Anexos

Reid Prausnitz & Poling, 1987, pp 42, 43

3-6 Cubic Equations of State

The term "cubic equation of state" implies an equation which, if expanded, would contain volume terms raised to either the first, second, or third power. Many of the common two-parameter cubic equations can be expressed by the equation

$$P = \frac{RT}{V - b} - \frac{a}{V^2 + ubV + wb^2} \tag{3-6.1}$$

An equivalent form of Eq. (3-6.1) is

$$Z^3 - (1 + B^* - uB^*)Z^2 + (A^* + wB^{*2} - uB^* - uB^{*2})Z - A^*B^* - wB^{*2} - wB^{*3} = 0 \tag{3-6.2}$$

where $$A^* = \frac{aP}{R^2T^2} \tag{3-6.3}$$

and $$B^* = \frac{bP}{RT} \tag{3-6.4}$$

TABLE 3-5 Constants for Four Common Cubic Equations of State

Equation	u	w	b	a
van der Waals	0	0	$\frac{RT_c}{8P_c}$	$\frac{27}{64}\frac{R^2T_c^2}{P_c}$
Redlich-Kwong	1	0	$\frac{0.08664RT_c}{P_c}$	$\frac{0.42748R^2T_c^{2.5}}{P_cT^{1/2}}$
Soave	1	0	$\frac{0.08664RT_c}{P_c}$	$\frac{0.42748R^2T_c^2}{P_c}[1+f\omega(1-T_r^{1/2})]^2$ where $f\omega = 0.48 + 1.574\omega - 0.176\omega^2$
Peng-Robinson	2	−1	$\frac{0.07780RT_c}{P_c}$	$\frac{0.45724R^2T_c^2}{P_c}[1+f\omega(1-T_r^{1/2})]^2$ where $f\omega = 0.37464 + 1.54226\omega - 0.26992\omega^2$

Reid Prausnitz & Poling, 1987, pp 82

4-5 Mixing Rules for Redlich-Kwong-Type Equations of State

The mixing rules recommended for all two-constant cubic equations of state (i.e., van der Waals, Redlich-Kwong, Soave, and Peng-Robinson) are

$$a_m = \sum_i \sum_j y_i y_j (a_i a_j)^{1/2} (1 - \bar{k}_{ij}) \tag{4-5.1}$$

$$b_m = \sum_i y_i b_i \tag{4-5.2}$$

a_i and b_i are given in Table 3-5. Some values of the binary interaction coefficient $\bar{k}_{ij}$ for the Soave and Peng-Robinson equations are given in Table 4-2. A more extensive tabulation is given in Ref. 28. Values for $\bar{k}_{ij}$ for specific systems and as a function of temperature are given in [9, 16, 23, 25, 33]. For hydrocarbon pairs, $\bar{k}_{ij}$ is usually taken as zero. If all $\bar{k}_{ij}$ are zero, Eq. (4-5.1) reduces to

$$a_m = \left(\sum_i y_i a_i^{1/2} \right)^2 \tag{4-5.3}$$

Reid Prausnitz & Poling, 1987, pp 102

Cubic, Secs. 3-6 and 4-5

$$P = \frac{RT}{V - b} - \frac{a}{V^2 + uVb + wb^2}$$

$$A - A^\circ = \frac{a}{b\sqrt{u^2 - 4w}} \ln \frac{2Z + B^*(u - \sqrt{u^2 - 4w})}{2Z + B^*(u + \sqrt{u^2 - 4w})} - RT \ln \frac{Z - B^*}{Z} - RT \ln \frac{V}{V^\circ}$$

$$S - S^\circ = R \ln \frac{Z - B^*}{Z} + R \ln \frac{V}{V^\circ} - \frac{1}{b\sqrt{u^2 - 4w}} \frac{\partial a}{\partial T} \ln \frac{2Z + B^*(u - \sqrt{u^2 - 4w})}{2Z + B^*(u + \sqrt{u^2 - 4w})}$$

where $$\frac{\partial a}{\partial T} = -\frac{R}{2} \left(\frac{\Omega_a}{T} \right)^{1/2} \sum_i \sum_j y_i y_j (1 - \bar{k}_{ij}) \left[f\omega_j \left(\frac{a_i T_{ci}}{P_{cj}} \right)^{1/2} + f\omega_i \left(\frac{a_j T_{ci}}{P_{ci}} \right)^{1/2} \right]$$

For the Soave Equation

$$f\omega_i = 0.480 + 1.574\omega_i - 0.176\omega_i^2$$
$$\Omega_a = 0.42748$$

For the Peng-Robinson Equation

$$f\omega_i = 0.37464 + 1.54226\omega_i - 0.26992\omega_i^2$$
$$\Omega_a = 0.45724$$

Note: u, w, a_i, a, and b are given in Table 3-5 and Eqs. (4-5.1) and (4-5.2).

Reid Prausnitz & Poling, 1987, pp 144, 145

With Eqs. (5-8.5), (5-8.6), and $\phi_i = \dfrac{\hat{f}_i}{Py_i}$

$$RT \ln \phi_i = -\int_{\infty}^{\underline{V}} \left[\left(\frac{\partial P}{\partial N_i} \right)_{T,\underline{V},N_{j|i}} - \frac{RT}{\underline{V}} \right] d\underline{V} - RT \ln Z \tag{5-8.7}$$

or

$$RT \ln \phi_i = \left(\frac{\partial(\underline{A} - \underline{A}^\circ)}{\partial N_i} \right)_{T,\underline{V},N_{j|i}} - RT \ln Z \tag{5-8.8}$$

ϕ_i is the fugacity coefficient of i in the gas mixture.

To obtain a usable relation for ϕ_i, Eq. (5-8.7) must be integrated; but before it can be, the derivative of P with respect to N_i must be found. Thus any pressure-explicit equation of state is convenient provided that the composition dependence of all the parameters can be expressed in analytical form.

