期末考试题目：

- 使用状态方程（vdw, RK或PR）计算丙烷在 60C 时的饱和压强 P^{sat} ?

- 丙烷（C3）和正丁烷（nC4）混合物在20C时，液相中丙烷摩尔分数 $x_1=0.49$, 求混合物的压力P=？和气相中丙烷摩尔分数 $y_1=?$

可参考EOS

- Van der Waals (1873)
  - $P = \frac{RT}{v-b} - \frac{a}{v^2}$,

    $,where\ a = \frac{27(RT_c)^2}{64P_c}, \mathrm{b} = \frac{RT_c}{8P_c}$
- Redlich- Kwong (RK, 1949)
  - $P = \frac{RT}{v-b} - \frac{a}{\sqrt{T}v(v+b)}$,

    $,where\ a = \frac{0.42748R^2{T_c}^{2.5}}{P_c}, b = \frac{0.08664RT_c}{P_c}$
- Soave-Redlich-Kwong (SRK, 1972)
  - $P = \frac{RT}{v-b} - \frac{a\alpha}{v(v+b)}$,

    $,where\ \alpha = (1 + (0.48508 + 1.55171\omega - 0.15613\omega^2)(1 - \sqrt{T/T_c}))^2$
- Peng-Robinson(RR, 1976)
  - $P = \frac{RT}{v-b} - \frac{a\alpha}{v(v+b)+b(v-b)}$,

    $,where\ \alpha = (1 + \kappa(1 - \sqrt{T/T_c}))^2, \kappa = 0.37464 + 1.54226\omega - 0.26992\omega^2$

可参考数据：(1/2)

▶ A.1 CRITICAL CONSTANTS, ACENTRIC FACTORS, AND ANTOINE COEFFICIENTS:[1]

The Antoine equation is of the form: $\ln(P^{sat}\,[\text{bar}]) = A - \dfrac{B}{T[K] + C}$

TABLE A.1.1 Organic compounds

Formula	Name	$MW_{[g/mol]}$	T_c [K]	P_c [bar]	ω	A	B	C	T_{min}	T_{max}
CH_2O	Formaldehyde	30.026	408	65.86	0.253	9.8573	2204.13	−30.15	185	271
CH_4	Methane	16.042	190.6	46.00	0.008	8.6041	897.84	−7.16	93	120
CH_4O	Methanol	32.042	512.6	80.96	0.559	11.9673	3626.55	−34.29	257	364
C_2H_4	Acetylene	26.038	308.3	61.40	0.184	9.7279	1637.14	−19.77	194	202
C_2H_3N	Acetonitrile	41.052	548	48.33	0.321	9.6672	2945.47	−49.15	260	390
C_2H_4	Ethylene	28.053	282.4	50.36	0.085	8.9166	1347.01	−18.15	120	182
C_2H_4O	Acetaldehyde	44.053	461	55.73	0.303	9.6279	2465.15	−37.15	210	320
C_2H_4O	Ethylene oxide	44.053	469	71.94	0.200	10.1198	2567.61	−29.01	300	310
$C_2H_4O_2$	Acetic acid	60.052	594.4	57.86	0.454	10.1878	3405.57	−56.34	290	430
C_2H_6	Ethane	30.069	305.4	48.74	0.099	9.0435	1511.42	−17.16	130	199
C_2H_6O	Ethanol	46.068	516.2	63.83	0.635	12.2917	3803.98	−41.68	270	369
C_3H_6	Propylene	42.080	365.0	46.20	0.148	9.0825	1807.53	−26.15	160	240
C_3H_6O	Acetone	58.079	508.1	47.01	0.309	10.0311	2940.46	−35.93	241	350
C_3H_8	Propane	44.096	370.0	42.44	0.152	9.1058	1872.46	−25.16	164	249
C_3H_8O	1-Propanol	60.095	536.7	51.68	0.624	10.9237	3166.38	−80.15	285	400
C_4H_6	1,3-Butadiene	54.090	425	43.27	0.195	9.1525	2142.66	−34.30	215	290
C_4H_8	*cis*-2-Butene	56.106	435.6	42.05	0.202	9.1969	2210.71	−36.15	200	305
C_4H_8	*trans*-2-Butene	56.106	428.6	41.04	0.214	9.1975	2212.32	−33.15	200	300
$C_4H_8O_2$	Ethyl acetate	88.105	523.2	38.30	0.363	9.5314	2790.50	−57.15	260	385
C_4H_{10}	*n*-Butane	58.122	425.2	37.90	0.193	9.0580	2154.90	−34.42	195	290
C_4H_{10}	Isobutane	58.122	408.1	36.48	0.176	8.9179	2032.76	−33.15	187	280
$C_4H_{10}O$	*n*-Butanol	74.122	562.9	44.18	0.590	10.5958	3137.02	−94.43	288	404
C_5H_{10}	1-Pentene	70.133	464.7	40.53	0.245	9.1444	2405.96	−39.63	220	325
C_5H_{12}	*n*-Pentane	72.149	469.6	33.74	0.251	9.2131	2477.07	−39.94	220	330
C_6H_6	Benzene	78.112	562.1	48.94	0.212	9.2806	2788.51	−52.36	280	377
C_6H_6O	Phenol	94.111	694.2	61.30	0.440	9.8077	3490.89	−98.59	345	481
C_6H_7N	Aniline	93.127	699	53.09	0.382	10.0546	3857.52	−73.15	340	500
C_6H_{12}	Cyclohexane	84.159	553.4	40.73	0.213	9.1325	2766.63	−50.50	280	380
C_6H_{12}	1-Hexene	84.159	504.0	31.71	0.285	9.1887	2654.81	−47.30	240	360
C_6H_{14}	*n*-Hexane	86.175	507.4	29.69	0.296	9.2164	2697.55	−48.78	245	370

(Continued)

…ds, consult ThermoSolver, the text software.

