_1, \log P_1)$ and $(1/T_2, \log P_2)$ on a plot of $\log P$ versus $1/T$. This two-point linear interpolation equation draws upon the Clausius–Clapeyron equation (a simpler version of the Antoine equation) and provides a method whereby the equation of the line between two adjacent data points is used to relate pressure and temperature between these points. Use of this equation to extrapolate a value for P_i^o at a temperature outside of the range bounded by T_1 and T_2 may result in loss of accuracy.

4.4 Stock Liquid Molecular Weight M_L

The stock liquid molecular weight M_L is the average molecular weight of the stock liquid on a weight basis and can be determined by the following methods.

- [Table 1](#) gives typical stock liquid molecular weights for selected petroleum liquids.
- When the weight fractions are known for all the components of a stock liquid, the stock liquid molecular weight can be calculated as:

$$M_L = 1 / \sum (w_i / M_i) \quad (8)$$

where

w_i weight fraction of component i in the liquid phase, and

M_i molecular weight of component i (lb/lb-mole).

- c) Two analytical methods are available: gel permeation chromatography (GPC) using a refractive index (RI) detector, and gas chromatography (GC) using a flame ionization detector (FID). More information on these methods can be found in Reference [14].

4.5 Stock Vapor Molecular Weight M_v

The stock vapor molecular weight is the average molecular weight of the stock vapor on a weight basis. The stock vapor molecular weight may be determined by the following methods.

- a) [Table 1](#) gives typical stock vapor molecular weights for selected petroleum liquids.
- b) When the mole fractions are known for all the components of a stock vapor, the stock vapor molecular weight can be calculated as:

$$M_v = \sum(y_i M_i) \quad (9)$$

where

y_i = mole fraction of component i in the vapor phase, and

M_i = molecular weight of component i (lb/lb-mole).

- c) Vapor samples may be analyzed.

4.6 Component Molecular Weight M_i

Molecular weights for selected petrochemicals are given in [Table 2](#).

Table 2—Properties of Selected Petrochemicals (See Table Footnote a)

Chemical Name	CAS Registry No.	Molecular Weight	Liquid Density ^b (lb/gal)	True Vapor Pressure ⁱ at 60 °F (psia)	Antoine's Equation ^c					Normal Boiling Point (°F)
					Constants			Temperature Range ^d		
					<i>c</i>	<i>B</i> (°C)	<i>C</i> (°C)	Min. (°F)	Max. (°F)	
Acetaldehyde					8.063	1,637.1	295.47	32	94	
Acetic acid					7.557	1,642.5	233.39	63	244	
Acetic anhydride	00075-07-0	44.05	6.54 64	12.19						69
{acetic acid anhydride}	00064-19-7	60.05	8.72	0.176	7.122	1,427.8	198.04	145	283	244
Acetone					7.300	1,312.3	240.71	7	454	
Acetonitrile	00108-24-7	102.09	9.03	0.053	7.154	1,355.4	235.30	59	192	282
Acrylamide ^{m, n}	00067-64-1	58.08	6.55	2.921	11.293	3,939.9	273.16			133
Acrylic acid	00075-05-8	41.05	6.56	1.090						179
{2-propenoic acid}	00079-06-1	71.08	9.36	8.57E-05	5.652	648.6	154.68	68	158	379
Acrylonitrile										
{2-propenenitrile}	00079-10-7	72.06	8.77	1.344	6.942	1,255.9	231.30	−60	172	282
Allyl alcohol					11.658	4,510.2	416.80	70	207	
Allyl chloride ^e {3-chloro-1-propene}	00107-13-1	53.06	6.73	1.383	5.297	418.4	128.68	55	111	172
Aniline	00107-18-6	58.08	7.13	0.326	7.221	1,661.9	199.10	88	363	206
Benzene ^e	00107-05-1	76.52	7.83	4.702	6.906	1,211.0	220.79	46	217	113
Benz[a]anthracene j	00062-53-3	93.13	8.53	0.0058	11.528	5,461	273.15	219	260	363
Benzo[a]pyrene j	00071-43-2	78.11	7.32	1.171	12.482	6,181	273.15	185	316	176
Benzo[ghi]perylene j	00056-55-3	228.29		7.92E-10	11.820	6,580	273.15	391	513	820
Biphenyl ^e	00050-32-8	252.31		2.29E-11	7.245	1,998.7	202.73	156	520	923
Butadiene (1,3)	00191-24-2	276.33		2.07E-13						
{divinyl}	00092-52-4	154.21	8.68	2.37E-04	6.873	941.7	240.40	−104	29	489
Butane (n)					6.725	909.7	237.00	−108	31	
Butene (1)	00106-99-0	54.09	5.13	30.22	7.122	1,099.2	264.89	−108	25	24
Butene (cis-2)	00106-97-8	58.12	4.78	25.67	6.863	957.1	236.65	−94	73	32
Butene (2-methyl-1)	00106-98-9	56.11	4.91	30.83	6.862	1,047.8	232.06	34	145	21

Table 2—Properties of Selected Petrochemicals (See Table Footnote a) (Continued)

Chemical Name	CAS Registry No.	Molecular Weight	Liquid Density ^b (lb/gal)	True Vapor Pressure ⁱ at 60 °F (psia)	Antoine's Equation ^c					Normal Boiling Point (°F)
					Constants			Temperature Range ^d		
					<i>c</i>	<i>B</i> (°C)	<i>C</i> (°C)	Min. (°F)	Max. (°F)	
Butene (trans-2)	00590-18-1	56.11	5.14	22.62	6.919	982.2	242.38	−97	34	39
Butyl alcohol (<i>n</i>)	00563-46-2	70.13	5.43	8.257						88
{butanol (1)}	00624-64-6	56.11	5.00	24.97	7.421	1,351.6	179.81	73	244	34
Butyl alcohol (tert)										
{1,1-dimethyl ethanol}	00071-36-3	74.12	6.76	0.062	7.373	1,174.9	179.23	103	180	243
Butyl chloride (<i>-n</i>)										
{1-chloro-butane}	00075-65-0	74.12	6.58	0.424	6.871	1,182.9	218.27	2	173	180
Butyl ether (di-tert)					6.590	1,157.7	203.05	39	228	
Carbon disulfide	00109-69-3	92.57	7.40	1.255	6.942	1,168.6	241.53	38	176	170
Carbon tetrachloride	06163-66-2	130.23	6.39	0.381	6.898	1,221.8	227.41	68	172	224
Chlorobenzene	00075-15-0	76.14	10.54	4.817	6.986	1,435.7	218.03	144	269	115
Chlorobutane (2) ⁿ	00056-23-5	153.82	13.31	1.431	6.871	1,182.9	218.27	2	173	170
Chloroform	00108-90-7	112.56	9.23	0.134	7.083	1,233.1	232.20	−73	142	269
Chloroprene	00078-86-4	92.57	7.27	1.255						170
{2-chloro-1,3-butadiene}	00067-66-3	119.38	12.38	2.468	6.291	841.9	187.79	68	140	142
Chlorotoluene (<i>o</i>)										
{1-chloro-2methylbenzene}	00126-99-8	88.54	7.98	2.736	7.363	1,768.1	234.76	42	319	140
Chrysene ^j										
{benzo[a]phenanthrene}	00095-49-8	126.58	9.04	0.039	12.320	6,160	273.15	185	374	318
Cresol (<i>m</i>)										
{3-methyl-phenol}	00218-01-9	228.29	10.63	1.86E-11	7.477	1,833.1	196.74	301	394	838
Cresol (<i>o</i>)										
{2-methyl-phenol}	00108-39-4	108.14	8.63	0.0013	6.843	1,391.3	160.18	248	376	396
Cresol (<i>p</i>)										

Table 2—Properties of Selected Petrochemicals (See Table Footnote a) (Continued)