For the analytical equations of state covered in Chap. 3, mixture combining rules are given in Chap. 4; thus evaluation of the integral in Eq. (5-8.7) is possible. For example, the original Redlich-Kwong equation is given as Eq. (3-6.1), and this same relation expressed in terms of total volume would be

$$P = \frac{NRT}{\underline{V} - Nb} - \frac{aN^2}{\underline{V}(\underline{V} + Nb)} \tag{5-8.9}$$

In the differentiation indicated in Eq. (5-8.7), the variables are N, a, and b, where the parameters a and b are shown as functions of composition in Eqs. (4-5.1), (4-5.2), and (3-6.1). The final result is

$$\ln \phi_i = \ln \frac{V}{V - b} + \frac{b_i}{V - b} - \ln Z + \frac{ab_i}{RTb^2} \left(\ln \frac{V + b}{V} - \frac{b}{V + b} \right) - \frac{2 \sum_j y_j a_{ij}}{RTb} \ln \frac{V + b}{V} \tag{5-8.10}$$

For all the analytical equations of state, the working equations for $\ln \phi_i$ are given in Table 5-13.

Virial, $Z = 1 + \dfrac{BP}{RT}$ [Eqs. (3-5.2a) and (4-4.1)]

$$\ln \phi_i = \left(2\sum_j y_j B_{ij} - B\right)\frac{P}{RT} \tag{5-8.11}$$

Cubic, $P = \dfrac{RT}{V-b} - \dfrac{a}{V^2 + ubV + wb^2}$ [Eqs. (3-6.1), (4-5.1), and (4-5.2) and Table 3-5]

$$\ln \phi_i = \frac{b_i}{b}(Z-1) - \ln(Z - B^*) + \frac{A^*}{B^*\sqrt{u^2-4w}}\left(\frac{b_i}{b} - \delta_i\right)\ln\frac{2Z + B^*(u + \sqrt{u^2-4w})}{2Z + B^*(u - \sqrt{u^2-4w})} \tag{5-8.12}$$

where
$$\frac{b_i}{b} = \frac{T_{ci}/P_{ci}}{\sum_j y_j T_{cj}/P_{cj}} \tag{5-8.13}$$

$$\delta_i = \frac{2a_i^{1/2}}{a}\sum_j x_j a_j^{1/2}(1 - \bar{k}_{ij}) \tag{5-8.14}$$

If all $\bar{k}_{ij} = 0$, this reduces to

$$\delta_i = 2\left(\frac{a_i}{a}\right)^{1/2} \tag{5-8.15}$$

Lee-Kesler [Eqs. (3-7.1) to (3-7.4) and Table 4-3]

$$\ln \phi_i = \ln\left(\frac{f}{P}\right)_m + \frac{H^\circ - H}{TRT_{cm}}\sum_{j\neq i} y_j\left(\frac{dT_{cm}}{dy_j}\right)_{y_k} + \frac{Z_m - 1}{P_{cm}}\sum_{j\neq i} y_j\left(\frac{dP_{cm}}{dy_j}\right)_{y_k} - \ln\left(\frac{f}{P}\right)_m^{(1)}\sum_{j\neq i} y_j\left(\frac{d\omega_m}{dy_j}\right)_{y_k} \tag{5-8.16}$$

$$\left(\frac{dT_{cm}}{dy_j}\right)_{y_k} = \left[2\sum_l y_l(V_{clj}^{1/4}T_{clj} - V_{cli}^{1/4}T_{cli}) - \frac{0.25}{V_{cm}^{5/4}}\left(\frac{dV_{cm}}{dy_j}\right)_{y_k} T_{cm}\right] \Big/ V_{cm}^{1/4} \tag{5-8.17}$$

$$\left(\frac{dV_{cm}}{dy_j}\right)_{y_k} = 2\sum_l y_l(V_{clj} - V_{cli}) \tag{5-8.18}$$

$$\left(\frac{dP_{cm}}{dy_j}\right)_{y_k} = P_{cm}\left[-\frac{0.085(\omega_j - \omega_i)}{Z_{cm}} + \frac{1}{T_{cm}}\left(\frac{dT_{cm}}{dy_j}\right)_{y_k} - \frac{1}{V_{cm}}\left(\frac{dV_{cm}}{dy_j}\right)_{y_k}\right] \tag{5-8.19}$$

Note: In Eqs. (5-8.16) to (5-8.19), $k \neq i, j$. $\ln (f/P)_m$ is given in Eq. (5-4.11); $(H^\circ - H)/RT_{cm}$ is given by Eq. (5-4.3); and T_{cm}, V_{cm}, ω_m, and P_{cm} are given in Table 4-3. $\log (f/P)_m^{(1)}$ [not $\ln (f/P)_m^{(1)}$] is given in Table 5-7.

Smith, van Ness & Abbott, 2007, pp 67

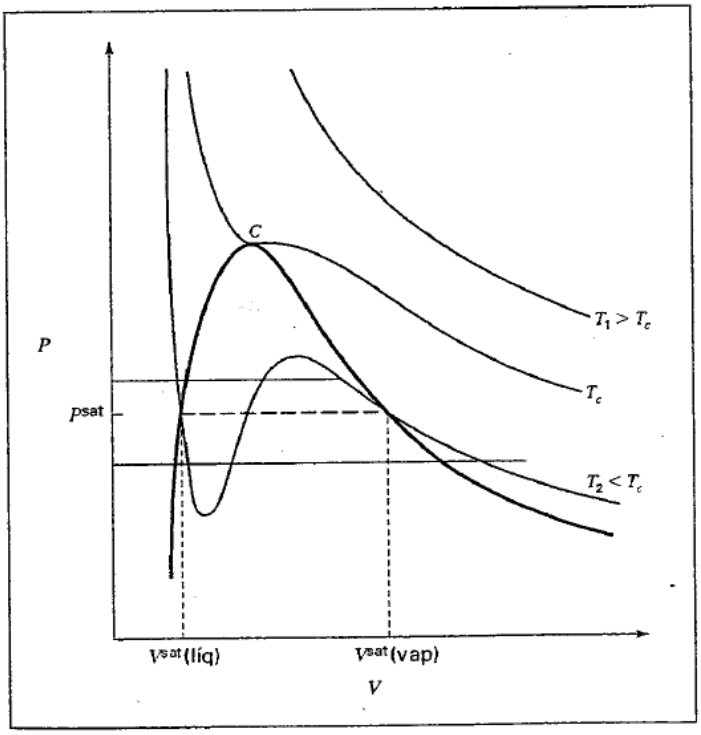


Figura 3.11 Isotermas fornecidas por uma equação de estado cúbica.

