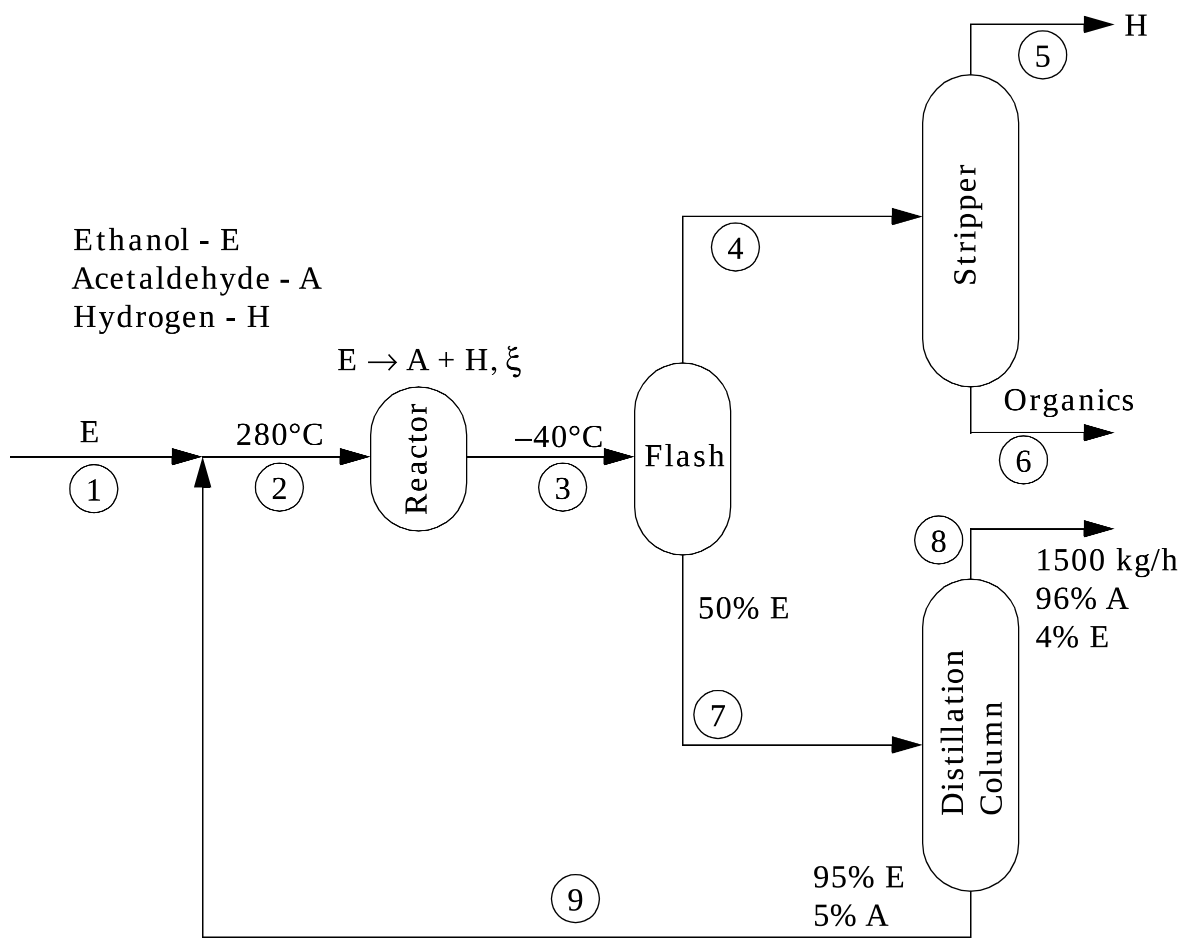
Problem 6.59 Using *Mathematica*

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. First, we'll calculate our molecular weights for M_{H}, M_{A}, and M_{E}.

In *Mathematica*-ese:

```
(* A Mathematica Solution for Problem 6.59 in Felder &
  Rousseau *)
```

Now, mole-to-mass and mass-to-mole conversions. We'll use as mole fraction and as mass flow rate.