Chemical Name	CAS Registry No.	Molecular Weight	Liquid Density ^b (lb/gal)	True Vapor Pressure ⁱ at 60 °F (psia)	Antoine's Equation ^c					Normal Boiling Point (°F)
					Constants			Temperature Range ^d		
					<i>c</i>	<i>B</i> (°C)	<i>C</i> (°C)	Min. (°F)	Max. (°F)	
{4-methyl-phenol}	00095-48-7	108.14	9.47	0.0016	7.016	1,498.6	160.55	262	395	376
Cyclohexane					6.845	1,203.5	222.86	68	179	
Cyclohexanol	00106-44-5	108.14	8.50	0.00062	5.956	777.4	91.11	201	321	395
Cyclohexanone	00110-82-7	84.16	6.46	1.212	5.978	1,495.5	209.55	193	330	177
Cyclohexene	00108-93-0	100.16	8.03	0.00090	5.872	1,221.9	223.17	98	196	320
Cyclopentane	00108-94-1	98.14	7.91	0.0042	6.878	1,119.2	230.74	60	122	311
Cyclopentanone	00110-83-8	82.14	6.77	0.110	3.958	376.4	104.65	32	78	181
Cyclopentene ^e	00287-92-3	70.13	6.22	4.171	6.921	1,121.8	223.45			121
Decane (- <i>n</i>)	00120-92-3	84.12	7.92	0.130	3.085	440.6	116.25	−21	99	266
Dibromopropane (1,2)	00142-29-0	68.12	6.44	3.264	7.314	1,667.0	234.85	19	287	111
Dibromopropane (1,3)	00124-18-5	142.28	6.09	0.011	7.309	1,776.7	233.46	49	333	345
Dichloroethane (1,1)	00078-75-1	201.89	16.13	0.088	7.097	1,229.2	233.95	−77	135	286
Dichloroethane (1,2)	00109-64-8	201.89	16.55	0.029	7.460	1,521.8	248.48	−23	211	314
Dichloroethylene (1,2) ^{e, k, n}	00075-34-3	98.96	9.81	2.863						135
{1,2 dichloroethene}	00107-06-2	98.96	10.40	0.961	7.022	1,205.4	230.60	32	183	182
Dichloroethylene (trans-1,2) ^e					6.965	1,141.9	231.90	−36	185	
Dichlorotoluene (3,4) ^e	00540-59-0	96.94	10.76	2.579	7.344	1,882.5	215.00	32	221	141
Diethoxyethane (1,1)	00156-60-5	96.94	10.49	4.333	7.625	1,574.0	229.47	−10	216	118
Diethoxymethane	00095-75-0	161.03	10.49	0.0029	6.986	1,270.2	221.26	32	167	408
Diethyl (n,n) aniline	00105-57-7	118.17	6.89	0.307						212
{N,N-diethylbenzenamine}	00462-95-3	104.15	6.94	0.810	8.258	2,652.8	277.32	122	425	191
Diethyl ketone										
{3-pentanone}	00091-66-7	149.23	7.77	0.0031	5.741	716.2	147.17	97	215	422
Diethyl sulfide					7.541	1,560.5	246.59	−39	190	

Table 2—Properties of Selected Petrochemicals (See Table Footnote a) (Continued)

Chemical Name	CAS Registry No.	Molecular Weight	Liquid Density ^b (lb/gal)	True Vapor Pressure ⁱ at 60 °F (psia)	Antoine's Equation ^c					Normal Boiling Point (°F)
					Constants			Temperature Range ^d		
					<i>c</i>	<i>B</i> (°C)	<i>C</i> (°C)	Min. (°F)	Max. (°F)	
Diethylamine	00096-22-0	86.13	6.76	0.423						215
{N-ethyl ethanamine}	00352-93-2	90.19	6.98	0.749	5.737	559.1	140.18	89	141	197
Diethylbenzene (1,2)					6.990	1,577.9	200.55	206	364	
Diethylbenzene (1,3)	00109-89-7	73.14	5.89	2.712	7.006	1,576.3	201.00	203	360	132
Diethylbenzene (1,4)	00135-01-3	134.22	7.34	0.0094	7.001	1,589.3	202.02	206	365	361
Di-isopropyl ether	00141-93-5	134.22	7.18	0.010	6.842	1,135.0	218.23	74	153	358
Dimethoxyethane (1,2)	00105-05-5	134.22	7.20	0.010	6.713	1,260.5	235.83	−55	199	363
Dimethyl formamide (n,n)	00108-20-3	102.17	6.04	1.877	6.806	1,337.7	190.50	86	194	155
Dimethyl hydrazine (1,1)	00110-71-4	90.12	7.25	0.966	7.588	1,388.5	232.54	−32	68	185
Dimethyl phthalate ^e	00068-12-2	73.09	7.88	0.040	4.522	700.3	51.42	180	304	307
Dimethylbutane (2,3)	00057-14-7	60.10	6.60	1.896	6.810	1,127.2	228.95	58	138	146
Dimethylcyclopentane (1,1)	00131-11-3	194.18	9.94	2.25E-08	6.830	1,226.6	222.76	60	192	540
Dimethylpentane (2,2)	00079-29-8	86.18	5.52	3.064	6.815	1,190.3	223.34	60	176	136
Dimethylpentane (2,3)	01638-26-2	98.19	6.26	0.932	6.862	1,242.6	222.34	64	195	190
Dimethylpentane (2,4)	00590-35-2	100.20	5.63	1.315	6.836	1,197.6	222.27	57	178	174
Dimethylpentane (3,3)	00565-59-3	100.20	5.80	0.842	6.831	1,231.0	225.58	56	189	194
Dioxane (1,4)	00108-08-7	100.20	5.62	1.221	7.456	1,570.1	241.85	68	221	177
Dipropyl ether	00562-49-2	100.20	5.79	1.029						187
{di-n-propyl ether}	00123-91-1	88.11	8.63	0.439	6.945	1,254.8	218.82	80	192	214
Dodecane (<i>n</i>)					6.981	1,625.9	180.31	259	423	
Epichlorohydrinm n	00111-43-3	102.17	6.23	0.754						
{chloromethyl oxirane}	00112-40-3	170.33	6.25	0.00093	8.229	2,086.8	273.16			241
Ethane					6.813	659.7	256.431	−215	−100	−127
Ethanolamine (mono)	00106-89-8	92.52	9.85	0.194	7.168	1,408.9	157.06	150	340	339

Table 2—Properties of Selected Petrochemicals (See Table Footnote a) (Continued)

Chemical Name	CAS Registry No.	Molecular Weight	Liquid Density ^b (lb/gal)	True Vapor Pressure ⁱ at 60 °F (psia)	Antoine's Equation ^c					Normal Boiling Point (°F)
					Constants			Temperature Range ^d		
					c	B (°C)	C (°C)	Min. (°F)	Max. (°F)	
Ethyl acetate	00074-84-0	30.07		472	7.103	1,245.7	217.96	60	168	171
Ethyl acrylate	00141-43-5	61.08	8.50	0.002						
{ethyl ester 2-propenoic acid}	00141-78-6	88.11	7.51	1.135	7.150	1,366.1	220.47	−21	211	211
Ethyl alcohol										
{ethanol}	00140-88-5	100.12	7.71	0.445	8.247	1,670.4	232.96	32	173	173
Ethyl chloride					7.037	1,052.8	241.07	−69	55	61
Ethyl ether	00064-17-5	46.07	6.59	0.648						
{diethyl ether}	00075-00-3	64.51	7.43	16.63	6.897	1,062.6	228.22	−10	132	94
Ethylamine					7.405	1,203.8	249.43	62	349	64
Ethylbenzene	00060-29-7	74.12	5.96	6.675	6.950	1,419.3	212.61	134	279	277
Ethylcyclopentane	00075-04-7	45.08	5.65	14.08	6.898	1,305.0	221.40	84	220	218
Ethylene	00100-41-4	106.17	7.24	0.104						
{ethene}	01640-89-7	98.19	6.40	0.475	6.748	584.1	254.84	−191	−120	−155
Ethyleneoxide					8.722	2,022.8	335.81	32	89	53
Ethylpentane (3)	00074-85-1	28.05	4.74-155	749	6.880	1,254.1	220.15	70	202	200
Fluoranthene ^{j, k}	00075-21-8	44.05	7.3650	17.84	12.836	5,348.1	273.15	77	230	723
Fluorobenzene	00617-78-7	100.20	5.83	0.701	7.237	1,409.8	238.36	0	183	185
Formic acid	00206-44-0	202.25	10.45	3.96E-08	4.876	515.0	133.74	33	93	213
Freon 11 ^{e, n}	00462-06-6	96.10	8.53	0.936						
{trichlorofluoromethane}	00064-18-6	46.03	10.18	0.516	6.884	1,043.0	236.88			75
Furan					6.975	1,060.8	227.73	37	143	89
Furfural	00075-69-4	137.37	12.48	10.93						
{2-furancarboxaldehyde}	00110-00-9	68.07	7.94	7.963	6.969	1,430.1	188.70	133	321	323
heneicosane (<i>n</i>)					8.796	3,571.2	253.20	307	663	679