Smith, van Ness & Abbott, 2007, pp 168

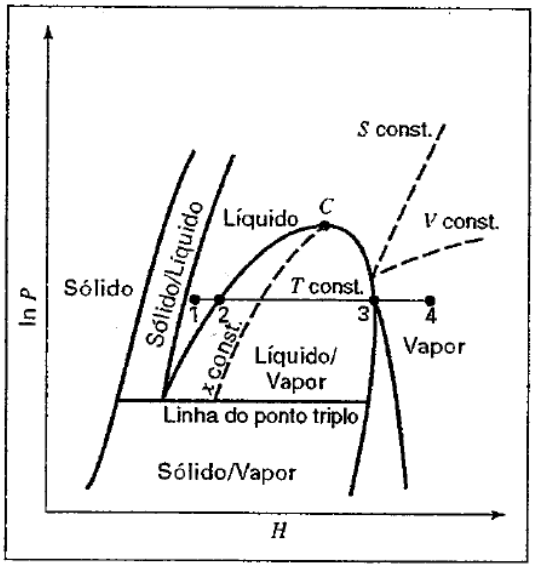


Figura 6.2 Diagrama *PH*.

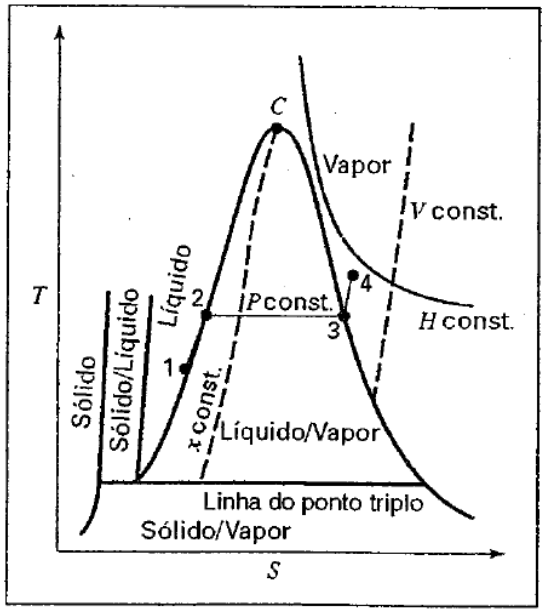


Figura 6.3 Diagrama *TS*.

Smith, van Ness & Abbott, 2007, pp 510

Tabela B.2: Constantes da Equação de Antoine para Pressões de Vapor de Espécies Puras

$$\ln P^{sat}/\text{kPa} = A - \frac{B}{t/°\text{C} + C}$$

Calor latente de vaporização no ponto normal de ebulição (ΔH_n) e ponto normal de ebulição (t_n)

Nome	Fórmula	Parâmetros para Eq. de Antoine A†	B	C	Faixa de Temperatura °C	ΔH_n kJ/mol	t_n °C
Acetona	C_3H_6O	14,3145	2756,22	228,060	−26 — 77	29,10	56,2
Ácido acético	$C_2H_4O_2$	15,0717	3580,80	224,650	24 — 142	23,70	117,9
Acetonitrila*	C_2H_3N	14,8950	3413,10	250,523	−27 — 81	30,19	81,6
Benzeno	C_6H_6	13,7819	2726,81	217,572	6 — 104	30,72	80,0
iso-Butano	C_4H_{10}	13,8254	2181,79	248,870	−83 — 7	21,30	−11,9
n-Butano	C_4H_{10}	13,6608	2154,70	238,789	−73 — 19	22,44	−0,5
1-Butanol	$C_4H_{10}O$	15,3144	3212,43	182,739	37 — 138	43,29	117,6
2-Butanol*	$C_4H_{10}O$	15,1989	3026,03	186,500	25 — 120	40,75	99,5
iso-Butanol	$C_4H_{10}O$	14,6047	2740,95	166,670	30 — 128	41,82	107,8
tert-Butanol	$C_4H_{10}O$	14,8445	2658,29	177,650	10 — 101	39,07	82,3
Tetracloreto de carbono	CCl_4	14,0572	2914,23	232,148	−14 — 101	29,82	76,6
Clorobenzeno	C_6H_5Cl	13,8635	3174,78	211,700	29 — 159	35,19	131,7
1-Clorobutano	C_4H_9Cl	13,7965	2723,73	218,265	−17 — 79	30,39	78,5
Clorofórmio	$CHCl_3$	13,7324	2548,74	218,552	−23 — 84	29,24	61,1
Ciclo-hexano	C_6H_{12}	13,6568	2723,44	220,618	9 — 105	29,97	80,7
Ciclopentano	C_5H_{10}	13,9727	2653,90	234,510	−35 — 71	27,30	49,2
n-Decano	$C_{10}H_{22}$	13,9748	3442,76	193,858	65 — 203	38,75	174,1
Diclorometano	CH_2Cl_2	13,9891	2463,93	223,240	−38 — 60	28,06	39,7
Éter dietílico	$C_4H_{10}O$	14,0735	2511,29	231,200	−43 — 55	26,52	34,4
1,4-Dioxano	$C_4H_8O_2$	15,0967	3579,78	240,337	20 — 105	34,16	101,3
n-Eicosano	$C_{20}H_{42}$	14,4575	4680,46	132,100	208 — 379	57,49	343,6
Etanol	C_2H_6O	16,8958	3795,17	230,918	3 — 96	38,56	78,2

