# Linear Mass Balances

*The buck stops here*

Anonymous
(sign on President Truman’s desk)

# Solution of Mass Balance Equations

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

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  - If flowsheet does not meet specifications, change $P$ and/or $T$ or modify flowsheet.

# Ethanol BFD

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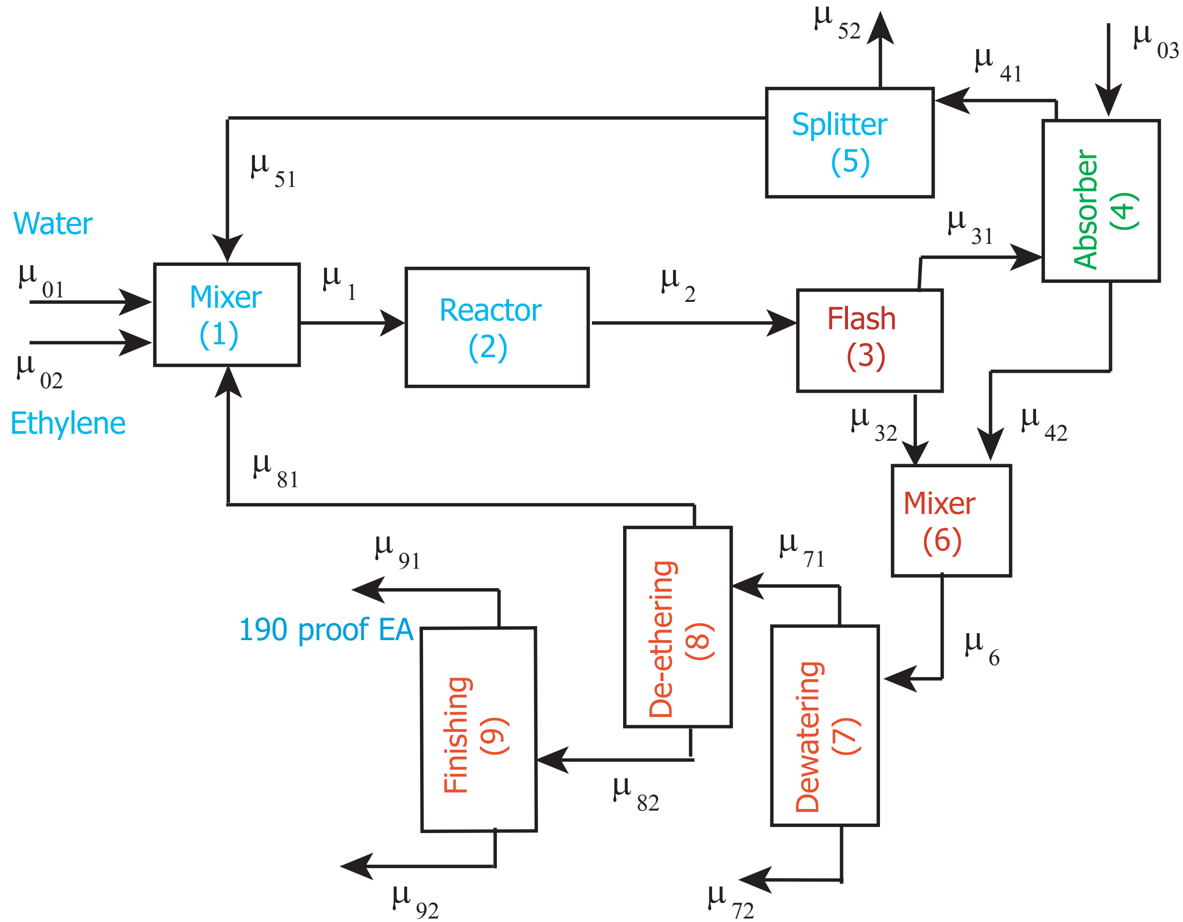

μ 52
μ 41
μ 03
Splitter
(5)
μ 51
Absorber
(4)
Water
μ 31
μ 01
Mixer
(1)
μ 1
Reactor
(2)
μ 2
Flash
(3)
μ 02
Ethylene
μ 32
μ 42
μ 81
Mixer
(6)
μ 91
μ 71
De-ethering
(8)
190 proof EA
μ 6
Finishing
(9)
Dewatering
(7)
μ 82
μ 92
μ 72

