Quiz 10
Chemical Engineering Thermodynamics
April 2, 2020

The K-ratio is used to calculate the equilibrium distribution of a component in a mixture between vapor and liquid phases. We went through five methods to determine the *K*-ratio. For n-octane at 100°C at 0.1 MPa calculate the K-ratio:

a) Using Raoult's Law and P_{sat} from:
   -The Antoine equation;
   Antoine Constants for n-Octane $P^{sat} = 10^{(A - B/(C+T))}$ $A = 4.049$; $B = 1355$; $C = -63.63$
   (P = bar; T = K; For 326-400K NIST Webbook)
   -The short-cut method;
   The shot-cut parameters are available as critical parameters in the PREOS.xls .
   -Using PREOS.xls
b) Calculate the *K*-ratio using the de Priester chart. (Show the chart in your answer.)
c) Calculate the *K*-ratio using the fugacity of the liquid and the vapor phases from PREOS.xls and Equation 10-70. $y_i f_i^V = x_i f_i^L$
d) Determine the bubble point temperature and the dew point temperature for a mixture of n-hexane, n-heptane, and n-octane in a 0.33:0.33:0.34 molar ratio at 0.1 MPa using the short-cut method.
e) For an isothermal flash at 100°C and 0.1 MPa what is the V/F ratio, for the mixture of part d, and what are the compositions of the vapor and liquid products using the short-cut method?

Show screen shots of the Excel sheets where you use them.

	Antoine	Short-Cut	PREO.xls	de Priester	f_i^L/f_i^V
$K_{n\text{-octane}}$					

	$T_{BubblePoint}$, °C	$T_{DewPoint}$, °C	V/F 100°C
0.1 MPa			

	x_i	y_i
n-C6		
n-C7		
n-C8		

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a) Using Raoult's Law and P_{sat} from:
   -The Antoine equation;
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b) Calculate the *K*-ratio using the de Priester chart. (Show the chart in your answer.)
c) Calculate the *K*-ratio using the fugacity of the liquid and the vapor phases from PREOS.xls and Equation 10-70. $y_i f_i^V = x_i f_i^L \quad f_i^L/f_i^V$
d) Determine the bubble point temperature and the dew point temperature for a mixture of n-hexane, n-heptane, and n-octane in a 0.33:0.33:0.34 molar ratio at 0.1 MPa using the short-cut method.
e) For an isothermal flash at 100°C and 0.1 MPa what is the V/F ratio, for the mixture of part d, and what are the compositions of the vapor and liquid products using the short-cut method?

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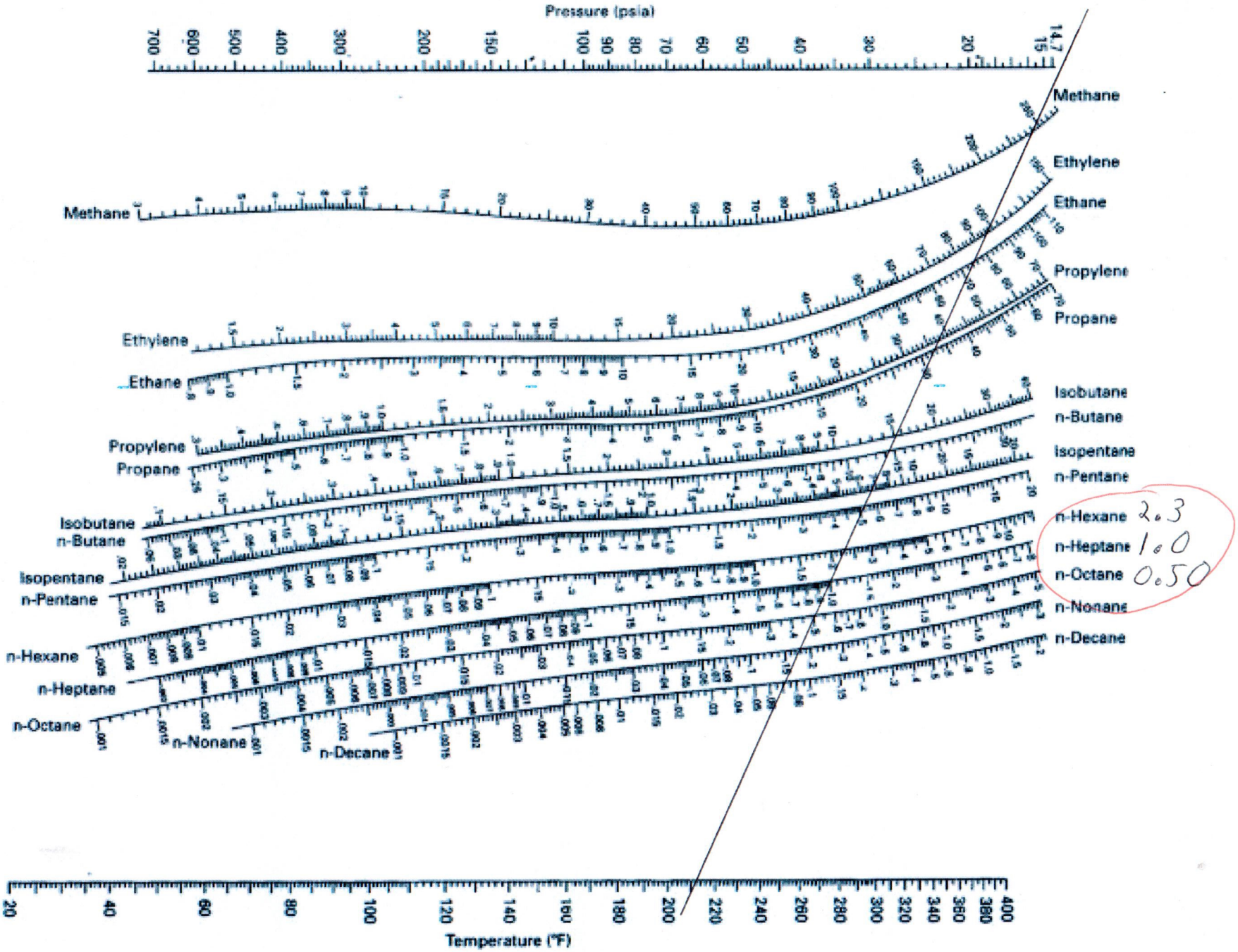
	Antoine	Short-Cut	PREO.xls	de Priester	f_i^L/f_i^V
$K_{n\text{-octane}}$	0.467	0.405	0.470	0.50	0.486

