CM 3450
Drills 2
9/8/2008

1. A stream containing compounds a, b, c and d are fed to a series of distillation columns as shown in Figure 1 with corresponding stream compositions given in Table 1.

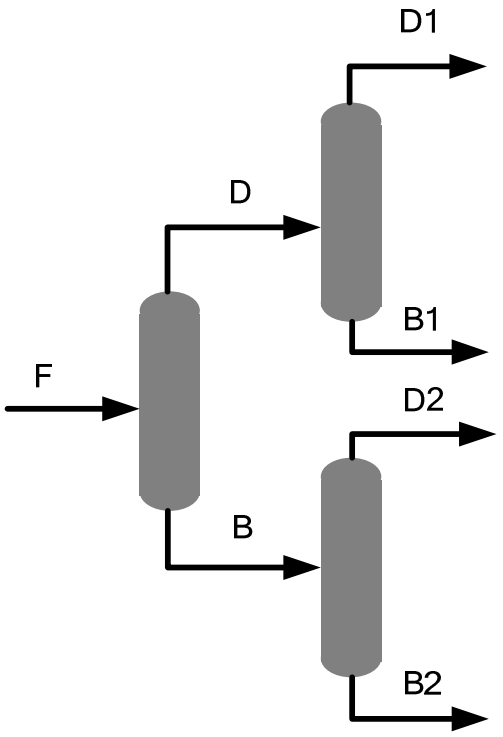

Figure 1. Distillation Train.

Table 1. Stream compositions.

Stream	Composition of Compounds (mol per cent)			
	a	*b*	*c*	*D*
F	26	25	24	25
D1	90	3	5	2
B1	15	40	30	15
D2	10	42	40	8
B2	2	10	20	68

Problem: Determine the molar flow rates of streams D1, B1, D2 and B2, if F=100 kmol/min.

Solution: Set up the spreadsheet shown in Figure 2.

	A	B	C	D	E	F	G	H	I	J	K	L	M
2		Composition					Stream	Flow Rate		Feed comp	F		flow in
3	*a*	0.9	0.15	0.1	0.02		D1			0.26	100		26
4	*b*	0.03	0.4	0.42	0.1	x	B1		=	0.25	100	=	25
5	*c*	0.05	0.3	0.4	0.2		D2			0.24	100		24
6	*d*	0.02	0.15	0.08	0.68		B2			0.25	100		25

Figure 2. Spreadsheet setup.

a) Name the range **B3:E6** as **Comp**
b) Name the range **M3:M6** as **FlowIn**
c) Mark (collect) the cell range **H3:H6**
d) Enter the formula: **=MMULT(MINVERSE(Comp), FlowIn)** then press **[CTRL-SHIFT-ENTER]**

Additional question: what is the molar flow rate of D and ?

2. Multi-linear regression of Antoine equation.

The Antoine equation is given by

$$\log_{10} P_v = A - \frac{B}{T + C}$$

where A, B and C are known as the Antoine coefficients, P_v is the vapor pressure in mm Hg and T is the temperature in $°C$.

The experimental data for vapor pressure at different temperatures are given in Table 2.

Table 2. Vapor Pressure Data.

T	P
29	20
30.5	21
40	35
45.3	46
53.6	68
60.1	92
72	152
79.7	206

T	P
83.5	238
90.2	305
105.2	512
110.5	607
123.2	897
130	1092
132	1152

Problem: Using the data given in Table 2, use multilinear regression to obtain the Antoine coefficients.

