Linear Mass Balances

Solution of Mass Balance Equations

The linear mass balances on various units are combined to analyze the ethanol process.

- Step 1: Guess P and T levels in the flowsheet. Specify recoveries, split fractions, ... (use degrees of freedom for each unit).
- Step 2: Determine coefficients for linear models in each unit $(\alpha_{k/n}, \beta, N, \xi)$.
- Step 3: Setup linear equations and solve for flowrates of each component.
- Step 4: Check guessed values from the first step.
 - Calculate P and T from flowrates. If different from Step 1, go to Step 2 using these values of P and T.
 - If flowsheet does not meet specifications, change Pand/or T or modify flowsheet.

Ethanol BFD



M: MethaneEL: EthylenePL: PropyleneDEE: Diethyl etherEA: EthanolIPA: Isopropyl alcoholW: WaterCroton aldehyde is neglected in the mass balance.

Linear Mass Balances - p.4/27

Mixer





 $\mu_{01} + \mu_{02} + \mu_{51} + \mu_{81} = \mu_1$

Reactor



The following reactions are occurring:

$$EL + W \longrightarrow EA \qquad \eta_1 = 0.07 \quad (EL \ to \ EA)$$
$$PL + W \longrightarrow IPA \qquad \eta_2 = 0.007 \quad (PL \ to \ IPA)$$
$$2EA \rightleftharpoons DEE + W$$

Equilibrium can be maintained via recycle at 590 K and 69 bar according to:

$$\frac{[DEE][W]}{[EA]^2} = 0.2$$

The mass balance for the reactor can be written as:

$$\mu_2(M) = \mu_1(M) \quad (Inert \ component)$$

$$\mu_2(EL) = (1 - \eta_1)\mu_1(EL)$$

$$\mu_2(PL) = (1 - \eta_2)\mu_1(PL)$$

$$\mu_2(DEE) = \frac{0.2[\mu_2(EA)]^2}{\mu_2(W)}$$

Solving for the remaining components:

$$\mu_{2}(EA) = \eta_{1}\mu_{1}(EL) + \mu_{1}(EA)$$

$$\mu_{2}(IPA) = \eta_{2}\mu_{1}(PL) + \mu_{1}(IPA)$$

$$\mu_{2}(W) = \mu_{1}(W) - \eta_{1}\mu_{1}(EL) - \eta_{2}\mu_{1}(PL)$$

We choose to use $\mu_1(W) = 0.6\mu_1(EL)$. Limiting component is actually *W*!



We want to take the reactor effluent to cooling water temperature and separate the liquid product from reactants.

- Assume a pressure drop of 0.5 bar from the reactor and operate the flash at 68.5 bar.
- Choose DEE as the key component, n, because of its intermediate volatility.
- Assume $\xi_n = 0.5$ for DEE and calculate split fractions of remaining components. It needs to be verified later that this recovery is possible.

Split Fraction Calculations at $T = 310 K$:								
k	M	EL	PL	DEE	EA	IPA	W	
P^0	211,000	55,500	11,360	824	114.5	75.1	47.1	
$lpha_{k/n}$	256.1	67.3	13.3	1.0	0.138	0.091	0.057	
ξ_k	0.996	0.985	0.932	0.5	0.121	0.083	0.054	
Given the solit fractions, we can write down linear mass								

Given the split fractions, we can write down linear mass balances.

$$\mu_{31}(M) = 0.996\mu_2(M)$$
 Vapor
 $\mu_{32}(M) = 0.004\mu_2(M)$ Liquid

Similarly

$$\begin{split} \mu_{31}(EL) &= 0.985 \mu_2(EL) & \mu_{32}(EL) = 0.015 \mu_2(EL) \\ \mu_{31}(PL) &= 0.932 \mu_2(PL) & \mu_{32}(PL) = 0.068 \mu_2(PL) \\ \mu_{31}(DEE) &= 0.5 \mu_2(DEE) & \mu_{32}(DEE) = 0.5 \mu_2(DEE) \\ \mu_{31}(EA) &= 0.121 \mu_2(EA) & \mu_{32}(EA) = 0.879 \mu_2(EA) \\ \mu_{31}(IPA) &= 0.083 \mu_2(IPA) & \mu_{32}(IPA) = 0.917 \mu_2(IPA) \\ \mu_{31}(W) &= 0.054 \mu_2(W) & \mu_{32}(W) = 0.946 \mu_2(W) \end{split}$$

Note that we ASSUMED a key component recovery. Once the flow rates are established, we need to verify if this assumption corresponds to our desired temperature and pressure specifications.

Absorber



There are 4 degrees of freedom: P, T, key component recovery and liquid feed rate.