可参考数据：(2/2)

Fugacity Coefficients for Three Cubic Equations of State

Van der Waals Equation of State

Pure species i

$$\ln \varphi_i = \frac{b_i}{v_i - b_i} - \ln\left(\frac{(v_i - b_i)P}{RT}\right) - \frac{2a_i}{RTv_i}$$

Species 1 in a binary mixture

$$\ln \hat{\varphi}_1 = \frac{b_1}{v - b} - \ln\left(\frac{(v - b)P}{RT}\right) - \frac{2(y_1 a_1 + y_2 a_{12})}{RTv}$$

Species i in a mixture

$$\ln \hat{\varphi}_i = \frac{b_i}{v - b} - \ln\left(\frac{(v - b)P}{RT}\right) - \frac{2\sum_{k=1}^{m} y_k a_{ik}}{RTv}$$

Redlich–Kwong Equation of State

Pure species i

$$\ln \varphi_i = z_i - 1 - \ln\left(\frac{(v_i - b_i)P}{RT}\right) - \frac{a_i}{b_i RT^{1.5}} \ln\left(1 + \frac{b_i}{v_i}\right)$$

Species 1 in a binary mixture

$$\ln \hat{\varphi}_1 = \frac{b_1}{b}(z - 1) - \ln\left(\frac{(v - b)P}{RT}\right) + \frac{1}{bRT^{1.5}}\left[\frac{ab_1}{b} - 2(y_1 a_1 + y_2 a_{12})\right]\ln\left(1 + \frac{b}{v}\right)$$

Species i in a mixture

$$\ln \hat{\varphi}_1 = \frac{b_1}{b}(z - 1) - \ln\left(\frac{(v - b)P}{RT}\right) + \frac{1}{bRT^{1.5}}\left[\frac{ab_1}{b} - 2\sum_{k=1}^{m} y_k a_{ik}\right]\ln\left(1 + \frac{b}{v}\right)$$

Peng–Robinson Equation of State

Pure species i

$$\ln \varphi_i = z_i - 1 - \ln\left(\frac{(v_i - b_i)P}{RT}\right) - \frac{(a\alpha)_i}{2\sqrt{2}b_i RT}\ln\left[\frac{v_i + (1 + \sqrt{2})b_i}{v_i + (1 - \sqrt{2})b_i}\right]$$

Species 1 in a binary mixture

$$\ln \hat{\varphi}_1 = \frac{b_1}{b}(z - 1) - \ln\left(\frac{(v - b)P}{RT}\right) + \frac{a\alpha}{2\sqrt{2}bRT}\left[\frac{b_1}{b} - \frac{2}{a\alpha}(y_1(a\alpha)_1 + y_2(a\alpha)_{12})\right]\ln\left[\frac{v + (1 + \sqrt{2})b}{v + (1 - \sqrt{2})b}\right]$$

Species i in a mixture

$$\ln \hat{\varphi}_i = \frac{b_i}{b}(z - 1) - \ln\left(\frac{(v - b)P}{RT}\right) + \frac{a\alpha}{2\sqrt{2}bRT}\left[\frac{b_i}{b} - \frac{2}{a\alpha}\sum_{k=1}^{m} y_k (a\alpha)_{ik}\right]\ln\left[\frac{v + (1 + \sqrt{2})b}{v + (1 - \sqrt{2})b}\right]$$

例题二：数值计算表参考

Values of the Iterative Bubble-point Calculation. The Column Labeled *n* Represents the Iteration Number.

n	a^v $\left[\frac{\mathrm{Jm^3}}{\mathrm{mol^2}}\right]$	b^v $\left[\frac{\mathrm{m^3}}{\mathrm{mol}}\right]$	v^v $\left[\frac{\mathrm{m^3}}{\mathrm{mol}}\right]$	v^l $\left[\frac{\mathrm{m^3}}{\mathrm{mol}}\right]$	$\hat{\varphi}_1^v$	$\hat{\varphi}_2^v$	$\hat{\varphi}_1^l$	$\hat{\varphi}_2^l$	y_1	y_2	$\sum y_i$	$P^{(k+1)}$ [bar]
1	0.238	$4.40\ 10^{-5}$	$2.55\ 10^{-4}$	$1.59\ 10^{-4}$	0.86	0.37	1.30	0.10	0.45	0.18	0.634	54.5
2	0.241	$4.72\ 10^{-5}$	$4.38\ 10^{-4}$	$1.65\ 10^{-4}$	0.91	0.56	1.78	0.12	0.59	0.15	0.739	40.3
3	0.328	$5.48\ 10^{-5}$	$5.97\ 10^{-4}$	$1.69\ 10^{-4}$	0.93	0.63	2.24	0.15	0.72	0.16	0.887	35.7
4	0.401	$6.07\ 10^{-5}$	$6.49\ 10^{-4}$	$1.70\ 10^{-4}$	0.94	0.61	2.47	0.16	0.79	0.19	0.971	34.7
5	0.433	$6.32\ 10^{-5}$	$6.43\ 10^{-4}$	$1.71\ 10^{-4}$	0.96	0.57	2.53	0.16	0.79	0.20	0.995	34.5
6	0.443	$6.40\ 10^{-5}$	$6.34\ 10^{-4}$	$1.71\ 10^{-4}$	0.96	0.56	2.54	0.16	0.79	0.21	0.999	34.5