Etilbenzeno	C_8H_{10}	13,9726	3259,93	212,300	33 — 163	35,57	136,2
Etileno glicol*	$C_2H_6O_2$	15,7567	4187,46	178,650	100 — 222	50,73	197,3
n-Heptano	C_7H_{16}	13,8622	2910,26	216,432	4 — 123	31,77	98,4
n-Hexano	C_6H_{14}	13,8193	2696,04	224,317	−19 — 92	28,85	68,7
Metanol	CH_4O	16,5785	3638,27	239,500	−11 — 83	35,21	64,7
Acetato de metila	$C_3H_6O_2$	14,2456	2662,78	219,690	−23 — 78	30,32	56,9
Metiletilcetona	C_4H_8O	14,1334	2838,24	218,690	−8 — 103	31,30	79,6
Nitrometano*	CH_3NO_2	14,7513	3331,70	227,600	56 — 146	33,99	101,2
n-Nonano	C_9H_{20}	13,9854	3311,19	202,694	46 — 178	36,91	150,8
iso-Octano	C_8H_{18}	13,6703	2896,31	220,767	2 — 125	30,79	99,2
n-Octano	C_8H_{18}	13,9346	3123,13	209,635	26 — 152	34,41	125,6
n-Pentano	C_5H_{12}	13,7667	2451,88	232,014	−45 — 58	25,79	36,0
Fenol	C_6H_6O	14,4387	3507,80	175,400	80 — 208	46,18	181,8
1-Propanol	C_3H_8O	16,1154	3483,67	205,807	20 — 116	41,44	97,2
2-Propanol	C_3H_8O	16,6796	3640,20	219,610	8 — 100	39,85	82,2
Tolueno	C_7H_8	13,9320	3056,96	217,625	13 — 136	33,18	110,6
Água	H_2O	16,3872	3885,70	230,170	0 — 200	40,66	100,0
o-Xileno	C_8H_{10}	14,0415	3358,79	212,041	40 — 172	36,24	144,4
m-Xileno	C_8H_{10}	14,1387	3381,81	216,120	35 — 166	35,66	139,1
p-Xileno	C_8H_{10}	14,0579	3331,45	214,627	35 — 166	35,67	138,3

Baseado principalmente nos dados apresentados por B. E. Poling, J. M. Prausnitz e J. P. O'Connell, *The Properties of Gases and Liquids*, 5.ª ed., Apêndice A, McGraw-Hill, Nova York, 2001.
*Parâmetros de Antoine adaptados de Gmehling et al. Ver nota de rodapé 2 do Apêndice H.
†Parâmetros de Antoine *A* estão ajustados para haver reprodução dos valores apresentados para t_n.

Smith, van Ness & Abbott, 2007, pp 507, 508, 509

Tabela B.1: Propriedades Características de Espécies Puras

	Massa molar	ω	T_c/K	P_c/bar	Z_c	V_c cm^3 mol^{-1}	T_n/K
Metano	16,043	0,012	190,6	45,99	0,286	98,6	111,4
Etano	30,070	0,100	305,3	48,72	0,279	145,5	184,6
Propano	44,097	0,152	369,8	42,48	0,276	200,0	231,1
n-Butano	58,123	0,200	425,1	37,96	0,274	255,	272,7
n-Pentano	72,150	0,252	469,7	33,70	0,270	313,	309,2
n-Hexano	86,177	0,301	507,6	30,25	0,266	371,	341,9
n-Heptano	100,204	0,350	540,2	27,40	0,261	428,	371,6
n-Octano	114,231	0,400	568,7	24,90	0,256	486,	398,8
n-Nonano	128,258	0,444	594,6	22,90	0,252	544,	424,0
n-Decano	142,285	0,492	617,7	21,10	0,247	600,	447,3
Isobutano	58,123	0,181	408,1	36,48	0,282	262,7	261,4
Isooctano	114,231	0,302	544,0	25,68	0,266	468,	372,4
Ciclopentano	70,134	0,196	511,8	45,02	0,273	258,	322,4
Ciclo-hexano	84,161	0,210	553,6	40,73	0,273	308,	353,9
Metilciclopentano	84,161	0,230	532,8	37,85	0,272	319,	345,0

(*Continua*)

Tabela B.1: Propriedades Características de Espécies Puras (Continuação)

	Massa molar	ω	T_c/K	P_c/bar	Z_c	V_c cm^3 mol^{-1}	T_n/K
Metilciclo-hexano	98,188	0,235	572,2	34,71	0,269	368,	374,1
Etileno	28,054	0,087	282,3	50,40	0,281	131,	169,4
Propileno	42,081	0,140	365,6	46,65	0,289	188,4	225,5
1-Buteno	56,108	0,191	420,0	40,43	0,277	239,3	266,9
cis-2-Buteno	56,108	0,205	435,6	42,43	0,273	233,8	276,9
trans-2-Buteno	56,108	0,218	428,6	41,00	0,275	237,7	274,0
1-Hexeno	84,161	0,280	504,0	31,40	0,265	354,	336,3
Isobutileno	56,108	0,194	417,9	40,00	0,275	238,9	266,3
1,3-Butadieno	54,092	0,190	425,2	42,77	0,267	220,4	268,7
Ciclo-hexeno	82,145	0,212	560,4	43,50	0,272	291,	356,1
Acetileno	26,038	0,187	308,3	61,39	0,271	113,	189,4
Benzeno	78,114	0,210	562,2	48,98	0,271	259,	353,2
Tolueno	92,141	0,262	591,8	41,06	0,264	316,	383,8
Etilbenzeno	106,167	0,303	617,2	36,06	0,263	374,	409,4
Cumeno	120,194	0,326	631,1	32,09	0,261	427,	425,6
o-Xileno	106,167	0,310	630,3	37,34	0,263	369,	417,6
m-Xileno	106,167	0,326	617,1	35,36	0,259	376,	412,3
p-Xileno	106,167	0,322	616,2	35,11	0,260	379,	411,5
Estireno	104,152	0,297	636,0	38,40	0,256	352,	418,3
Naftaleno	128,174	0,302	748,4	40,51	0,269	413,	491,2
Bifenil	154,211	0,365	789,3	38,50	0,295	502,	528,2
Formaldeído	30,026	0,282	408,0	65,90	0,223	115,	254,1
Acetaldeído	44,053	0,291	466,0	55,50	0,221	154,	294,0
Acetato de metila	74,079	0,331	506,6	47,50	0,257	228,	330,1
Acetato de etila	88,106	0,366	523,3	38,80	0,255	286,	350,2
Acetona	58,080	0,307	508,2	47,01	0,233	209,	329,4
Metiletilcetona	72,107	0,323	535,5	41,50	0,249	267,	352,8