Table 2—Properties of Selected Petrochemicals (See Table Footnote a) (Continued)

Chemical Name	CAS Registry No.	Molecular Weight	Liquid Density ^b (lb/gal)	True Vapor Pressure ⁱ at 60 °F (psia)	Antoine's Equation ^c					Normal Boiling Point (°F)
					Constants			Temperature Range ^d		
					<i>c</i>	<i>B</i> (°C)	<i>C</i> (°C)	Min. (°F)	Max. (°F)	
Heptane (<i>n</i>)	00098-01-1	96.09	9.68	0.018	6.903	1,268.6	216.95	79	211	209
Heptene (1)	00629-94-7	296.57	6.61	6.23E-07	7.093	1,400.7	238.96	32	192	201
Hexadiene (1,5)	00142-82-5	100.20	5.71	0.541	6.563	1,008.1	214.16	32	138	140
Hexane (<i>n</i>)	00592-76-7	98.19	5.82	0.752	6.878	1,171.5	224.37	55	157	156
Hexanol (1)	00592-42-7	82.14	5.74	2.890	7.288	1,422.0	165.44	126	315	314
Hexene (1)	00110-54-3	86.18	5.47	1.913	6.866	1,153.0	225.85	61	148	147
Hydrogen cyanide	00111-27-3	102.17	6.79	0.005						
{hydrocyanic acid}	00592-41-6	84.16	5.62	2.378	7.549	1,340.8	261.56	2	115	79
Isobutane										
{methylpropane (2)}	00074-90-8	27.03	5.74	9.931	6.819	912.1	243.34	−121	11	12
Isobutene										
{methylpropene (2)}	00075-28-5	58.12	4.60	38.22	6.522	799.1	226.54	−70	32	20
Isobutyl alcohol										
{2-methyl 1-propanol}	00115-11-7	56.11	4.92	32.18	7.306	1,237.0	171.62	176	240	226
Isooctane										
{2,2,4-trimethylpentane}	00078-83-1	74.12	6.69	0.096	6.812	1,257.8	220.74	76	212	211
Isopentane										
{2-methyl butane}	00540-84-1	114.23	5.74	0.596	6.790	1,020.0	233.10	61	83	82
Isopentene										
{2-methyl 2-butene}	00078-78-4	72.15	5.18	9.426	6.922	1,098.6	233.26	37	159	100
Isoprene										
{2-methyl 1,3-butadiene}	00513-35-9	70.13	5.53	6.210	6.091	706.9	186.10	62	93	93
Isopropyl alcohol										
{isopropanol}	00078-79-5	68.12	5.67	7.446	7.736	1,357.4	197.34	134	193	180
Isopropyl benzene										
{cumene}	00067-63-0	60.10	6.52	0.443	6.929	1,455.8	207.20	158	308	305

Table 2—Properties of Selected Petrochemicals (See Table Footnote a) (Continued)

Chemical Name	CAS Registry No.	Molecular Weight	Liquid Density ^b (lb/gal)	True Vapor Pressure ⁱ at 60 °F (psia)	Antoine's Equation ^c					Normal Boiling Point (°F)
					Constants			Temperature Range ^d		
					<i>c</i>	<i>B</i> (°C)	<i>C</i> (°C)	Min. (°F)	Max. (°F)	
Isopropylbenzene (1-methyl-2)					7.417	1,880.5	236.27	178	355	350
Methacrylonitrile	00098-82-8	120.19	7.19	0.048						
{2-methyl 2-propenenitrile}	00527-84-4	134.22	7.32	0.017	6.999	1,353.6	238.03	−48	194	194
Methane					7.096	516.7	284.37	−262	−117	−260
Methyl acetate	00126-98-7	67.09	6.68	0.886						
{methyl ester acetic acid}	00074-82-8	16.04	3.53-260	4567	7.079	1,164.4	220.46	35	133	134
Methyl acrylate										
{methyl ester 2-propenoic acid}	00079-20-9	74.08	7.80	2.703	7.198	1,338.7	229.63	−47	176	177
Methyl alcohol										
{methanol}	00096-33-3	86.09	7.96	1.058	8.079	1,581.3	239.65	59	183	148
Methyl ethyl ketone										
{2-butanone}	00067-56-1	32.04	6.61	1.476	6.864	1,150.2	209.25	106	207	176
Methyl isobutyl ketone					6.828	1,254.1	201.61	71	241	241
Methyl methacrylate	00078-93-3	72.11	6.68	1.081	8.253	1,945.6	265.58	102	192	213
Methyl propyl ether	00108-10-1	100.16	6.65	0.219	6.563	903.6	206.46	31	103	102
Methyl styrene (α) ^e	00080-62-6	100.12	7.88	0.416	6.924	1,486.9	202.40			329
Methylcyclohexane ^e	00557-17-5	74.12	6.14 55	6.017	6.823	1,270.8	221.42	27	261	214
Methylcyclopentane	00098-83-9	118.18	7.60	0.024	6.863	1,186.1	226.04	59	163	161
Methyldichlorosilane ^{e, n}	00108-87-2	98.19	6.42	0.558	7.028	1,167.8	240.70	34	106	
Methylene chloride	00096-37-7	84.16	6.25	1.738	7.412	1,327.0	252.68	−40	104	104
Methylhexane (2)	20156-50-7	115.03	8.91	5.718	6.882	1,240.9	220.10	65	196	194
Methylhexane (3) ⁿ	00075-09-2	84.93	11.07	5.640	6.874	1,243.8	219.63	68	199	197
Methylpentane (2)	00591-76-4	100.20	5.66	0.799	6.839	1,135.4	226.57	55	142	142

Table 2—Properties of Selected Petrochemicals (See Table Footnote a) (Continued)

