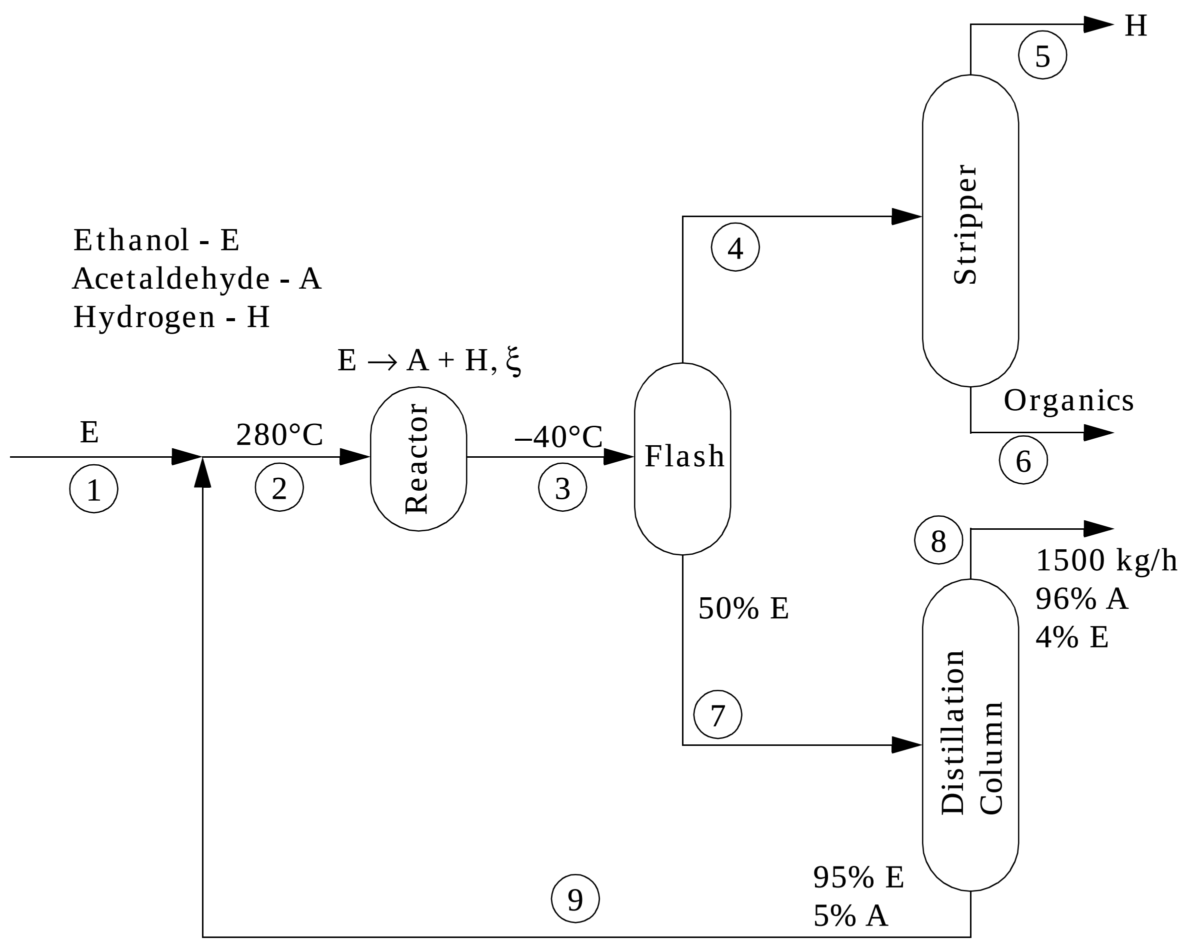
Problem 6.59 Using *Excel* as a calculator

Acetaldehyde is produced by the catalytic dehydrogenation of ethanol.

$$C_2H_5OH(g) \rightarrow CH_3CHO(g) + H_2(g)$$

A fresh feed (pure ethanol) and a recycle stream (95 mol% ethanol and 5 mol% acetaldhyde) combine and enter a reactor at 280°C. The exit gasses are cooled to –40°C to condense the acetaldehyde and unreacted ethanol. The gas leaving the condenser is scrubbed to remove the remaining organics, and hydrogen is sold as a valuable reaction by-product. The condensate, which is 50 mol% ethanol, passes to a distillation column. The distillate, which is 96 mol% acetaldehyde, is sold for use as is or for additional refining, and the bottom stream is recycled to the reactor. The pressure of each gas stream may be taken to be 1 atm. The production rate of the 96% acetaldehyde stream is 1500 kg/hr. Calculate the mole flow rates of the fresh feed, the recycle stream, and the hydrogen; the volumetric flow rate of the feed to the reactor; the overall and single-pass conversions; and the rates at which ethanol and acetaldehyde are removed in the hydrogen scrubber. (*Suggestion:* Use Raoult's law and the Antoine equation in your analysis of the condenser.)