- We want to run the absorber at low temperature and high pressure because:
 - Reactor is at high pressure.
 - We want to condense as much of the product as possible.
 - Choose $P = 68 \ bar$ and $T = 310 \ K$

- ● Choose ethanol recovery to be 99% ($\xi_n = 0.99$)
 - Choose liquid flow rate of solvent from:

$$A = \frac{L_0}{V_{n+1}K_{EA}} = 1.4$$

$$K_{EA} = \frac{P_{EA}^0(310)}{P} = 2.25 \times 10^{-3}$$

Thus:

$$\mu_{03} = \mu_{31} (2.25 \times 10^{-3})(1.4) = 3.15 \times 10^{-3} \mu_{31}$$

How much water do we lose in the overhead vapor (in μ_{41})?

—For $\xi_{EA} = 0.99$ and $A_{EA} = 1.4$, the number of equilibrium trays is:

$$N = \frac{\ln\left\{\frac{r - A_{EA}}{-A_{EA}(1-r)}\right\}}{\ln(A_{EA})} = 10$$

We determine the split fractions for the other components from:

$$A_{k} = \frac{1.4}{\alpha_{k/EA}} = \frac{L}{VK_{k}} \quad \beta_{N}^{k} = \frac{1 - A_{k}^{N+1}}{1 - A_{k}} \quad \beta_{N-1}^{k} = \frac{1 - A_{k}^{N}}{1 - A_{k}}$$
$$v_{1}^{k} = \frac{v_{N+1}^{k}}{\beta_{N}^{k}} + \frac{\beta_{N-1}^{k}}{\beta_{N}^{k}} l_{0}^{k} \quad l_{N}^{k} = \left(1 - \frac{\beta_{N-1}^{k}}{\beta_{N}^{k}}\right) l_{0}^{k} + \left(1 - \frac{1}{\beta_{N}^{k}}\right) v_{N+1}^{k}$$

Note that
$$rac{eta_{N-1}^k}{eta_N^k} =$$
 fraction of l_0 in vapor v_1

$$-$$
At $T = 310 K$ we have:

$$\begin{aligned} \alpha_{W/EA} &= \frac{47.1}{114.5} = 0.41 \quad A_W = \frac{1.4}{\alpha_{W/EA}} = 3.415 \\ \beta_N^W &= 3.05 \times 10^5 \qquad \beta_{N-1}^W = 8.93 \times 10^4 \\ \text{Thus } \frac{\beta_N^W}{\beta_N^W} = 0.293 \end{aligned}$$

Thus, 29.3% of the solvent goes into the vapor phase. The assumption of isothermal operation is probably violated.

- Increase P Expensive
- Decrease T Expensive
- Increase Absorption factor A_{EA} and hence increase solvent flow rate

Suppose
$$A_{EA} = 10$$

Then, $\mu_{03} = 0.0225\mu_{31}$ and $N = 1.95$.
 $A_W = \frac{10}{\alpha_{W/EA}} = 24.39$
 $\beta_N^W = 528.7$ and $\beta_{N-1}^W = 21.68$.
Loss of water in the overhead vapor is $\frac{\beta_{N-1}^W}{\beta_N^W} = 0.041$
A loss of 4.1% is acceptable.

$$\mu_{41}(W) = \frac{\mu_{31}(W)}{\beta_N^W} + \frac{\beta_{N-1}^W}{\beta_N^W} \mu_{03}(W)$$

= 0.0019\mu_{31}(W) + 0.00092\mu_{31}

Since μ_{03} is pure water, $\mu_{03}(k)$ where $k \neq water$ is zero. We can calculate $\mu_{41}(k)$ and $\mu_{42}(k)$ in terms of μ_{31} .

It can be sho	own that:
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k	$\alpha_{k/n}$	A_k	β_N	β_{N-1}	$\mu_{41}(k)$	$\mu_{42}(k)$	
M	1854	0.0054	1	1	$\mu_{31}(M)$	0	
EL	486.3	0.021	1.021	1.021	$0.979\mu_{31}(EL)$	$0.021\mu_{31}(EL)$	
PL	99.5	0.101	1.11	1.10	$0.901\mu_{31}(PL)$	$0.099\mu_{31}(PL)$	
DEE	7.24	1.38	4.17	2.30	$0.24\mu_{31}(DEE)$	$0.76\mu_{31}(DEE)$	
EA	1.0	10	98.92	9.79	$0.01\mu_{31}(EA)$	$0.99\mu_{31}(EA)$	
IPA	0.79	12.66	153.2	12.02	$0.0065\mu_{31}(IPA)$	$0.993\mu_{31}(IPA)$	
Note that the component balance of each component k in							
streams 41 and 42 can be written in terms of linear relation							
of stream 31.							

Splitter



- We need to specify the purge rate ξ to avoid accumulation of inerts.
- Specifically, methane entering the reactor should be less than 10%.

From mass balance:

$$\mu_{52} = \xi \mu_{41} \\ \mu_{51} = (1 - \xi) \mu_{41}$$

Assume that EA, IPA, and DEE are negligible in the recycle.