Chemical Name	CAS Registry No.	Molecular Weight	Liquid Density ^b (lb/gal)	True Vapor Pressure ⁱ at 60 °F (psia)	Antoine's Equation ^c					Normal Boiling Point (°F)
					Constants			Temperature Range ^d		
					<i>c</i>	<i>B</i> (°C)	<i>C</i> (°C)	Min. (°F)	Max. (°F)	
Methyl-tert-butyl ether ^g	00589-34-4	100.20	5.72	0.744						
{MTBE}	00107-83-5	86.18	5.43	2.730	6.867	1,116.1	224.74	125	431	131
Morpholine ^e					7.718	1,745.8	235.00	32	111	263
Naphthalene	01634-04-4	88.15	6.18	3.226	7.146	1,831.6	211.82	177	354	422
Nitrobenzene	00110-91-8	87.12	8.35	0.109	7.091	1,727.6	199.71	273	411	412
Nitromethane	00091-20-3	128.17	8.56	0.0024	7.281	1,446.2	227.52	132	277	214
Nonadecane (<i>n</i>)	00098-95-3	123.11	10.05	0.0022	33.303	28,197	725.94	91	131	624
Nonane (<i>n</i>)	00075-52-5	61.04	9.49	0.415	6.700	1,492.9	217.26	−64	94	303
Octadecane (<i>n</i>)	00629-92-5	268.52	6.56	3.64E-07	7.207	2,069.0	161.22	346	602	592
Octane (<i>n</i>)	00111-84-2	128.26	5.99	0.037	8.076	1,936.3	253.01	−70	75	258
Octanol (1)	00593-45-3	254.49	6.4882	6.16E-07	9.352	2,603.4	224.35	68	176	383
Octene (1)	00111-65-9	114.23	5.8377	0.142	6.933	1,353.5	212.76	113	252	251
Pentachloroethane	00111-87-5	130.23	6.9077	0.00061	6.643	1,342.3	196.51	77	324	324
Pentadiene (1,2)	00111-66-0	112.21	5.97	0.196	6.936	1,125.5	231.88	−76	−19	113
Pentadiene (1,4)	00076-01-7	202.29	14.02	0.040	7.035	1,108.2	241.05	−110	65	79
Pentadiene (2,3)	00591-95-7	68.12	5.78	4.718	7.263	1,256.2	239.57	−76	−15	119
Pentane (<i>n</i>)	00591-93-5	68.12	5.52	10.06	6.864	1,070.6	232.70	24	155	97
Pentene (1)	00591-96-8	68.12	5.80	4.223	6.786	1,014.3	229.78	55	87	88
Pentyne (1) ^e	00109-66-0	72.15	5.23	6.884	6.967	1,092.5	227.18	−47	142	104
Phenanthrene	00109-67-1	70.13	5.35	8.671	7.394	2,428.5	202.19	212	302	635
Phenol	00627-19-0	68.12	5.76	5.657	7.122	1,509.7	174.20	225	359	359
Phosgene	00085-01-8	178.23	8.18	3.37E-06	7.146	1,072.7	243.30	47	345	46

Table 2—Properties of Selected Petrochemicals (See Table Footnote a) (Continued)

Chemical Name	CAS Registry No.	Molecular Weight	Liquid Density ^b (lb/gal)	True Vapor Pressure ⁱ at 60 °F (psia)	Antoine's Equation ^c					Normal Boiling Point (°F)
					Constants			Temperature Range ^d		
					c	B (°C)	C (°C)	Min. (°F)	Max. (°F)	
Picoline (3)	00108-95-2	94.11	8.80 113	0.003						
{3-methyl pyridine}	00075-44-5	98.92	11.45	19.43	7.054	1,484.3	211.54	165	364	291
Propane					6.858	819.3	248.73	−45	117	−44
Propanethiol (1)	00108-99-6	93.13	7.98	0.064	6.929	1,183.4	224.63	76	216	154
Propanethiol (2)	00074-98-6	44.10	4.12	111	6.877	1,113.9	226.16	51	186	131
Propyl alcohol (<i>n</i>)	00107-03-9	76.16	7.02	1.943						
{propanol (1)}	00075-33-2	76.16	6.80	3.590	8.189	1,690.9	221.35	67	207	207
Propyl nitrate (<i>n</i>) ^e										
{propyl ester nitric acid}	00071-23-8	60.10	6.67	0.218	6.955	1,294.4	206.70	32	158	231
Propylamine (<i>n</i>)										
{1-propanamine}	00627-13-4	105.09	8.80	0.261	6.926	1,044.0	210.84	73	172	120
Propylene										
{propene}	00107-10-8	59.11	5.99	3.990	6.850	795.8	248.27	−161	−53	−54
Propylene glycol (1,2) m										
{1,2 propanediol}	00115-07-1	42.08	4.22	132	8.208	2,085.9	203.54			368
Propylene oxide					6.970	1,065.3	226.28	−100	94	95
Pyridine	00057-55-6	76.09	8.65	0.00094	7.038	1,371.4	214.65	153	307	240
Resorcinol	00075-56-9	58.08	7.1732	7.101	8.398	2,687.2	210.99	305	530	532
Styrene	00110-86-1	79.10	8.20	0.233	7.095	1,525.1	216.77	86	293	295
Tetrachloroethane (1,1,1,2)	00108-46-3	110.11	10.61	6.65E-06	6.906	1,370.4	210.25	139	266	271
Tetrachloroethane (1,1,2,2)	00100-42-5	104.15	7.56	0.066	6.091	959.6	149.78	77	266	295
Tetrachloroethylene	00630-20-6	167.85	12.86	0.133	7.056	1,440.8	223.98	82	226	250
Tetrahydrofuran	00079-34-5	167.85	13.32	0.037	6.996	1,202.9	226.33	74	211	151
Toluene	00127-18-4	165.83	13.54	0.213	7.017	1,377.6	222.64	32	122	231

Table 2—Properties of Selected Petrochemicals (See Table Footnote a) (Continued)

Chemical Name	CAS Registry No.	Molecular Weight	Liquid Density ^b (lb/gal)	True Vapor Pressure ⁱ at 60 °F (psia)	Antoine's Equation ^c					Normal Boiling Point (°F)
					Constants			Temperature Range ^d		
					<i>c</i>	<i>B</i> (°C)	<i>C</i> (°C)	Min. (°F)	Max. (°F)	
Trichloroethane (1,1,1)	00109-99-9	72.11	7.42	2.039	8.761	2,210.2	308.05	22	62	165
Trichloroethane (1,1,2)	00108-88-3	92.14	7.24	0.331	6.945	1,310.3	208.74	122	237	237
Trichloroethylene	00071-55-6	133.40	11.18	1.650	6.429	974.5	187.34	64	188	189
Trichloropropane (1,2,3)	00079-00-5	133.40	12.02	0.245	7.532	1,818.9	232.52	48	316	313
Tridecane (<i>n</i>)	00079-01-6	131.39	12.22	0.817	7.003	1,689.1	174.28	283	457	453
Trifluoroethane	00096-18-4	147.43	11.59	0.031						
(1,1,2-trichloro-1,2,2) ^e	00629-50-5	184.36	6.31	2.46E-04	6.880	1,099.9	227.50	−13	181	118
Trimethylbenzene (1,2,4) ^e					7.044	1,573.3	208.56	126	388	337
Trimethylchlorosilane	00076-13-1	187.37	13.05	4.376						
{chlorotrimethylsilane}	00095-63-6	120.19	7.31	0.020	6.951	1,191.0	235.15	37	132	136
Trimethylpentane (2,2,3) ^e					6.825	1,294.9	218.42			230
Trimethylpentane (2,3,3) ^e	00075-77-4	108.64	7.15	3.068	6.844	1,328.1	220.38			238
Trimethylpentane (2,3,4)	00564-02-3	114.23	5.74	0.378	7.031	1,420.7	228.53	−59	308	237
Undecane (<i>n</i>)	00560-21-4	114.23	6.06	0.317	6.977	1,572.5	188.02	220	387	383
Vinyl acetate	00565-75-3	114.23	6.00	0.314						
{acetic acid ethenyl ester}	01120-21-4	156.31	6.18	0.0035	7.215	1,299.1	226.97	71	162	163
Vinylidene chloride										
{1,1-dichloro ethene}	00108-05-4	86.09	7.78	1.396	6.983	1,104.7	237.75	−19	90	88
Xylene (<i>m</i>) ^e										
{1,3-dimethyl benzene}	00075-35-4	96.94	10.13	8.096	7.009	1,462.3	215.11	82	331	283
Xylene (<i>o</i>) ^e										

Table 2—Properties of Selected Petrochemicals (See Table Footnote a) (Continued)