First we'll draw the PFD and label the streams



We can either pick a basis of Stream 1, and scale everything at the end or we can work from Stream 8.

Starting from Stream 8, we must do some mole-to-mass and mass-to-mole conversions. We'll use x as mole fraction and m as mass flow rate.

$$n_{8_A} = x_{8_A} n_8$$

$$m_{8_A} = M_A n_{8_A} = M_A x_{8_A} n_8$$

$$n_{8_E} = x_{8_E} n_8$$

$$m_{8_E} = M_E n_{8_E} = M_E x_{8_E} n_8$$

Combining:

$$m_8 = m_{8_A} + m_{8_E} = M_A x_{8_A} n_8 + M_E x_{8_E} n_8 = n_8 (M_A x_{8_A} + M_E x_{8_E})$$

$$n_8 = \frac{m_8}{M_A x_{8_A} + M_E x_{8_E}}$$

We'll next do a mole balance on both A and E around the Distillation Column.

$$n_7 = n_8 + n_9$$

$$n_7 x_{7_A} = n_8 x_{8_A} + n_9 x_{9_A}$$

$$n_7 x_{7_E} = n_8 x_{8_E} + n_9 x_{9_E}$$

Substituting in compositions and known flows

$$0.5 n_7 = n_{8_A} + 0.05 n_9$$

$$0.5 n_7 = n_{8_E} + 0.95 n_9$$

Subtracting

$$n_{8_A} + 0.05 n_9 = n_{8_E} + 0.95 n_9$$

$$n_9 = \frac{n_{8_A} - n_{8_E}}{0.9}$$

With the usual substitutions we know all of the flows in Streams 7, 8, and 9.

There is a temptation to ignore the E and A in Stream 4 (because they will be in low concentration) and solve the rest of the problem. We'll resist that temptation. Working backwards into the Flash unit, we have vapor-liquid equilibrium between Stream 7 and 4. We know T, P, and the liquid composition. We need the y_i's. We'll make the assumption that H is insoluble in the liquid phase (our other choice is to look up Henry's law constants for H in E and H in A, which aren't in the book). Then from Raoult's law,

$$y_A = \frac{x_A p^*_A}{P},$$

$$y_E = \frac{x_E p^*_E}{P}$$

and

$$y_H = 1 - y_A - y_E.$$

From the problem statement

$$P = 1 \text{ atm} = 760 \text{ mm Hg}.$$

To find p^*_i we'll use the Antoine equation

$$\log_{10}(p^*) = A - \frac{B}{T + C}$$

with T in °C and p^* in mm Hg.

For A

$$A = 6.81089,$$

$$B = 992.0,$$

and

$$C = 230$$

For E

$$A = 8.04494,$$

$$B = 1554.3,$$

and

$$C = 222.65$$

We have the compositions in Stream 4 but not the overall flow rate n_4. For completeness, we'll do a mole balance on the stripper now.

$$n_{5_H} = n_{4_H}$$

$$n_{5_A} = 0$$

$$n_{5_E} = 0$$

and

$$n_{6_H} = 0$$

$$n_{6_A} = n_{4_A}$$

$$n_{6_E} = n_{4_E}$$

We'll briefly treat Stream 4 as an outlet stream. If we perform an overall mole balance on the process, treating it like a reactor, we have

$$n_{4_H} = x_{4_H} n_4 = \nu_H \xi = \xi$$

$$n_{4_A} + n_{8_A} = x_{4_A} n_4 + n_{8_A} = \nu_A \xi = \xi$$

$$n_{4_E} + n_{8_E} = x_{4_E} n_4 + n_{8_E} = n_{1_E} + \nu_E \xi = n_{1_E} - \xi$$

These last three equations can be solved simultaneously for ξ, n_4, and n_{1_E}.