	$T_{BubblePoint}$ °C	$T_{DewPoint}$ °C	V/F 100°C
0.1 MPa	105°C (378K)	90.2°C (363K)	0.646

	xi	yi
n-C6	0.173	0.416
n-C7	0.318	0.337
n-C8	0.509	0.247

Antoine Constants for n-Octane $P^{sat} = 10^{(A - B/(C+T))}$ $A = 4.049$; $B = 1355$; $C = -63.63$
(P = bar; T = K; For 326-400K NIST Webbook)
The shot-cut parameters are available as critical parameters in the PREOS.xls worksheet.


Pressure (psia)
700
600
500
400
300
200
150
100
90
80
70
60
50
40
30
20
14.7
15
Methane
Ethylene
Ethane
Propylene
Propane
Isobutane
n-Butane
Isopentane
n-Pentane
n-Hexane
n-Heptane
n-Octane
n-Nonane
n-Decane
2.3
1.0
0.50
20
40
60
80
100
120
140
160
180
200
220
240
260
280
300
320
340
360
380
400
Temperature (°F)

Dew Point Temperature

		T, °C	
Temp, K	363.237081	90.23708116	
			Dew Point Temp
	zi	Ki	yi
C6	0.33	1.863561579	0.61497532
C7	0.33	0.799392277	0.26379945
C8	0.34	0.356543833	0.1212249
			0.99999968

$$K_i = \frac{P_i^{sat}}{P} \approx \frac{P_{c,i}10^{\frac{7}{3}(1+\omega)\left(1-\frac{1}{T_{r,i}}\right)}}{P}$$

Shortcut *K*-ratio

Gas	T_c (K)	P_c (MPa)	ω
n-HEXANE	507.4	3.012	0.305
n-HEPTANE	540.3	2.736	0.349
n-OCTANE	568.8	2.486	0.396

Bubble Point Temperature

		T, °C		
Temp, K	377.808075	104.8080752		
			Dew Point Temp	
	zi	Ki	yi	xi
C6	0.33	2.718877892		0.1213736
C7	0.33	1.211525025		0.27238397
C8	0.34	0.560832794		0.6062413
				0.99999887

$$K_i = \frac{P_i^{sat}}{P} \approx \frac{P_{c,i}10^{\frac{7}{3}(1+\omega)\left(1-\frac{1}{T_{r,i}}\right)}}{P}$$

Shortcut *K*-ratio

Gas	T_c (K)	P_c (MPa)	ω
n-HEXANE	507.4	3.012	0.305
n-HEPTANE	540.3	2.736	0.349
n-OCTANE	568.8	2.486	0.396

Isothermal Flash

				T, °C	V/F	L/F	
P, Mpa	0.1	Temp, K	373	100	0.64572049	0.35427951	
					Dew Point Temp		
			zi	Ki	yi	xi	Di
		C6	0.33	2.408104575	0.41622514	0.17284347	-0.2433817
		C7	0.33	1.060003806	0.33675351	0.31769085	-0.0190627
		C8	0.34	0.484863447	0.24702132	0.50946574	0.26244443
					0.99999997	1.00000006	9.1174E-08

$$K_i = \frac{P_i^{sat}}{P} \approx \frac{P_{c,i}10^{\frac{7}{3}(1+\omega)\left(1-\frac{1}{T_{r,i}}\right)}}{P}$$

Shortcut *K*-ratio

$$\sum_i \frac{z_i(1-K_i)}{1_i+(V/F)(K_i-1)} = 0$$

Gas	T_c (K)	P_c (MPa)	ω
n-HEXANE	507.4	3.012	0.305
n-HEPTANE	540.3	2.736	0.349
n-OCTANE	568.8	2.486	0.396

Increase Indent

	Antoine	Short-Cut	PREO.xls	de Priester	f_i^L/f_i^V
n-C6	out of range	2.41	2.42	2.3	2.29
n-C7	out of range	1.06	1.05	1	1.05
n-C8	0.467	0.485	0.47	0.5	0.486

Gas	T_c (K)	P_c (MPa)	w
n-HEXANE	507.4	3.012	0.305
n-HEPTANE	540.3	2.736	0.349
n-OCTANE	568.8	2.486	0.396

Gas	A	B	C	Range K
n-HEXANE	4.003	1172	-48.78	286-343
n-HEPTANE	4.028	1269	-56.2	299-373
n-OCTANE	4.049	1355	-63.63	326-400
	P= Bar	T = K		