Éter dietílico	74,123	0,281	466,7	36,40	0,263	280,	307,6
Éter metil-*t*-butílico	88,150	0,266	497,1	34,30	0,273	329,	328,4
Metanol	32,042	0,564	512,6	80,97	0,224	118,	337,9
Etanol	46,069	0,645	513,9	61,48	0,240	167,	351,4
1-Propanol	60,096	0,622	536,8	51,75	0,254	219,	370,4
1-Butanol	74,123	0,594	563,1	44,23	0,260	275,	390,8
1-Hexanol	102,177	0,579	611,4	35,10	0,263	381,	430,6
2-Propanol	60,096	0,668	508,3	47,62	0,248	220,	355,4
Fenol	94,113	0,444	694,3	61,30	0,243	229,	455,0
Etileno glicol	62,068	0,487	719,7	77,00	0,246	191,0	470,5
Ácido acético	60,053	0,467	592,0	57,86	0,211	179,7	391,1
Ácido *n*-butírico	88,106	0,681	615,7	40,64	0,232	291,7	436,4
Ácido benzóico	122,123	0,603	751,0	44,70	0,246	344,	522,4
Acetonitrila	41,053	0,338	545,5	48,30	0,184	173,	354,8
Metilamina	31,057	0,281	430,1	74,60	0,321	154,	266,8
Etilamina	45,084	0,285	456,2	56,20	0,307	207,	289,7
Nitrometano	61,040	0,348	588,2	63,10	0,223	173,	374,4
Tetracloreto de carbono	153,822	0,193	556,4	45,60	0,272	276,	349,8
Clorofórmio	119,377	0,222	536,4	54,72	0,293	239,	334,3
Diclorometano	84,932	0,199	510,0	60,80	0,265	185,	312,9
Cloreto de metila	50,488	0,153	416,3	66,80	0,276	143,	249,1
Cloreto de etila	64,514	0,190	460,4	52,70	0,275	200,	285,4
Clorobenzeno	112,558	0,250	632,4	45,20	0,265	308,	404,9
Tetrafluoroetano	102,030	0,327	374,2	40,60	0,258	198,0	247,1
Argônio	39,948	0,000	150,9	48,98	0,291	74,6	87,3
Criptônio	83,800	0,000	209,4	55,02	0,288	91,2	119,8
Xenônio	131,30	0,000	289,7	58,40	0,286	118,0	165,0
Hélio 4	4,003	−0,390	5,2	2,28	0,302	57,3	4,2
Hidrogênio	2,016	−0,216	33,19	13,13	0,305	64,1	20,4
Oxigênio	31,999	0,022	154,6	50,43	0,288	73,4	90,2

(*Continua*)

Sandler, 2006, 561, 562

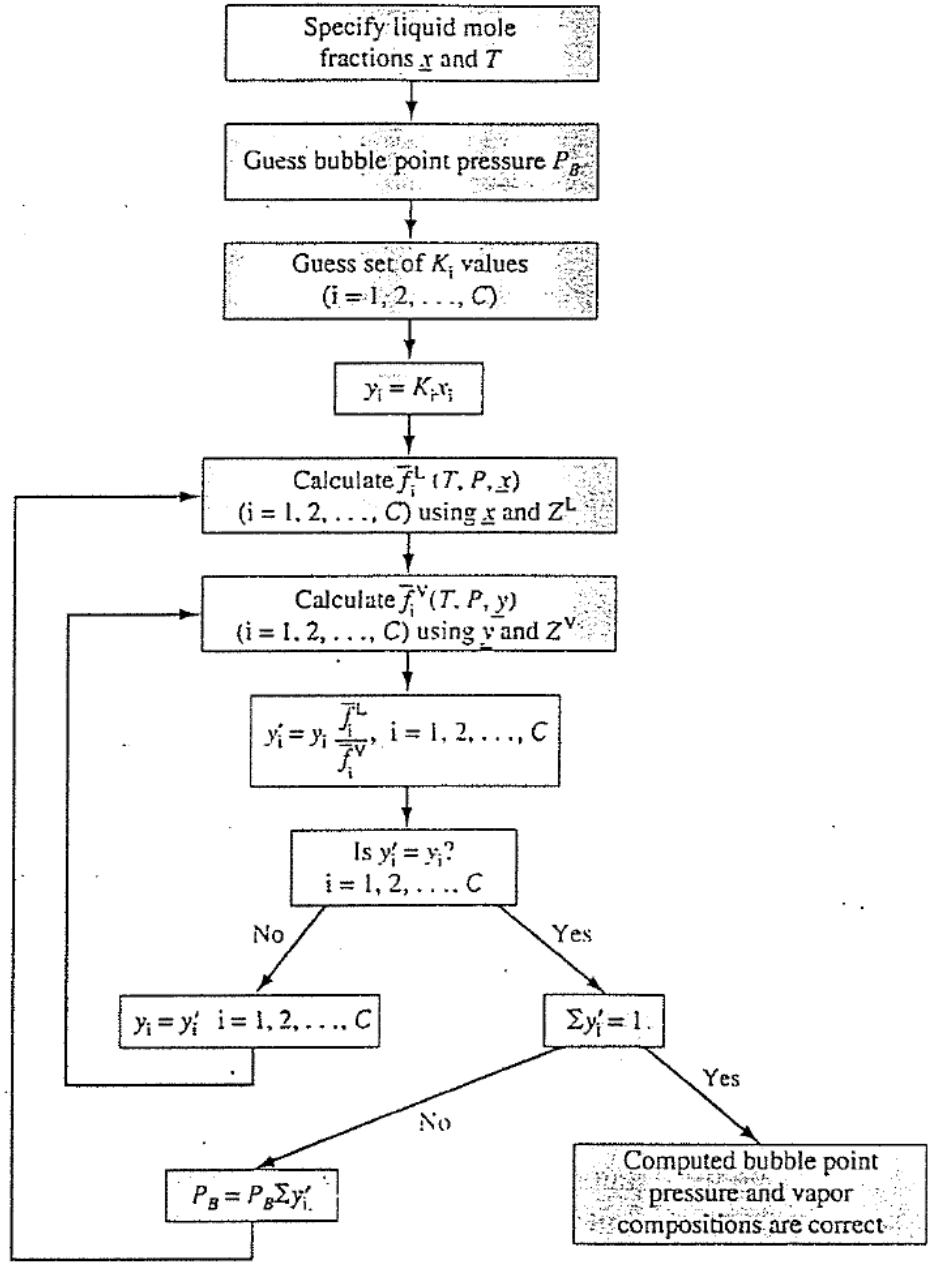
The initial guesses for the bubble point pressure P_B and for the $K_i = y_i/x_i$ values for all species in the mixture do not affect the final solution to the problem, but may influence the number of iterations required to obtain the solution. One possible set of initial guesses is obtained by assuming ideal liquid and vapor mixtures so that