$$x_{4_A} n_4 + n_{8_A} = x_{4_H} n_4$$

$$n_4 = \frac{n_{8_A}}{x_{4_H} - x_{4_A}}$$

$$\xi = x_{4_H} n_4 = \frac{x_{4_H} n_{8_A}}{x_{4_H} - x_{4_A}}$$

$$n_{1_E} = n_4 x_{4_E} + n_{8_E} + \xi = n_{8_A} \frac{x_{4_H} + x_{4_E}}{x_{4_H} - x_{4_A}} + n_{8_E}$$

We can now work either direction around the recycle loop.

$$n_{3_A} = n_{4_A} + n_{7_A}$$

$$n_{3_E} = n_{4_E} + n_{7_E}$$

$$n_{3_H} = n_{4_H}$$

And

$$n_{2_A} = n_{9_A}$$

$$n_{2_E} = n_{1_E} + n_{9_E}$$

The single-pass conversion is:

$$f_{E_{\text{One Pass}}} = \frac{n_{2_E} - n_{3_E}}{n_{2_E}}.$$

The overall conversion is:

$$f_{E_{\text{Overall}}} = \frac{n_{1_E} - n_{6_E} - n_{8_E}}{n_{1_E}}.$$

Finally, the volumetric flow rate in Stream 2 is found by assuming ideal gas behavior (acetaldehyde boils at 20.2°C and ethanol at 78.5°C).

$$PV = nRT$$

or

$$V = \frac{nRT}{P}$$

where

$$R = 62.36\frac{\mathrm{m^3 mm\ Hg}}{\mathrm{kmol\ K}}$$

Since the product rate was specified in kg/h, we can also calculate all of the flows in kg/h with very little additional effort.

The finished spreadsheet looks like:

T in Flash	*-40*	°C							
Species	Nickname	Molec Wt	A	B	C	log10p*	p* in Flash (mm Hg)		
C2H5OH	E	*46.0695*	*8.04494*	*1554.3*	*222.65*	-0.46478	0.34294		
CH3CHO	A	*44.0536*	*6.81089*	*992*	*230*	1.589837	38.8899		
H2	H	*2.01594*							
	Stream 1	Stream 2	Stream 3	Stream 4	**Stream 5**	**Stream 6**	Stream 7	Stream 8	**Stream 9**
n E (kmol/h)	**34.87502**	67.8804	34.37263	0.00776	0	**0.00776**	34.3649	1.35949	**33.00538**
n A (kmol/h)	**0**	1.73713	35.2449	0.88003	0	**0.880027**	34.3649	32.6277	**1.737125**
n H (kmol/h)	**0**	0	33.50777	33.5078	**33.50777**	0	0	0	**0**
n tot (kmol/h)	**34.87502**	69.6175	103.1253	34.3956	33.50777	0.887788	68.7297	33.9872	**34.74251**
m E (kg/h)	1606.676	3127.22	1583.531	0.35752	0	0.357515	1583.17	62.631	1520.542
m A (kg/h)	0	76.5266	1552.664	38.7684	0	38.76835	1513.9	1437.37	76.52659
m H (kg/h)	0	0	67.54966	67.5497	67.54966	0	0	0	0
m tot (kg/h)	1606.676	3203.74	3203.744	106.676	67.54966	39.12587	3097.07	*1500*	1597.069
x E	*1*	0.97505	0.333309	0.00023	*0*	0.008741	*0.5*	0.04	*0.95*
x A	*0*	0.02495	0.341768	0.02559	*0*	0.991259	*0.5*	*0.96*	0.05
x H	*0*	*0*	0.324923	0.97419	*1*	*0*	*0*	*0*	*0*
f E Overall	**0.960796**		P	*760*	mm Hg	R	*62.36*	m^3 mm Hg/kmol K	
f E Reactor	**0.49363**		T (Strm 2)	*280*	°C				
extent	33.50777		**V (Strm 2)**	**3159.76**	**m^3/h**				

Nomenclature: In a spreadsheet, the cells containing entries that can be changed are in *italics*, the intermediate calculated quantities are in plain text, and the answers are in **bold text**.

If you are running this tutorial in *FrameMaker* and you have *Microsoft Excel* available, you can double-click the spreadsheets above and below and they will operate just like in *Excel*.