Chemical Name	CAS Registry No.	Molecular Weight	Liquid Density ^b (lb/gal)	True Vapor Pressure ⁱ at 60 °F (psia)	Antoine's Equation ^c					Normal Boiling Point (°F)
					Constants			Temperature Range ^d		
					c	B (°C)	C (°C)	Min. (°F)	Max. (°F)	
{1,2-dimethyl benzene}	00108-38-3	106.17	7.21	0.090	6.999	1,474.7	213.69	90	342	291
Xylene (<i>p</i>)										
{1,4-dimethyl benzene}	00095-47-6	106.17	7.3550	0.071	7.021	1,474.4	217.77	56	355	281
NOTE Synonyms are shown in braces { }. Prefixes are shown in parentheses ().										
a Properties are from the NIST Standard Reference Database Number 69 ^[4] , except where noted otherwise.										
b Liquid densities are from CRC Handbook of Chemistry and Physics, 83 rd Edition ^[18] . The superscript denotes the temperature in °F; if no superscript is given, the density is 68 °F.										
c Vapor pressure <i>P</i> in psia = $(0.019337) \cdot 10^{\frac{B}{(T_{Li}-32)5/9+C}}$ where <i>T</i> is the temperature in °F.										
d Use of this equation for temperatures outside the indicated temperature range may result in loss of accuracy.										
e Values of <i>A</i> , <i>B</i> , and <i>C</i> and the temperature range (if any) for the 3-constant Antoine's equation are from <i>Lange's Handbook of Chemistry</i> ^[5] .										
g Values of <i>A</i> , <i>B</i> , and <i>C</i> and the temperature range for the 3-constant Antoine's equation are from Lisal et al. ^[34] .										
i Vapor pressures are calculated from the Antoine constants provided in this table.										
j Values of <i>A</i> , <i>B</i> , and <i>C</i> and the temperature range for the 3-constant Antoine's equation are from Stephenson and Malanowski ^[35] .										
k Boiling point from <i>Lange's Handbook of Chemistry</i> ^[5] .										
m Antoine constants from API <i>MPMS</i> Chapter 19.1, Third Edition ^[3] and not confirmed from a primary source.										
n Density from API <i>MPMS</i> Chapter 19.1, Third Edition ^[3] ; not confirmed from a primary source.										

4.7 Concentrations for Selected Compounds in Petroleum Liquids

[Table 3](#) and [Table 4](#) provide concentrations of some HAP and TRI chemicals in selected petroleum liquids. [Table 5](#) provides concentrations of PAHs in selected petroleum liquids.

Table 3—Concentrations (Weight Percent) of Selected Components in Selected Petroleum Liquids

Compound	Gasoline	JP-4 ^a (Jet Naphtha)	Jet A (Jet Kerosene)	Diesel (Distillate Fuel Oil No. 2)	Crude Oil
n-hexane	1.0	1.5	0.005	0.0001	0.4
benzene	1.8 (3)	0.6	0.004	0.0008	0.6
iso-octane {2,2,4 trimethylpentane}	4.0	0.0	0.0	0.0	0.1
toluene	7.0	2.0	0.133	0.032	1.0
ethylbenzene	1.4	0.5	0.127	0.013	0.4
xylene ^b	7.0	2.5	0.31	0.29	1.4
cumene {isopropylbenzene}	0.5	0.2	0.0	0.0	0.1
MTBE	(5)	0.0	0.0	0.0	0.0
1,2,4 trimethylbenzene	2.5	0.0	0.0	1.0	0.33
cyclohexane	0.24	1.2	0.0	0.0	0.7
NOTE 1 Concentrations in this table are the default values in EPA's TANKS software ^[24] . Actual product profiles may differ greatly from the TANKS default values, and TANKS has the ability to accept custom profiles.					
NOTE 2 The benzene content shown for gasoline in this table was based on 1990 data. Benzene content in gasoline has been driven to significantly lower levels than this by the EPA Fuels Specifications.					
NOTE 3 MTBE concentrations vary significantly. EPA ^[24,33] suggested in the early 1990s the following liquid-phase concentrations (weight percent). Subsequently, however, the use of MTBE as a gasoline additive has been phased out in the United States. Normal gasoline—0; Reformulated with MTBE—8.8; Oxygenated with MTBE—12.0					
^a The use of JP-4 in the United States was phased out in 1998.					
^b Xylenes includes mixed isomers; for convenience, TANKS ^[24] uses <i>m</i> -xylene to represent all isomers of xylene.					

**Table 4—Concentrations (Weight Percent) of
Selected Components in No. 6 Fuel Oil**

Species	Suggested Default (weight percent)
PACs	0.07
benzo(g,h,i)perylene	0.007
phenanthrene	0.09
benzene	0.002
biphenyl	0.02
cumene	0.002
cyclohexane	0.001
ethylbenzene	0.009
hexane (-n)	0.002
naphthalene	0.1
phenol	0
styrene	0
toluene	0.01
trimethylbenzene (1,2,4-)	0.1
xylene (<i>m</i> , <i>o</i> , and <i>p</i>)	0.05
NOTE Source: Annex G (see G.3 and Table G.4).	

Table 5—Concentrations of PAHs in Selected Petroleum Liquids (See NOTE 1)

Compound	CAS No.	Concentrations (ppmw) in Selected Petroleum Liquids							
		Crude Oil	Gasoline	Diesel	Jet Fuel	Heavy Fuel Oil (Bunker)	Light Cycle Oil	Heavy Cycle Oil	Asphalt
benzo[a]anthracene	56-55-3	6.4	5.3	2.5	0.0	144.9	11.3	344.0	8.2
benzo[a]phenanthrene {chrysene}	218-01-9	25.7	3.0	4.3	6.8	256.9	13.5	680.0	0.0
benzo[a]pyrene	50-32-8	2.4	2.4	0.0	0.0	127.6	1.6	61.4	0.0
benzo[b]fluoranthene	205-99-2	6.1	4.1	0.0	0.0	67.4	3.5	49.0	0.0
benzo[j]fluoranthene	205-82-3	See NOTE 2	See NOTE 2	0.0	0.0	See NOTE 2	See NOTE 2	See NOTE 2	0.0
benzo[k]fluoranthene	207-08-9	2.3	4.1	0.0	0.0	11.1	0.0	5.8	0.0
dibenzo[a,h]anthracene	53-70-3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
indeno[1,2,3-cd]pyrene	193-39-5	2.4	3.6	3.0	0.0	0.0	0.0	0.0	0.0
benzo[j,k]fluorene {fluoranthene}	206-44-0	5.7	3.0	10.2	0.0	34.1	88.1	390.0	0.0
benzo(r,s,t)pentaphene {dibenzo[a,i]pyrene}	189-55-9	0.0	0.0	2.6	0.0	9.4	0.0	0.0	0.0
Total PACs (ppm) (see NOTE 3)		51.0	25.5	22.6	6.8	651.4	118.0	1530.2	8.2
Other PAHs (not in the EPCRA Section 313 category for PACs)									
benzo(g,h,i)perylene	191-24-2	3.6	3.1	9.3	4.3	70.0	0.0	12.5	0.0
naphthalene	91-20-3	368.4	4150.0	756.5	796.7	630.7	4713.3	880.0	2.1

NOTE 1 The Canadian Petroleum Products Institute (CPPI) commissioned a speciation study of refinery streams ^[36], which included analyzing the streams for the presence of numerous polycyclic aromatic hydrocarbons (PAHs)—also known as polycyclic aromatic compounds (PACs). This study represents the most comprehensive data set available for the concentration of these compounds in petroleum liquids. Results for the more common streams from that study are summarized in this table, with concentrations for compounds that are potentially subject to Toxic Chemical Release Inventory (TRI) reporting under EPCRA Section 313. See [Annex F](#) for additional background on the EPA characterization of PAHs and PACs.

NOTE 2 Included with benzo[b]fluoranthene.

NOTE 3 Total PACs includes all the compounds from the EPCRA Section 313 category for PACs that are identified by EPA as detected in these petroleum liquids ^[31]. EPCRA Section 313 specifies that these compounds are to be reported in aggregate, rather than individually. These PACs may be speciated in aggregate by using the Total PACs concentration given in this table (in the absence of more accurate data) and applying the physical properties of chrysene (from [Table 2](#)) as being representative of the entire group.

