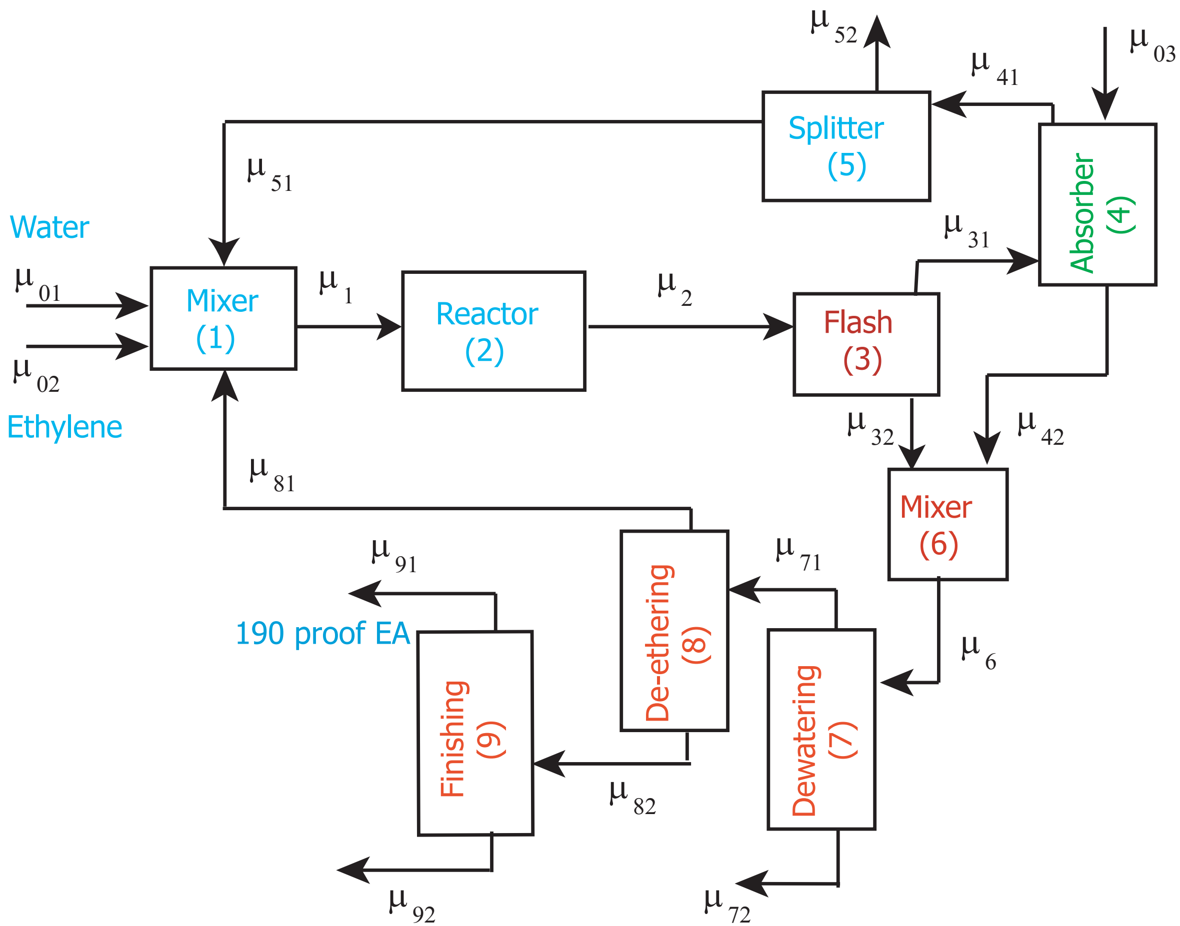
Solving Flowsheet Equations

Solving Linear Mass Balance Equations

- All units except the reactor have independent split fractions for each component.
- The reactor mass balance relates flows to limiting components in the reaction.
  - If we solve for the limiting components first, we can solve for all other flows.
- Option 1: Solve simultaneously, the linear mass balances for the flowsheet.
- Option 2: Solve sequentially, using a tearing algorithm.

1. Choose tear streams that break all recycle loops in flowsheet (typically at the reactor inlet).
2. Trace path backwards from reactor until all loops are covered (end up at the reactor inlet again).
3. Fill all streams by using split fractions and moving forward from the reactor feed.