The formulas that are entered are

T in Flash	*-40*	°C		
Species	Nickname	Molec Wt	A	B
C2H5OH	E	*46.06952*	*8.04494*	*1554.3*
CH3CHO	A	*44.05358*	*6.81089*	*992*
H2	H	*2.01594*		
	Stream 1	Stream 2	Stream 3	Stream 4
n E (kmol/h)	**=E12*E17+I9+B23**	=J9+B9	=E9+H9	=E$12*E17
n A (kmol/h)	**=B$12*B18**	=J10	=E10+H10	=E$12*E18
n H (kmol/h)	**=B$12*B19**	=J11+B11	=E11+H11	=E$12*E19
n tot (kmol/h)	**=B9**	=SUM(C9:C11)	=E12+H12	=I10/(E19-E18)
m E (kg/h)	=B9*$C4	=C9*$C4	=E13+H13	=E9*$C4
m A (kg/h)	=B10*$C5	=C10*$C5	=E14+H14	=E10*$C5
m H (kg/h)	=B11*$C6	=C11*$C6	=E15+H15	=E11*$C6
m tot (kg/h)	=SUM(B13:B15)	=SUM(C13:C15)	=E16+H16	=SUM(E13:E15)
x E	*1*	=C9/C$12	=D9/D$12	=H17*H4/E$21
x A	*0*	=C10/C$12	=D10/D$12	=H18*H5/E$21
x H	*0*	*0*	=D11/D$12	=1-E18-E17
f E Overall	**=(B9-G9-I9)/B9**		P	*760*
f E Reactor	**=(C9-D9)/C9**		T (Strm 2)	*280*
extent	=E19*E12		**V (Strm 2)**	**=C12*H21*(E22+273.15)/E21**

C	log10p*	p* in Flash (mm Hg)		
222.65	=D4-E4/(B1+F4)	=10^G4		
230	=D5-E5/(B1+F5)	=10^G5		
Stream 5	**Stream 6**	Stream 7	Stream 8	**Stream 9**
=F17	**=E9-F9**	=I9+J9	=I$12*I17	**=J$12*J17**
=F18	**=E10-F10**	=I10+J10	=I$12*I18	**=J$12*J18**
=E11	=E11-F11	=I11+J11	=I$12*I19	**=J$12*J19**
=SUM(F9:F11)	=SUM(G9:G11)	=I12+J12	=I16/(I18*C5+I17*C4)	**=(I10-I9)/(J17-J18)**
=F9*$C4	=G9*$C4	=I13+J13	=I9*$C4	=J9*$C4
=F10*$C5	=G10*$C5	=I14+J14	=I10*$C5	=J10*$C5
=F11*$C6	=G11*$C6	=I15+J15	=I11*$C6	=J11*$C6
=SUM(F13:F15)	=SUM(G13:G15)	=I16+J16	*1500*	=SUM(J13:J15)
0	=E17/(E17+E18)	*0.5*	=1-I18	*0.95*
0	=1-G17	*0.5*	*0.96*	=1-J17
1	*0*	*0*	*0*	*0*
mm Hg	R	*62.36*	m^3 mm Hg/kmol K	
°C				
m^3/h				

There are a number of techniques for entering formulas that speed entry immensely. First, you should (almost) never enter a cell reference by hand. For example, in cell C9 the formula reads “=J9+B9”. You enter this formula by clicking on cell C9, typing “=”, clicking on cell J9, typing “+”, clicking on cell B9, and finally pressing the *Enter* key.

The second is autogeneration of a series. To label the streams as “Stream 1” through “Stream 9”: Click on cell B8 and enter “Stream 1”. You should see a small black handle in the bottom right corner. Click and drag the little black handle to the right and *Excel* will automatically autofill the labels to “Stream 9”.

The third is similar. Click on cell E13. Type “=”. Click on cell E9. Type “*”. Click on Cell C4. Click on the formula entry bar between the * and the C4. Type a “$” and press *Enter* (The “$” is an *Absolute Reference* symbol. It means “Refer to the cell in Column C no matter where the cell is copied-and-pasted or dragged”). Click and drag the little black handle to the right (to cell G13) and then down (to cell G15) and *Excel* will automatically calculate the mass flowrates in Streams 4, 5,and 6.

You can also select cell E13 to E15 after having filled them as described above. Choose *Copy* from the *Edit* menu. Click in cell I13 and choose *Paste* from the *Edit* menu. Click in cell J13 and choose *Paste* from the *Edit* menu. The mass flows for Streams 8 and 9 have now been calculated.