4.8 Tank Solar Absorptance α

The tank outside surface solar absorptance α is a function of its color and reflective condition. [Table 6](#) provides solar absorptance values.

- If the tank color is unknown, use the solar absorptance for white paint.
- If the tank roof and shell have different solar absorptances, $\alpha = (\alpha_R + \alpha_S)/2$.

Table 6—Solar Absorptance α for Selected Tank Surfaces

Surface Color	Shade or Type	Reflective Condition (See NOTE 1)		
		Good	Average	Aged
White		0.17	0.25	0.34
Aluminum	Specular	0.39	0.44	0.49
Aluminum	Diffuse	0.60	0.64	0.68
Beige/Cream		0.35	0.42	0.49
Brown		0.58	0.62	0.67
Gray	Light	0.54	0.58	0.63
Gray	Medium	0.68	0.71	0.74
Green	Dark	0.89	0.90	0.91
Red	Primer	0.89	0.90	0.91
Rust	red iron oxide	0.38	0.44	0.50
Tan		0.43	0.49	0.55
Aluminum (see NOTE 2)	mill finish, unpainted	0.10	0.12	0.15

NOTE 1 Reflective condition definitions:
 Good—For paint, paint is in good condition; i.e. the studies that the white factors were taken from clearly used a factor of 0.17 (83 % reflectance) for tanks “in good condition” (and this was the condition of the majority of the tanks studied), ^[47] and there is no evidence to support the idea that this factor only applies to paint that still “retains a fresh shine of having been recently applied”. For mill-finish aluminum, surface is shiny. If specific information is not available, a white shell and roof, with the paint in good condition, can be assumed to represent the most common or typical tank surface in use.
 Average—For mill-finish aluminum, surface is oxidized but still bright. The value given in each case is the average of the Good and the Aged values for that case and does not represent new data.
 Aged—For paint, paint is noticeably faded and dull; for mill-finish aluminum, surface is dull.
 NOTE 2 This refers to aluminum as the base metal, rather than aluminum-colored paint.

5 Speciation Methods

5.1 Speciation Based on Liquid Profiles

5.1.1 General

This method uses Raoult's Law to calculate the concentrations of components in the vapor phase from given weight fractions in the liquid phase. See [Section 7](#) for additional discussion of Raoult's Law.

5.1.2 Full Speciation Versus Partial Speciation

When the weight fraction is known for every component in a petroleum liquid, then a full speciation may be performed. This does not require any information on the properties of the petroleum liquid itself—the overall stock liquid properties may be calculated from the properties and weight fractions of the components.

A full speciation by Raoult's Law is generally not feasible with typical petroleum liquids. Petroleum liquids tend to consist of a high number of components, each of which represents a small fraction of the total stock. Neglecting even a trace amount of certain components has the potential for a disproportionate impact on the calculated stock liquid properties. The presence of a few thousandths of a percent (by weight) of methane in a refined product, for example, may be undetected in a chemical analysis, yet have a significant impact on the stock true vapor pressure and the stock vapor molecular weight.

When sufficient properties are known for the stock liquid (i.e. the stock true vapor pressure, stock liquid molecular weight, and stock vapor molecular weight), then a partial speciation may be performed. A partial speciation does not require the weight fraction of every component, but rather requires only the weight fractions of those components that are to be speciated.

Speciation of emissions is commonly performed to report the emissions of certain chemicals of interest. When speciation results are required for only a partial list of the components, a partial speciation is generally preferred.

5.1.3 Steps

Problem—Given the weight fraction, w_i , of some or all of the components of a liquid, calculate the weight fraction, z_i , of these components in the vapor produced by evaporation of the liquid.

STEP 1—Determine the stock liquid surface temperature, T_{LA} . If not known, see [4.1](#).

STEP 2—List the components of the liquid that are to be speciated. For each component, i , list its weight fraction, w_i . [Tables 3, 4, and 5](#) give default weight fractions for selected compounds in selected petroleum liquids.

STEP 3—For each component, i , list its molecular weight, M_i . [Table 2](#) gives molecular weights for selected petrochemicals.

STEP 4—Determine the stock liquid molecular weight, M_L .

Partial Speciation—Typical stock liquid molecular weights for selected petroleum liquids are presented in [Table 1](#). Alternatively, the stock liquid molecular weight can be determined by analysis (see [4.4](#)).

Full Speciation—The stock liquid molecular weight can be calculated as:

$$M_L = 1/\Sigma(w_i/M_i) \quad (8)$$

STEP 5—Calculate the mole fraction in the liquid phase, x_i , for each component, i :

$$x_i = w_i M_L / M_i \quad (10)$$

STEP 6—Calculate the saturated vapor pressure, P_i^o (psia), at the stock liquid surface temperature, T_{LA} (°F), for each component, i , using the Antoine constants A , B , and C given in [Table 2](#):

$$P_i^o = 0.019337 \log^{-1} \left[A - \frac{B}{(T_{LA} - 32) 5/9 + C} \right] \quad (6)$$

where

T_{LA} the stock liquid surface temperature in °F.

STEP 7—Calculate the partial pressure, P_i , for each component, i :

$$P_i = x_i P_i^o \quad (11)$$

STEP 8—Determine the stock true vapor pressure, P_v .

Partial Speciation—Typical stock true vapor pressures may be calculated for selected petroleum liquids from Equation (5) using the vapor pressure constants A and B given in [Table 1](#).

$$P_v = \exp \left[A - \frac{B}{(T_{LA} + 459.7)} \right] \quad (5)$$

where

T_{LA} the stock liquid surface temperature in °F.

Values for the vapor pressure constants A and B may also be calculated, using Equation (1) and Equation (2) for refined stocks and Equation (3) and Equation (4) for crude oils. See [4.2](#) for additional guidance.

Full Speciation—The stock true vapor pressure can be calculated as:

$$P_v = \Sigma(P_i) \quad (12)$$

STEP 9—Calculate the mole fraction in the vapor phase, y_i , for each component, i :

$$y_i = P_i / P_v \quad (13)$$

STEP 10—Determine the stock vapor molecular weight M_v .

Partial Speciation—Typical stock vapor molecular weights for selected petroleum liquids are presented in [Table 1](#). Alternatively, the stock vapor molecular weight can be determined by analysis. See [4.5](#).

Full Speciation—The stock vapor molecular weight can be calculated as:

$$M_v = \Sigma(y_i M_i) \quad (9)$$

STEP 11—Calculate the weight fraction in the vapor phase, z_i , for each component, i :

$$z_i = y_i M_i / M_v \quad (14)$$

STEP 12—Calculate the emissions (weight) for each component, i :

$$L_i = z_i L_t \quad (15)$$

where

L_i emissions (by weight) of component, i , and

L_t total emissions (by weight) of all components.

5.2 Speciation Based on Vapor Profiles

Many of the problems associated with converting liquid composition data to vapor concentrations could be avoided if vapor profiles were available for petroleum stocks. Such profiles might resemble the one presented in

[Table 7](#). These data were obtained from laboratory testing of a simulated 11–component gasoline at 77 °F ^[17], and they illustrate how the light ends evaporate preferentially versus the heavy ends. For example, the concentration of the lightest component, butane, is almost 70 times greater in the vapor phase than in the liquid phase, whereas the heaviest components of the liquid phase are not detected at all in the vapor phase.

The proper use of vapor profiles would require developing a vapor profile for each individual stock and storage temperature. Too often, profiles in the literature provide very limited or no information on some of the important hydrocarbon species present in low concentrations. Frequently, they are not derived from actual measurements; instead they are taken from engineering evaluation of literature data. However, once vapor profiles have been measured or calculated for a system, they should be appropriate for future applications with the same petroleum stock and temperature.