Ethanol BFD



μ 52
μ 41
μ 03
Splitter
(5)
μ 51
Absorber
(4)
Water
μ 31
μ 01
Mixer
(1)
μ 1
Reactor
(2)
μ 2
Flash
(3)
μ 02
Ethylene
μ 32
μ 42
μ 81
Mixer
(6)
μ 91
μ 71
De-ethering
(8)
190 proof EA
μ 6
Finishing
(9)
Dewatering
(7)
μ 82
μ 92
μ 72

Balance for EL and PL

$$
\begin{aligned}
\mu_1(EL) &= \mu_{02}(EL) + \mu_{51}(EL) + \mu_{81}(EL) \\
&= \mu_{02}(EL) + (0.995)(0.979)(0.985)(0.93)\mu_1(EL) + \\
&\quad (1)(1)\{0.021(0.985) + 0.015\}(0.93)\mu_1(EL) \\
&= 96 + 0.9255\mu_1(EL)
\end{aligned}
$$

Solving for $\mu_1(EL)$, we get: $\mu_1(EL) = 1289\ gmol/s$
Similarly, for PL:

$$
\begin{aligned}
\mu_1(PL) &= \mu_{02}(PL) + \mu_{51}(PL) + \mu_{81}(PL) \\
&= 3 + (0.995)(0.901)(0.932)(0.993)\mu_1(PL) + \\
&\quad (1)(1)\{0.099(0.932) + 0.068\}(0.993)\mu_1(PL)
\end{aligned}
$$

Solving for $\mu_1(PL)$, we get: $\mu_1(PL) = 268.6\ gmol/s$

Once we have the limiting reactant flow rate, we can determine other component flow rates as well.

Balance for EA

$$\mu_1(EA) = \mu_{51}(EA) + \mu_{81}(EA) \qquad (No\ EA\ in\ feed)$$

$$\mu_{51}(EA) = (1-\xi)\mu_{41}(EA) = 0.995\mu_{41}(EA)$$
$$\mu_{41}(EA) = \xi_{41}\mu_{31}(EA) = 0.01\mu_{31}(EA)$$
$$\mu_{31}(EA) = 0.121\mu_2(EA)$$
$$\mu_2(EA) = \eta_1\mu_1(EL) + \mu_1(EA)$$
$$= 0.07 \times 1289 + \mu_1(EA)$$

Thus: $\mu_{51}(EA) = (0.995)(0.01)(0.121)\{90.23 + \mu_1(EA)\}$

Similarly:

$\mu_{81}(EA) = (0.005)(0.995)\{879 + 0.121(0.99)\}\{90.23 + \mu_1(EA)\}$

Substituting in $\mu_1(EA) = \mu_{51}(EA) + \mu_{81}(EA)$ and solving for $\mu_1(EA)$, we get: $\mu_1(EA) = 0.56\ gmol/s$

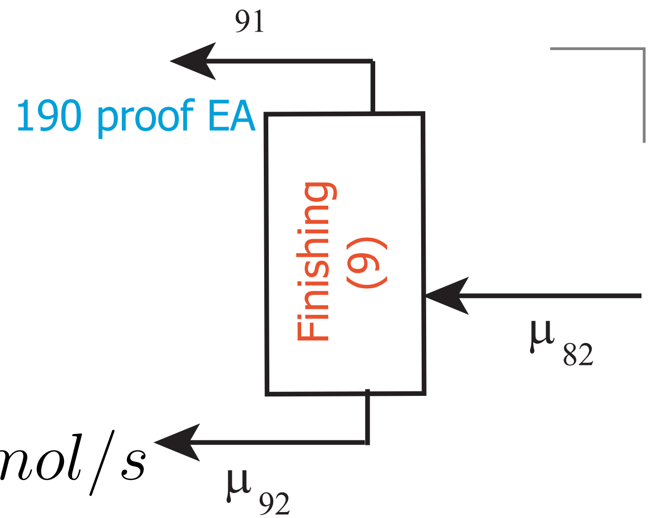
Once $\mu_1(EA)$ is known, we can calculate the flow rates $\mu_2(EA)$, $\mu_{31}(EA)$, ...

$$\mu_{31}(EA) = 10.99\ gmol/s \qquad \mu_{32}(EA) = 79.81\ gmol/s$$
$$\mu_{41}(EA) = 0.11\ gmol/s \qquad \mu_{42}(EA) = 10.88\ gmol/s$$
$$\mu_{51}(EA) = 0.1093\ gmol/s \qquad \mu_{52}(EA) = 0.0005\ gmol/s$$
$$\mu_{6}(EA) = 90.68\ gmol/s$$
$$\mu_{71}(EA) = 90.73\ gmol/s \qquad \mu_{72}(EA) = 0.45\ gmol/s$$
$$\mu_{81}(EA) = 0.45\ gmol/s \qquad \mu_{82}(EA) = 89.77\ gmol/s$$