Solution:

First, transform the original equation into a multi-linear formulation as follows

$$\log_{10} P_v = A - \frac{B}{T + C}$$
$$(T + C)\log_{10} P_v = A(T + C) - B$$
$$T\log_{10} P_v + C\log_{10} P_v = AT + AC - B$$
$$T\log_{10} P_v = -C\log_{10} P_v + AT + (AC - B)$$

Rename the group of variables and parameters as follows:

$$y = T\log_{10} P_v \qquad x = \log_{10} P_v \quad w = T$$
$$a_1 = -C \quad a_2 = A \quad a_3 = AC - B$$

Then,

$$y = a_1 x + a_2 w + a_3$$

which is multilinear. Once the parameters a_1, a_2 and a_3 have been estimated, recover the original coefficients,

$$C = -a_1 \quad ; \quad A = a_2 \quad ; \quad B = AC - a_3 = -a_1 a_2 - a_3$$

a) Prepare the following spreadsheet:

	B	C	D	E	F	G	H	I	J	K	L
2	Raw Data										
3	T	P		log(P)	T	1					T log(P)
4	29	20		1.30103	29	1		a1			37.72987
5	30.5	21		1.322219	30.5	1		a2			40.32769
6	40	35		1.544068	40	1		a3			61.76272
7	45.3	46		1.662758	45.3	1					75.32293
8	53.6	68		1.832509	53.6	1					98.22248
9	60.1	92		1.963788	60.1	1	x			=	118.0236
10	72	152		2.181844	72	1					157.0927
11	79.7	206		2.313867	79.7	1					184.4152
12	83.5	238		2.376577	83.5	1					198.4442
13	90.2	305		2.4843	90.2	1					224.0838
14	105.2	512		2.70927	105.2	1					285.0152
15	110.5	607		2.783189	110.5	1					307.5424
16	123.2	897		2.952792	123.2	1					363.784
17	130	1092		3.038223	130	1					394.9689
18	132	1152		3.061452	132	1					404.1117

Figure 2. Setup for multilinear regression.

b) Name the range **E4:G18** as A, and range **L4:L18** as b.

c) Select range J4:J6 and input the formula below and then press **[ctrl-shift-enter]:**

=MMULT(MINVERSE(MMULT(TRANSPOSE(A),A)), MMULT(TRANSPOSE(A), b))

d) Recover the original parameters.

	N	O
3	Antoine Coefficient	
4	C	223.4209
5	A	7.400909
6	B	1541.979

Figure 3. Recover the Antoine coefficients.

e) Create a range of values for T, then calculate for P_v using the coefficients.

	A	B	C	D
19				
20		New Data		
21		T	P	
22		20	11.649	
23		21.18812	12.50	
24		22.37624	13.413	
113		128.1188	1034.07	
114		129.3069	1069.857	
115		130.495	1106.628	
116		131.6832	1144.403	
117		132.8713	1	
118		134.0594	1	
119		135.2475	1263.956	
120		136.4356	1305.95	
121		137.6238	1349.048	
122		138.8119	1393.272	
123		140	1438.642	

=10^($O$5-$O$6/(B22+$O$4))

Figure 4. Generate new data using model equation.

f) Plot the predicted values together with raw data.

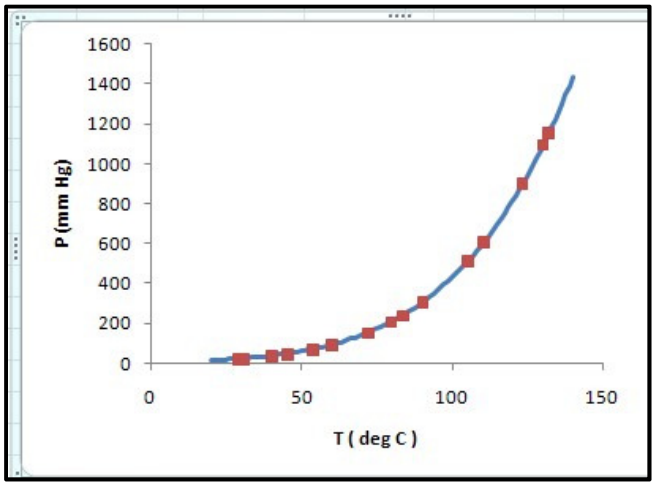

Figure 5. Compare model data with raw data.