Hydrocarbon emissions can be speciated by directly sampling the vapor emissions from the modeled system. However, there are multiple problems associated with direct vapor phase sampling. Such samples are only snapshots of the system, representing only the conditions under which the samples were collected, and are not necessarily applicable to the average conditions associated with the operation. The logistics of collecting vapor samples from the variety of emission points associated with tanks are difficult and often impossible. The vapors in tanks may be stratified, creating difficulties in obtaining a representative sample, and the analysis of vapor samples is generally less accurate than that of liquid samples.

Table 7—Vapor Profile for Simulated Gasoline

Species	Mole Fraction Liquid Phase	Mole Fraction Vapor Phase (at 77 °F)
Butane	0.018	0.123
2-Methylbutane	0.202	0.627
2-Methylpentane	0.052	0.068
Benzene	0.024	0.018
2,2,4-trimethylpentane	0.166	0.057
1-Heptene	0.104	0.038
Methylcyclohexane	0.073	0.024
Toluene	0.121	0.029
<i>p</i> -Xylene	0.183	0.016
Undecane	0.035	0.000
Hexylbenzene	0.022	0.000
Total	1.00	1.00
NOTE Mole fraction data source: Reference [17].		

6 Speciation Example

Problem: A floating-roof tank stores normal gasoline with an average annual liquid surface temperature, T_{LA} = 75.9 °F, a Reid vapor pressure, RVP = 10.4 psi, and a distillation slope, *s* = 3. Total estimated emissions from this tank are 5,480 lb/yr, of which 5,220 lb are standing loss and 260 lb are working loss. Calculate the portion (weight) of these annual emissions that is attributable to each of the first eight compounds listed in [Table 3](#).

STEP 1—The stock liquid surface temperature is given as:

$$T_{LA} = 75.9 \text{ °F}$$

STEP 2—The components that are to be speciated are listed in [Table 8](#). The weight fractions in the liquid phase, *w_i*, are taken as the typical values from Table 3, in that actual weight fractions were not given. The listed HAPs

constitute 22.7 % of the liquid, with the constitution of the remainder being unknown. This will, then, be a partial speciation. (A full speciation would require knowing the weight fraction of every component of the liquid.)

STEP 3—The molecular weight, M_i (taken from [Table 2](#)), is listed for each component in [Table 8](#).

STEP 4—The stock liquid molecular weight, M_L , is taken as 92 from [Table 1](#).

STEP 5—The mole fraction in the liquid phase, x_i , is calculated for each component from Equation (10), and then listed in [Table 8](#).

For example, for n-hexane:

$$\begin{aligned} x_i &= w_i M_L / M_i \\ &= (0.01)(92/86.18) \\ &= 0.01068 \end{aligned}$$

STEP 6—The saturated vapor pressure, P_i^o , is calculated at the stock liquid surface temperature, T_{LA} , for each component from Equation (6), using the Antoine constants A , B , and C given in [Table 2](#), and then listed in [Table 8](#).

For example, for n-hexane:

$$\begin{aligned} P_i^o &= 0.019337 \log^{-1} \left[A - \frac{B}{(T_{LA} - 32)5/9 + C} \right] \\ &= (0.019337) 10^{\left[6.878 - \frac{1171.5}{(75.9 - 32)(5/9) + 224.37} \right]} \\ &= 2.85 \text{ psia} \end{aligned}$$

STEP 7—The partial pressure, P_i , is calculated for each component from Equation (11), and then listed in [Table 8](#).

For example, for n-hexane:

$$\begin{aligned} P_i &= x_i P_i^o \\ &= 0.01068 (2.85) \\ &= 0.0304 \text{ psia} \end{aligned}$$

STEP 8—The stock true vapor pressure, P_v , is determined by first calculating the vapor pressure constants, A and B . For refined petroleum stocks, the constants A and B are calculated from Equation (1) and Equation (2), given the stock RVP of 10.4 and distillation slope, S , of 3:

$$\begin{aligned} A &= 15.64 - 1.854 \sqrt{S} - (0.8742 - 0.328 \sqrt{S}) \ln(\text{RVP}) \\ &= 15.64 - 1.854 \sqrt{3} - (0.8742 - 0.328 \sqrt{3}) \ln(10.4) \\ &= 11.712 \\ B &= 8742 - 1042 \sqrt{S} - (1049 - 179.4 \sqrt{S}) \ln(\text{RVP}) \\ &= 8742 - 1042 \sqrt{3} - (1049 - 179.4 \sqrt{3}) \ln(10.4) \end{aligned}$$

$$= 5208.3$$

The stock true vapor pressure, P_v , is then calculated from Equation (5):

$$\begin{aligned} P_v &= \exp \left[A - \frac{B}{(T_{LA} + 459.7)} \right] \\ &= e^{(11.712 - 5208.3/535.6)} \\ &= 7.34 \text{ psia} \end{aligned}$$

STEP 9—The mole fraction in the vapor phase, y_i , is calculated for each component from Equation (13), and then listed in [Table 8](#).

For example, for n-hexane:

$$\begin{aligned} y_i &= P_i / P_v \\ &= 0.0304 / 7.34 \\ &= 0.0041 \end{aligned}$$

STEP 10—The stock vapor molecular weight, M_v , is taken as 66, which is given as an average value for RVP 10 gasoline in [Table 1](#).

STEP 11—The weight fraction in the vapor phase, z_i , is calculated for each component from Equation (14), and then listed in [Table 8](#):

For example, for n-hexane:

$$\begin{aligned} z_i &= y_i M_i / M_v \\ &= 0.0041(86.18) / 66 \\ &= 0.0054, \text{ or } 0.54 \% \end{aligned}$$

STEP 12—The total standing loss, L_s , is given as 5,220 lb. The standing loss, L_i , is calculated for each component from Equation (15):

For example, for n-hexane:

$$\begin{aligned} L_i &= z_i L_s \\ &= 0.0054 (5,220) \\ &= 28.2 \text{ lb} \end{aligned}$$

The total working loss, L_w , is given as 260 lb. The working loss does not occur as evaporation from the surface of a bulk liquid, but rather is the evaporation of the thin film of liquid that is left behind on the inside of the tank shell as the liquid level is lowered in the tank. This film of liquid is assumed to entirely evaporate. The working loss, then, is speciated on the basis of the liquid profile, rather than using Raoult's Law to account for differential evaporation of the light ends from the surface of a bulk liquid. The working loss is calculated for each component, i , as follows:

$$L_i = w_i (\text{total working loss}) \quad (16)$$

For example, for n-hexane:

$$\begin{aligned} L_i &= w_i(260) \\ &= 0.01(260) \\ &= 2.6 \text{ lb} \end{aligned}$$

The standing, working, and total emissions of each listed component are summarized in [Table 9](#).

Table 8—Speciation Example Worksheet

Components	Liquid Phase			Vapor Pressure Equation Constants (for pressure in mm Hg and temperature in °C)			P_i^o	P_i	Vapor Phase	
	M_i	W_i	X_i						y_i	z_i
	(lb/lb-mole)	(weight fraction)	(mole fraction)	A	B	C	(psia)	(psia)	(mole fraction)	(weight fraction)
n-hexane	86.18	0.0100	0.011	6.878	1171.5	224.37	2.8482	0.0304	0.0041	0.0054
benzene	78.11	0.0180	0.021	6.906	1211.0	220.79	1.7890	0.0379	0.0052	0.0061
iso-octane (2,2,4-trimethylpentane)	114.23	0.0400	0.032	6.812	1257.8	220.74	0.9265	0.0298	0.0041	0.0070
toluene	92.14	0.0700	0.070	7.017	1377.6	222.64	0.5328	0.0372	0.0051	0.0071
ethylbenzene	106.17	0.0140	0.012	6.950	1419.3	212.61	0.1769	0.0021	0.0003	0.0005
xylene (<i>m</i> -xylene) ^a	106.17	0.0700	0.061	7.009	1462.3	215.11	0.1548	0.0094	0.0013	0.0021
cumene (isopropylbenzene)	120.19	0.0050	0.004	6.929	1455.8	207.20	0.0850	0.0003	0.0000	0.0001
MTBE (methyl tert-butyl ether)	88.15	0.0000	0.000	6.867	1116.1	224.74	4.7344	0.0000	0.0000	0.0000
Totals		0.2270								0.0283

^a Xylenes includes mixed isomers; for convenience, use *m*-xylene to represent all xylenes.