 $\left[\begin{array}{c}Mole\ fraction\ of\ M\\entering\ reactor\end{array}\right] =$

$$= \frac{\mu_1(M)}{\mu_1(M) + \mu_1(PL) + \mu_1(EL) + \mu_1(W)}$$

<u>EL Balance</u>

$$\mu_1(EL) = \mu_{51}(EL) + 96$$

$$\mu_{51}(EL) = (1 - \xi)\mu_{41}(EL)$$

$$\mu_{41}(EL) = 0.979\mu_{31}(EL)$$

$$\mu_{31}(EL) = 0.985\mu_2(EL)$$

$$\mu_2(EL) = 0.93\mu_1(EL)$$

Thus $\mu_1(EL) = (1 - \xi)(0.979)(0.985)(0.93)\mu_1(EL) + 96$ This implies that $\mu_1(EL) = \frac{96}{0.1 + 0.9\xi}$

We can write down similar component balances for PL and M. PL Balance

$$\mu_1(PL) = \mu_{51}(PL) + 3$$

$$\mu_{51}(PL) = (1 - \xi)\mu_{41}(PL)$$

$$\mu_{41}(PL) = 0.901\mu_{31}(PL)$$

$$\mu_{31}(PL) = 0.932\mu_2(PL)$$

$$\mu_2(PL) = 0.993\mu_1(PL)$$

Thus $\mu_1(PL) = (1 - \xi)(0.901)(0.932)(0.993)\mu_1(PL) + 3$ This implies that $\mu_1(PL) = \frac{3}{0.17 + 0.83\xi}$

M Balance

Т

$$\mu_1(M) = \mu_{51}(M) + 1$$

$$\mu_{51}(M) = (1 - \xi)\mu_{41}(M)$$

$$\mu_{41}(M) = \mu_{31}(M)$$

$$\mu_{31}(M) = 0.996\mu_2(M)$$

$$\mu_2(M) = 0.93\mu_1(M)$$

Thus $\mu_1(M) = (1 - \xi)(0.996)\mu_1(M) + 1$
This implies that $\mu_1(M) = \frac{1}{0.004 + 0.996\xi}$
W Balance

$$\mu_1(W) = 0.6\mu_1(EL) \qquad Assumed \ earlier$$
$$= \frac{53.6}{0.1 + 0.9\xi}$$

If the mole fraction of M entering the reactor is equal to 0.1, then using the equation:

$$\begin{bmatrix} Mole \ fraction \ of \ M \\ entering \ reactor \end{bmatrix} = \frac{\mu_1(M)}{\mu_1(M) + \mu_1(PL) + \mu_1(EL) + \mu_1(W)}$$

we have:

$$0.1 = \frac{1}{\frac{1}{0.004 + 0.996\xi}}$$
$$\frac{1}{\frac{1}{0.004 + 0.996\xi} + \frac{3}{0.17 + 0.83\xi} + \frac{96}{0.1 + 0.9\xi} + \frac{53.6}{0.1 + 0.9\xi}}$$

Solving for ξ by trial and error, we get $\xi = 0.0019$. We need to choose ξ to be greater than 0.0019 to ensure that M entering the reactor is less than 10%. Let us choose $\xi = 0.005$.



We can write down a mass balance for each component as follows:

$$\mu_{42}(k) + \mu_{32}(k) = \mu_6(k)$$

where k = M, EL, PL, DEE, EA, IPA, WNote that we wrote component balances for $\mu_{32}(k)$ and $\mu_{42}(k)$ earlier.

Dewatering Column



Specifications:

- 90% of the water goes to the bottom product.
- 99.5% of the EA goes as the top product.
- We operate this column at low pressure so that all the DEE goes out in the top.
- We want to recycle as much of the DEE as possible.

Key Components:

$$lk = EA \qquad \xi_{EA} = 0.995$$
$$hk = W \qquad \xi_W = 0.1$$

- \blacksquare *EL*, *PL*, and *DEE* are lighter than the light key.
- \blacksquare *IPA* is distributed between *EA* and *W*.
- If we run this column with cooling water (at T = 310 K), a partial condenser may be needed to remove trace low boiling components of EL and PL.

$$\alpha_{EA/W} = \frac{P_{EA}^0}{P_W^0} = \frac{114}{47.1} = 2.43$$

From Fenske Equation:

$$N = \frac{\ln \left[\frac{\xi_{lk}(1-\xi_{hk})}{\xi_{hk}(1-\xi_{lk})}\right]}{\ln \left[\alpha_{lk/hk}\right]} = 8.4 \ stages$$

$$\xi_{IPA} = \frac{\alpha_{IPA/W}^{N} \xi_{W}}{1 + (\alpha_{IPA/W}^{N} - 1)\xi_{W}} = 0.96$$

Thus we have:

De-ethering Column

- DEE is removed overhead and recycled.
- Specify \$\xi_{DEE}\$ = 0.995 (light key) and \$\xi_{EA}\$ = 0.005 (heavy key).



M, EL and PL are lighter than the light key. IPA and W are heavier than the heavy key. There are no distributed components.

Thus we have:

Final Azeotropic Separation



- To follow these specifications, it is necessary to know the molar flow rate μ_{82} .
- Once μ_{82} is known, a simple mass balance can be used to calculate μ_{91} and μ_{22} .