Similarly, molar flow rates for all components can be calculated.

$$\begin{aligned}\mu_{82} &= \mu_{82}(M) + \mu_{82}(EL) + \mu_{82}(PL) + \\ &\quad \mu_{82}(DEE) + \mu_{82}(EA) + \mu_{82}(IPA) + \mu_{82}(W) \\ &= 0 + 0 + 0 + 0.1065 + 89.775 + 1.804 + 71.686 \\ &= 163.77\ gmol/s\end{aligned}$$

Final Azeotropic Separation



We want to recover 99.5% of azeotropic composition ((85.5% EA and 14.5% W).

$$\Longrightarrow \quad 99.5\% \; EA + necessary \; water$$

$$\Longrightarrow \quad \mu_{91}(EA) = 0.995 \times 89.775 = 89.33 \; gmol/s$$

$$\mu_{91}(W) = \frac{14.5}{85.5} \times 89.33 = 15.17 \; gmol/s$$

$$\mu_{91}(DEE) = 0.01065 \; gmol/s \qquad (lighter \; than \; azeotrope)$$

We want IPA to be less than 0.1% in the top product. Thus:

$$\frac{\mu_{91}(IPA)}{\mu_{91}(IPA) + \mu_{91}(DEE) + \mu_{91}(W) + \mu_{91}(EA)} = 0.001$$

Solving for $\mu_{91}(IPA)$, we get: $\mu_{91}(IPA) = 0.1046 \; gmol/s$

Flowsheet Solution

	μ_{01}	μ_{02}	μ_1	μ_2	μ_{31}	μ_{32}	μ_{41}	μ_{42}	μ_{03}
Methane (gmol/s)		0	200	200	199.2	0.8	199.2	0	0
Ethylene	96	0	1289	1198.77	1180.78	17.98	1155.99	24.796	0
Propylene	3	0	268.6	266.71	248.58	18.136	223.97	24.609	0
Diethyl Ether	0	0	0	2.421	1.210	1.2108	0.2906	0.9202	0
Ethanol	0	0	0.56	90.79	10.98	79.80	0.1098	10.87	0
Isopropanol	0	0	0	1.8802	0.156	1.724	0.001018	0.1550	0
Water	0	771.797	773.4	680.72	36.75	643.97	1.610	72.896	37.747
Total	100	771.797	2531.56	2441.31	1677.68	763.62	1581.177	134.25	37.747
Temperature, K	300	300	590	590	393	393	381.57	338.7	310
Pressure, bar		1	69	69	68.5	68.5	68	68	68
Vap. Frac	1	0			1	0	1	0	0
Enthalpy, kcal/s	1198.85	−52097.04	−21683.63	−22689.24	11515.18	−47920.28	13439.75	−5324.42	−2544.97

	μ_{51}	μ_{52}	μ_6	μ_{71}	μ_{72}	μ_{81}	μ_{82}	μ_{91}	μ_{92}
Methane (gmol/s)	198.204	0.996	0.8	0.8	0	0.8	0	0	0
Ethylene	1150.21	5.780	42.778	42.778	0	42.7781	0	0	0
Propylene	222.85	1.1198	42.746	42.746	0	42.7466	0	0	0
Diethyl Ether	0.2891	0.00145	2.131	2.131	0	2.1205	0.01065	0.01065	0
Ethanol	0.1093	0.000549	90.680	90.226	0.4534	0.451	89.775	89.3267	0.4489
Isopropanol	0.001013	5.09323E-06	1.879	1.804	0.075	0	1.804	0.1046	1.6994
Water	1.6024	0.00805	716.867	71.68	645.18	0	71.686	15.1490	56.537
Total	1573.27	7.9058	897.882	252.173	645.70	88.896	163.277	104.591	58.686
Temperature, K	381.57	381.57	372	310	480	310	418	350	383
Pressure, bar	67.5	67.5	68	17.56	18.06	10.7	11.2	1	1.5
Vap. Frac			0	0	0		0	0	0
Enthalpy, kcal/s	13372.55	67.197	−53244.70	−10436.14	−42629.37	590.10	−10576.78	−6787.79	−3930.30