$$P_B = \sum x_i P_i^{vap}(T) \tag{10.3-2}$$

and

$$K_i = \frac{y_i}{x_i} = \frac{P_i^{vap}(T)}{P_B} \tag{10.3-3}$$

where the pure component vapor pressure can be estimated using the Antoine equation, Eq. 7.7-8, with parameters for the fluid of interest, or by using the equation of state as described in Sec. 7.5.


Specify liquid mole fractions $\underline{x}$ and T
Guess bubble point pressure P_B
Guess set of K_i values ($i = 1, 2, \ldots, C$)
$y_i = K_i x_i$
Calculate $\bar{f}_i^L(T, P, \underline{x})$ ($i = 1, 2, \ldots, C$) using $\underline{x}$ and Z^L
Calculate $\bar{f}_i^V(T, P, \underline{y})$ ($i = 1, 2, \ldots, C$) using $\underline{y}$ and Z^V
$y_i' = y_i \frac{\bar{f}_i^L}{\bar{f}_i^V}$, $i = 1, 2, \ldots, C$
Is $y_i' = y_i$? $i = 1, 2, \ldots, C$
No
Yes
$y_i = y_i'$ $i = 1, 2, \ldots, C$
$\Sigma y_i' = 1$.
Yes
No
$P_B = P_B \Sigma y_i'$
Computed bubble point pressure and vapor compositions are correct

Smith, van Ness & Abbott, 2007, pp 48

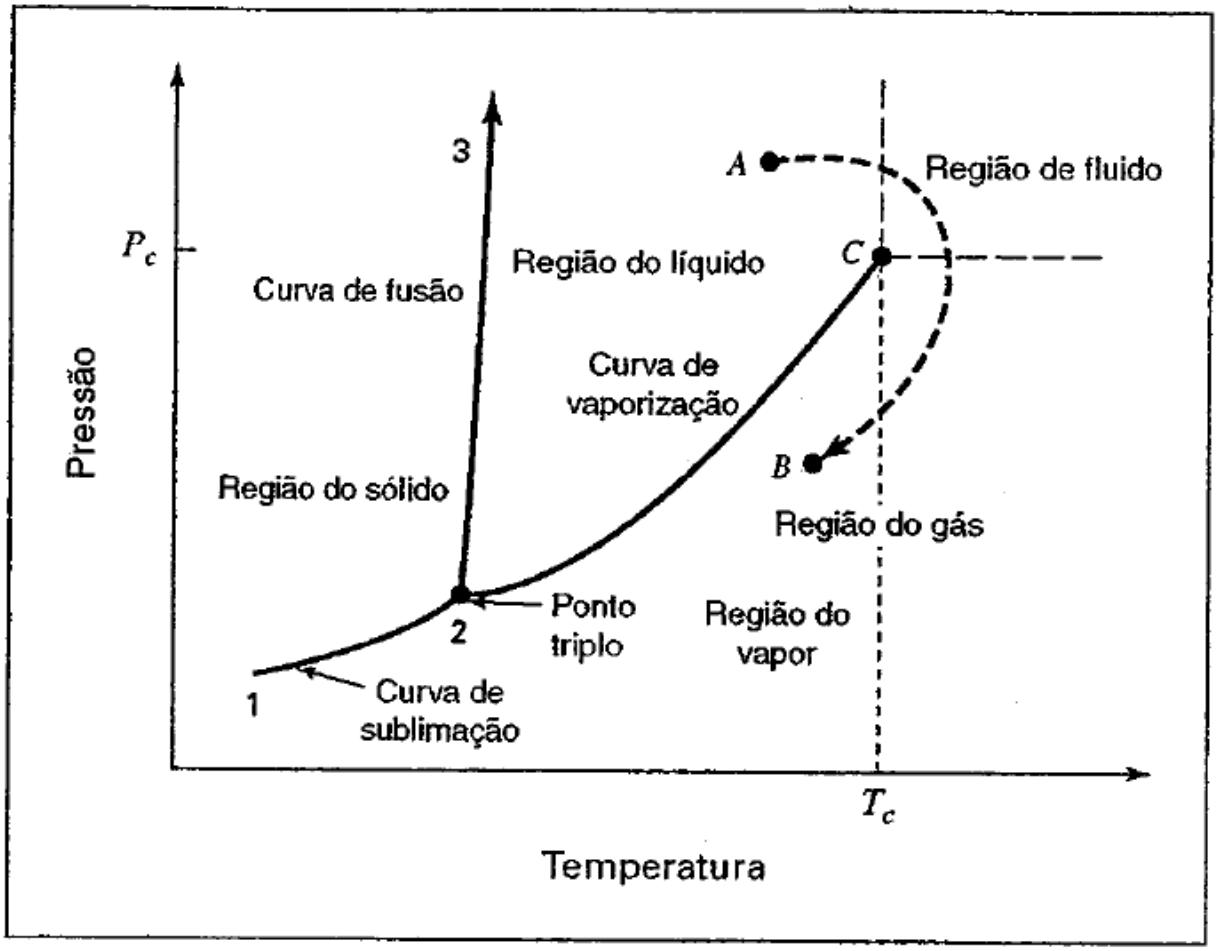


Figura 3.1 Diagrama *PT* para uma substância pura.