In *Mathematica*-ese:

```
0.96 n8
m8A = MA n8A
42.291 n8
n8E = x8E n8
0.04 n8
m8E = ME n8E
1.84276 n8
```

Combining:

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

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

In *Mathematica*-ese:

```
eq1 = m8 == m8A + m8E
1500 == 44.1338 n8
Solve[eq1, n8]
{{n8 → 33.9876}}
n8 = n8 /. %[[1]]
33.9876
```

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

$$n_7 = n_8 + n_9$$

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

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

In *Mathematica*-ese:

```
(* Mole Balance around Distillation Column *)
eq2 = n7 == n8 + n9
n7 == 33.9876 + n9
eq3 = n7 x7A == n8 x8A + n9 x9A
n7 x7A == 32.6281 + n9 x9A
eq4 = n7 x7E == n8 x8E + n9 x9E
n7 x7E == 1.3595 + n9 x9E
x7A = 0.5
```

```
0.5
x7E = 1 - x7A
0.5
x9E = 0.95
0.95
x9A = 1 - x9E
0.05
```

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.

In *Mathematica*-ese:

```
sol1 = Solve[{eq3, eq4}, {n7, n9}]
{{n7 → 68.7304, n9 → 34.7428}}
n7 = n7 /. sol1[[1]]
68.7304
n9 = n9 /. sol1[[1]]
34.7428
n7A = n7 x7A
34.3652
n7E = n7 x7E
34.3652
n9A = n9 x9A
1.73714
n9E = n9 x9E
33.0057
```

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

$$C = 222.65$$

In *Mathematica*-ese:

```
(* Raoult's Law and Antoine equation in Flash *)
T3 = -40
-40
log10pA = 6.81089 - 992 / (T3 + 230)
```

```
1.58984
pA = 10^log10pA
38.8899
log10pE = 8.04494 - 1554.3 / (T3 + 222.65)
General::spell1 : Possible spelling error: new symbol
   name "log10pE" is similar to existing symbol "log10pA".
-0.464778
pE = 10^log10pE
0.342943
pressure = 760
760
y4A = x7A pA / pressure
0.0255855
y4E = x7E pE / pressure
0.00022562
y4H = 1 - y4A - y4E
0.974189
```

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

$n_{6_H} = 0$

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

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

In *Mathematica*-ese:

```
(* Mole Balance around Stripper *)
n5H = n4H
n4H
n4H = y4H n4
0.974189 n4
n6A = n4A
```

```
n4A
n4A = n4 y4A
0.0255855 n4
n6E = n4E
n4E
n4E = n4 y4E
0.00022562 n4
```

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

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

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

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

In *Mathematica*-ese:

```
(* Overall Mole Balance *)
eq5 = n4H == ξ
0.974189 n4 == ξ
eq6 = n4A + n8A == ξ
32.6281 + 0.0255855 n4 == ξ
eq7 = n4E + n8E == n1E - ξ
1.3595 + 0.00022562 n4 == n1E - ξ
```

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

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

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

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

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

In *Mathematica*-ese:

```
sol2 = Solve[{eq5, eq6, eq7}, {ξ, n4, n1E}]
```

```
{{ξ → 33.5081, n4 → 34.3959, n1E → 34.8754}}
ξ = ξ /. sol2[[1]]
33.5081
n4 = n4 /. sol2[[1]]
34.3959
n1 = n1E = n1E /. sol2[[1]]
34.8754
```

We can now work either direction around the recycle loop.

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

In *Mathematica*-ese:

```
(* Finish around Loop *)
n3A = n4A + n7A
35.2452
n3E = n4E + n7E
34.373
n3H = n4H
33.5081
```

And

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

In *Mathematica*-ese:

```
n2A = n9A
1.73714
n2E = n1E + n9E
67.8811
```

The single-pass conversion is:

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

In *Mathematica*-ese:

```
(* Fractional Conversion in Reactor *)
fEone = (n2E - n3E) / n2E
0.49363
```

The overall conversion is:

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

In *Mathematica*-ese:

```
(* Fractional Conversion Overall *)
fEover = (n1E - n6E - n8E) / n1E
0.960796
```

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

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

In *Mathematica*-ese:

```
(* Volumentric Flowrate in Reactor Feed *)
n2 = n2A + n2E
69.6182
R = 62.36
62.36
V2 = n2 R (280 + 273.15) / pressure
3159.79
```

Since our answers are scattered throuought the notebook, we probably ought to gather them all together in on spot, for the grader's sake. The problem statement says we are to: 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.

In *Mathematica*-ese:

```
(* Assemble all of the answers in one place *)
answers = {n1E, n9, n5H, V2, fEover, fEone, n6E, n6A}
{34.8754, 34.7428, 33.5081, 3159.79, 0.960796, 0.49363,
 0.00776041, 0.880036}
```