Table 9—Speciation Example Summary

Components	Working Loss $L_w = 260$		+	Standing Loss $L_s = 5,220$		=	Total 5,480
	w_i Liquid Weight Fraction	L_i This Component (lb)		z_i Vapor Weight Fraction	L_i This Component (lb)		This Component (lb)
n-hexane	0.0100	2.6	+	0.0054	28.2	=	30.8
benzene	0.0180	4.7	+	0.0061	31.8	=	36.5
iso-octane (2,2,4-trimethylpentane)	0.0400	10.4	+	0.0070	36.5	=	46.9
toluene	0.0700	18.2	+	0.0071	37.1	=	55.3
ethylbenzene	0.0140	3.6	+	0.0005	2.6	=	6.2
xylene (<i>m</i> -xylene)	0.0700	18.2	+	0.0021	11.0	=	29.2
cumene (isopropylbenzene)	0.0050	1.3	+	0.0001	0.5	=	1.8
MTBE (methyl tert-butyl ether)	0.0000	0.0	+	0.0000	0.0	=	0.0
Totals	0.2270	59.0	+	0.0283	147.7	=	206.7

7 Speciation Theory

7.1 Introduction

Typically, representative tank vapor profiles are not available, and it is not feasible to collect a vapor sample. In most situations, it is adequate to use a typical liquid profile to calculate the concentrations of constituents in the vapor phase. In some instances, a representative liquid sample should be collected and analyzed. In the latter case, proper sampling procedures and appropriate methods of analysis should be used. Once the liquid component concentrations are known, the constituents in the vapor phase can be approximated by using a vapor-liquid relationship such as Raoult's Law. More complex approaches should be used when some constituents are not typical hydrocarbons and their liquid and vapor relationships deviate widely from ideal relationships at low concentrations. Examples of compounds that have non-ideal interactions with hydrocarbons include polars such as water, alcohols, and similar oxygenates.

The quality of the vapor speciation calculation depends on the accuracy of the liquid composition profile. Due to averaging effects, calculations based on standard profiles for a large number of sources achieve better accuracy. As the number of sources decreases and for periods of time less than one year, these calculations have the potential for less accuracy.

7.2 Raoult's Law

In a multicomponent gas-liquid system at equilibrium, the compositions of the two phases at a given temperature and pressure are directly related. The composition of the vapor phase is uniquely determined by the physical properties of the components in the liquid phase ^[6, 11].

Raoult's Law and Dalton's Law can be used to estimate the composition of the vapor in equilibrium above a liquid where constituents form a near ideal mixture in both the liquid and vapor phases ^[12].

Raoult's Law states:

$$P_i = P_i^o x_i \quad (17)$$

where

P_i partial pressure of component i in the vapor phase (psia).

P_i^o saturated vapor pressure of component i at the equilibrium temperature (psia).

x_i mole fraction of component i in the liquid.

Equation (17) is the same as Equation (11) given earlier. Dalton's Law extends this relationship to the total composition of the vapor phase. Partial pressure, P_i , is defined as:

$$P_i = y_i P_T \quad (18)$$

where

P_i partial pressure of component i in the vapor phase (psia).

y_i mole fraction of component i in the vapor phase.

P_T total pressure of the system analyzed (psia).

Combining Raoult's Law and Dalton's Law yields an expression which can be used to predict the vapor phase composition:

$$y_i = P_i^o x_i / P_T \quad (19)$$

where the terms are as previously defined above.

Raoult's Law is an approximation that is generally valid when the liquid components are chemically similar, such as paraffinic hydrocarbons, and when the total pressure of the system is atmospheric or less ^[6].

In systems where Raoult's Law does not apply, the phase composition can be predicted using component vapor-liquid equilibrium constants, K_i , defined by the relationship ^[10]:

$$y_i = K_i x_i \quad (20)$$

where

K_i vapor-liquid equilibrium constant of component i (dimensionless).

K is a function of the system temperature, pressure, and composition. When Raoult's Law applies, i.e. for an ideal liquid:

$$K_i = P_i^o / P_T$$

and the relationship shown in Equation (20) then reverts to that shown in Equation (19).

Studies performed for the API (summarized in [Annex A](#)) show that, when the liquid composition is known, Raoult's Law will adequately characterize the vapor phase composition for multicomponent hydrocarbon mixtures such as crude oils and gasoline ^[14].

7.3 Precision, Accuracy, and Variability of Methods

7.3.1 General

Raoult's Law was examined for precision and accuracy in predicting vapor phase composition for several petroleum feedstocks and gasolines. Details of the study are given in [Annex A](#) and summarized below.

7.3.2 Gasolines

Winter and summer blend gasolines were studied ^[13]. Raoult's Law predicted the vapor phase concentrations within 79 % of the measured values; generally under predicting the winter blend vapors by 63 % and over predicting the summer blend vapors by 36 %. The Peng-Robinson (PR) and Redlich-Kwong-Soave (RKS)

equations of state were found to be comparable to Raoult's Law in their accuracy. There were no significant differences between the vapor phase compositions predicted by Raoult's Law and those predicted by either the PR or RKS equations of state.

7.3.3 Heavier Stocks

When heavier petroleum stocks, such as crude oils, jet fuel, and fuel oil were studied, the vapor phase compositions that were estimated using Raoult's Law were found to be ~5 % below those predicted by the RKS equation of state, and ~18 % below those predicted by the PR equation of state ^[14]. However, for many of the species measured, the vapor concentrations that were predicted by Raoult's Law appeared to be within the confidence intervals computed from the precision and accuracy of the analytical techniques that were used in the project.

The liquid molecular weight was the most important factor affecting the predicted vapor phase compositions. This value varied by up to a factor of five with different determination methods, and directly affected the calculated vapor concentrations.

7.3.4 Deviations from Raoult's Law

7.3.4.1 General

Vapors from some petroleum stocks often display marked variations from Raoult's Law. In these cases, it might be necessary to sample and speciate the vapor phase directly, or to experimentally develop and utilize a relationship such as that shown previously in Equation (20):

$$y_i = K_i x_i \quad (20)$$

where

y_i	mole fraction of component i in the vapor.
K_i	vapor-liquid equilibrium constant at equilibrium pressure and temperature (dimensionless).
x_i	mole fraction of component i in the liquid.

Some workable guidelines have been proposed for determining deviations from Raoult's Law. These guidelines are based on the idea that liquid properties are related to the degree of bonding between molecules. The hydrogen bond is the most important bond and serves as the most important criterion. This concept gives rise to five classifications of compounds ^[8]:

Class 1—Liquids capable of forming three-dimensional networks of strong hydrogen bonds. This includes water, glycol, glycerol, amino alcohols, hydroxy acids, amides, and so forth.

Class 2—Other liquids composed of molecules containing both active hydrogen atoms and donor atoms of oxygen, nitrogen, and fluorine. This includes alcohols, acids, primary phenols, oximes, primary and secondary amines, ammonia, hydrogen fluoride, hydrogen cyanide, nitro compounds with α -hydrogen atoms, and so forth.

Class 3—Liquids that contain donor atoms but do not contain active hydrogen atoms. This includes ethers, aldehydes, esters, ketones, tertiary amines, nitro compounds and nitriles without α -hydrogen atoms, and so forth.

Class 4—Liquids composed of molecules with active hydrogen atoms, but no donor atoms. These include molecules with two or three chlorine atoms on the same carbon atom as a hydrogen atom, or one chlorine atom on the same carbon and one or more chlorine atoms on adjacent carbon atoms.

Class 5—All other liquids (those without hydrogen-bond forming capability). These include hydrocarbons, carbon disulfide, mercaptans, halohydrocarbons not in class 4, and nonmetallic elements.