Smith, van Ness & Abbott, 2007, pp 260

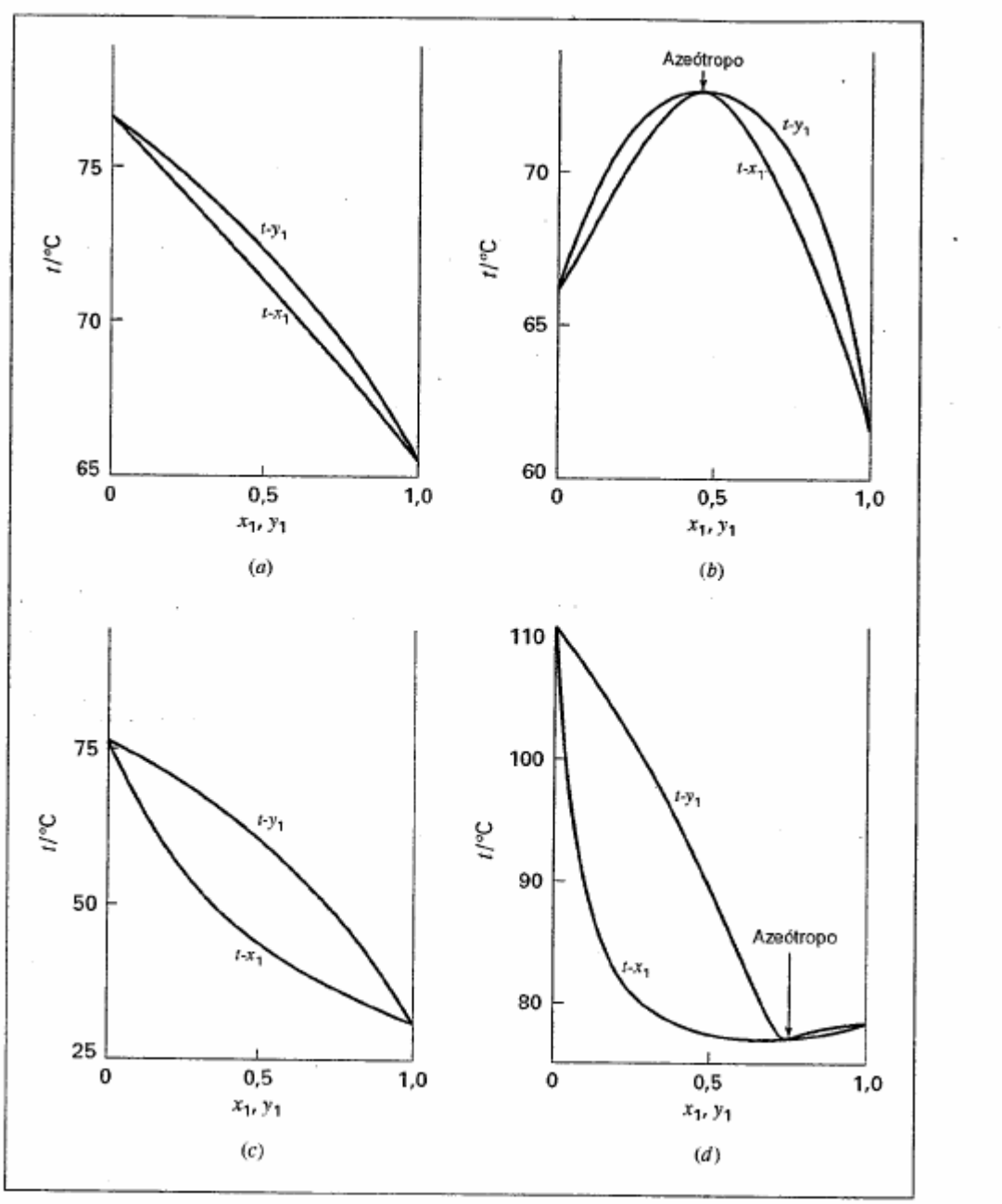


Figura 10.9 Diagramas *txy* a 1(atm). (*a*) tetraidrofurano(1)/tetracloreto de carbono(2); (*b*) clorofórmio(1)/tetraidrofurano(2); (*c*) furano(1)/tetracloreto de carbono(2); (*d*) etanol(1)/tolueno(2).

Smith, van Ness & Abbott, 2007, pp 119

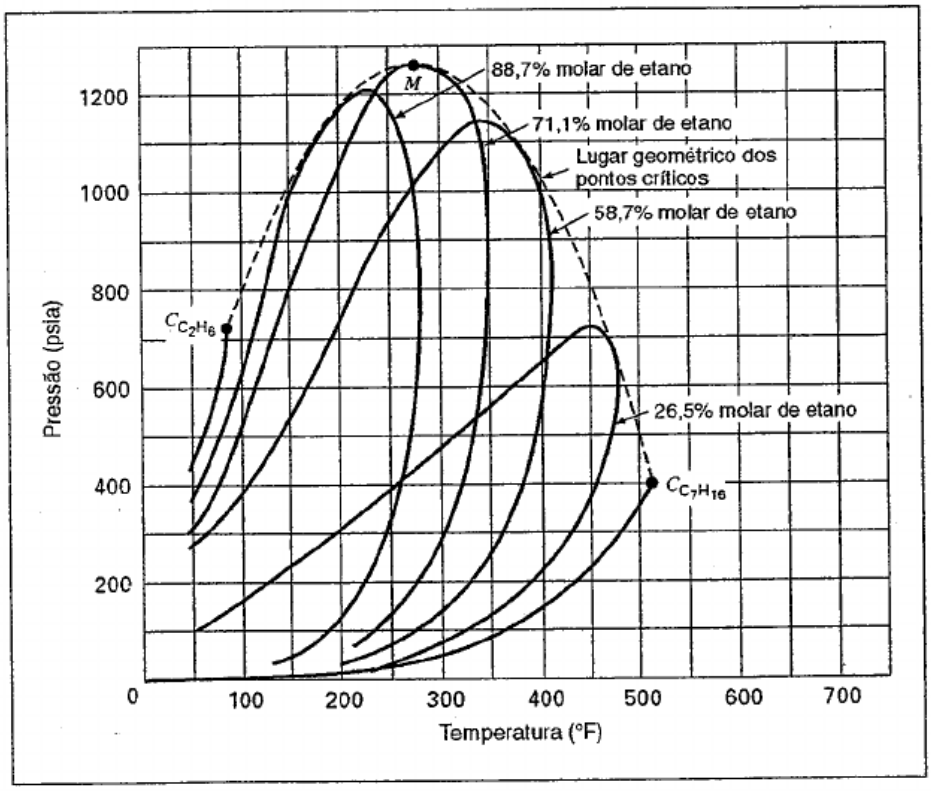


Figura 10.5 Etano/*n*-heptano. Diagrama *PT*. (Reproduzido com permissão. F.H. Barr-David, *AIChE J.*, vol. 2, p. 426-427, 1956.)

$$\frac{C_P^{gi}}{R} = A + BT + CT^2 + DT^{-2}$$

Os valores dos parâmetros para um conjunto de gases orgânicos e inorgânicos comuns são fornecidos na Tabela C.1 do Apêndice C. Equações mais precisas, porém mais complexas, são encontradas na literatura.[1]

Como resultado da Eq. (3.19), as duas capacidades caloríficas de gás ideal são relacionadas:

$$\frac{C_V^{gi}}{R} = \frac{C_P^{gi}}{R} - 1 \tag{4.5}$$

Smith, van Ness & Abbott, 2007, pp 512

Tabela C.1: Capacidades Caloríficas de Gases no Estado de Gás Ideal†

Constantes da equação $C_P^{gi}/R = A + BT + CT^2 + DT^{-2}$ T (kelvins), de 298 K até $T_{máx}$

Espécies químicas		$T_{máx}$	$C_{P_{298}}^{gi}/R$	A	$10^3\,B$	$10^6\,C$	$10^{-5}\,D$
Parafinas:							
Metano	CH_4	1500	4,217	1,702	9,081	−2,164	
Etano	C_2H_6	1500	6,369	1,131	19,225	−5,561	
Propano	C_3H_8	1500	9,011	1,213	28,785	−8,824	
n-Butano	C_4H_{10}	1500	11,928	1,935	36,915	−11,402	
iso-Butano	C_4H_{10}	1500	11,901	1,677	37,853	−11,945	
n-Pentano	C_5H_{12}	1500	14,731	2,464	45,351	−14,111	
n-Hexano	C_6H_{14}	1500	17,550	3,025	53,722	−16,791	
n-Heptano	C_7H_{16}	1500	20,361	3,570	62,127	−19,486	
n-Octano	C_8H_{18}	1500	23,174	4,108	70,567	−22,208	
1-Alcenos:							
Etileno	C_2H_4	1500	5,325	1,424	14,394	−4,392	
Propileno	C_3H_6	1500	7,792	1,637	22,706	−6,915	
1-Buteno	C_4H_8	1500	10,520	1,967	31,630	−9,873	
1-Penteno	C_5H_{10}	1500	13,437	2,691	39,753	−12,447	
1-Hexeno	C_6H_{12}	1500	16,240	3,220	48,189	−15,157	
1-Hepteno	C_7H_{14}	1500	19,053	3,768	56,588	−17,847	
1-Octeno	C_8H_{16}	1500	21,868	4,324	64,960	−20,521	

Vários orgânicos:							
Acetaldeído	C_2H_4O	1000	6,506	1,693	17,978	−6,158	
Acetileno	C_2H_2	1500	5,253	6,132	1,952	.....	−1,299
Benzeno	C_6H_6	1500	10,259	−0,206	39,064	−13,301	
1,3-Butadieno	C_4H_6	1500	10,720	2,734	26,786	−8,882	
Ciclo-hexano	C_6H_{12}	1500	13,121	−3,876	63,249	−20,928	
Etanol	C_2H_6O	1500	8,948	3,518	20,001	−6,002	
Etilbenzeno	C_8H_{10}	1500	15,993	1,124	55,380	−18,476	
Óxido de etileno	C_2H_4O	1000	5,784	−0,385	23,463	−9,296	
Formaldeído	CH_2O	1500	4,191	2,264	7,022	−1,877	
Metanol	CH_4O	1500	5,547	2,211	12,216	−3,450	
Estireno	C_8H_8	1500	15,534	2,050	50,192	−16,662	
Tolueno	C_7H_8	1500	12,922	0,290	47,052	−15,716	
Vários inorgânicos:							
Ar		2000	3,509	3,355	0,575	.....	−0,016
Amônia	NH_3	1800	4,269	3,578	3,020	.....	−0,186
Bromo	Br_2	3000	4,337	4,493	0,056	.....	−0,154
Monóxido de carbono	CO	2500	3,507	3,376	0,557	.....	−0,031
Dióxido de carbono	CO_2	2000	4,467	5,457	1,045	.....	−1,157
Dissulfeto de carbono	CS_2	1800	5,532	6,311	0,805	.....	−0,906
Cloro	Cl_2	3000	4,082	4,442	0,089	.....	−0,344
Hidrogênio	H_2	3000	3,468	3,249	0,422	.....	0,083
Dissulfeto de hidrogênio	H_2S	2300	4,114	3,931	1,490	.....	−0,232
Cloreto de hidrogênio	HCl	2000	3,512	3,156	0,623	.....	0,151
Cianeto de hidrogênio	HCN	2500	4,326	4,736	1,359	.....	−0,725
Nitrogênio	N_2	2000	3,502	3,280	0,593	.....	0,040
Óxito nitroso	N_2O	2000	4,646	5,328	1,214	.....	−0,928
Óxito nítrico	NO	2000	3,590	3,387	0,629	.....	0,014
Dióxido de nitrogênio	NO_2	2000	4,447	4,982	1,195	.....	−0,792
Tetraóxido de dinitrogênio	N_2O_4	2000	9,198	11,660	2,257	.....	−2,787
Oxigênio	O_2	2000	3,535	3,639	0,506	.....	−0,227
Dióxido de enxofre	SO_2	2000	4,796	5,699	0,801	.....	−1,015
Trióxido de enxofre	SO_3	2000	6,094	8,060	1,056	.....	−2,028
Água	H_2O	2000	4,038	3,470	1,450	.....	0,121

[t]Retirados de H.M. Spencer, *Ind. Eng. Chem.*, vol. 40, pp. 2152-2154, 1948; K.K. Kelley, *U.S. Bur. Mines Bull. 584*, 1960; L.B. Pankratz, *U.S. Bur. Mines Bull. 672*, 1982.

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