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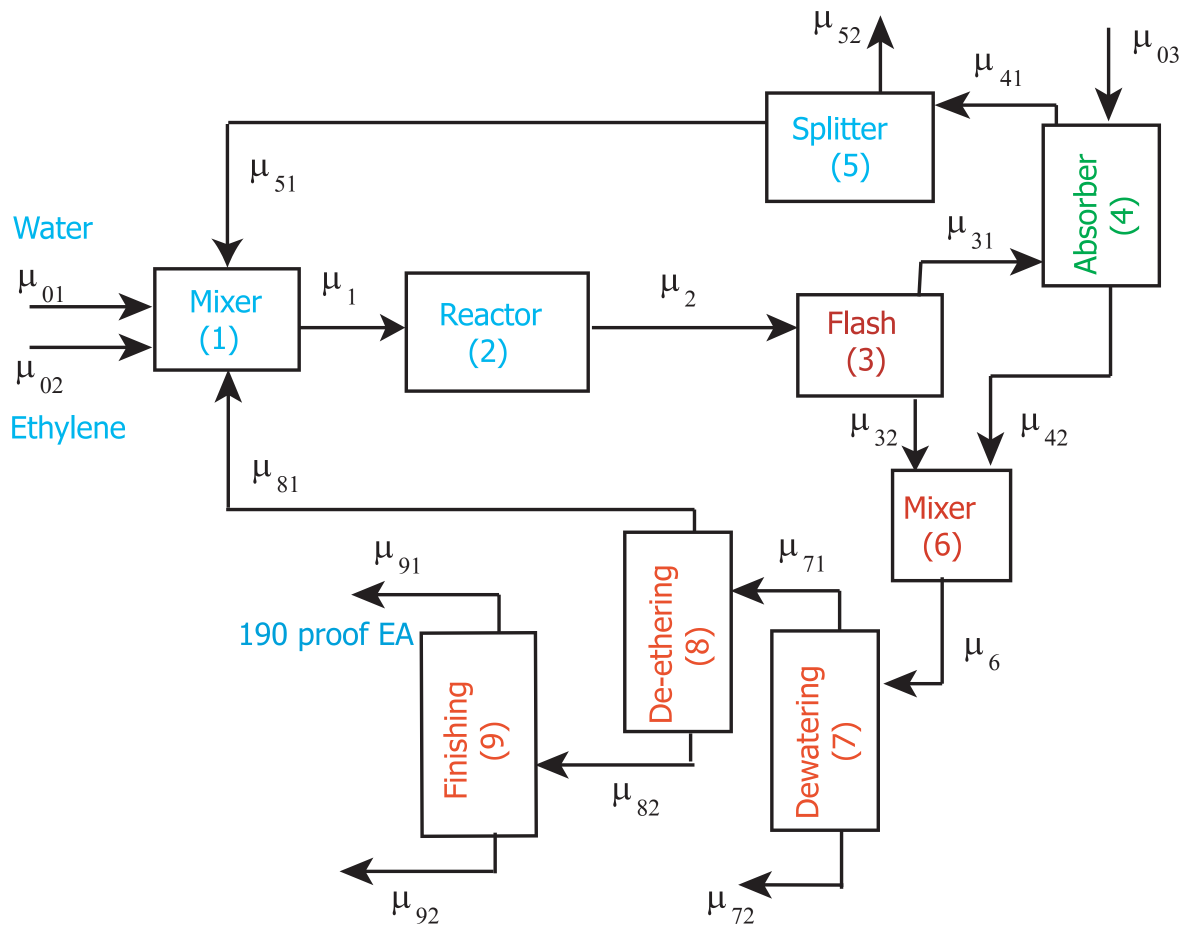


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$DEE:\ Diethyl\ ether \qquad EA:\ Ethanol$

$IPA:\ Isopropyl\ alcohol \qquad W:\ Water$

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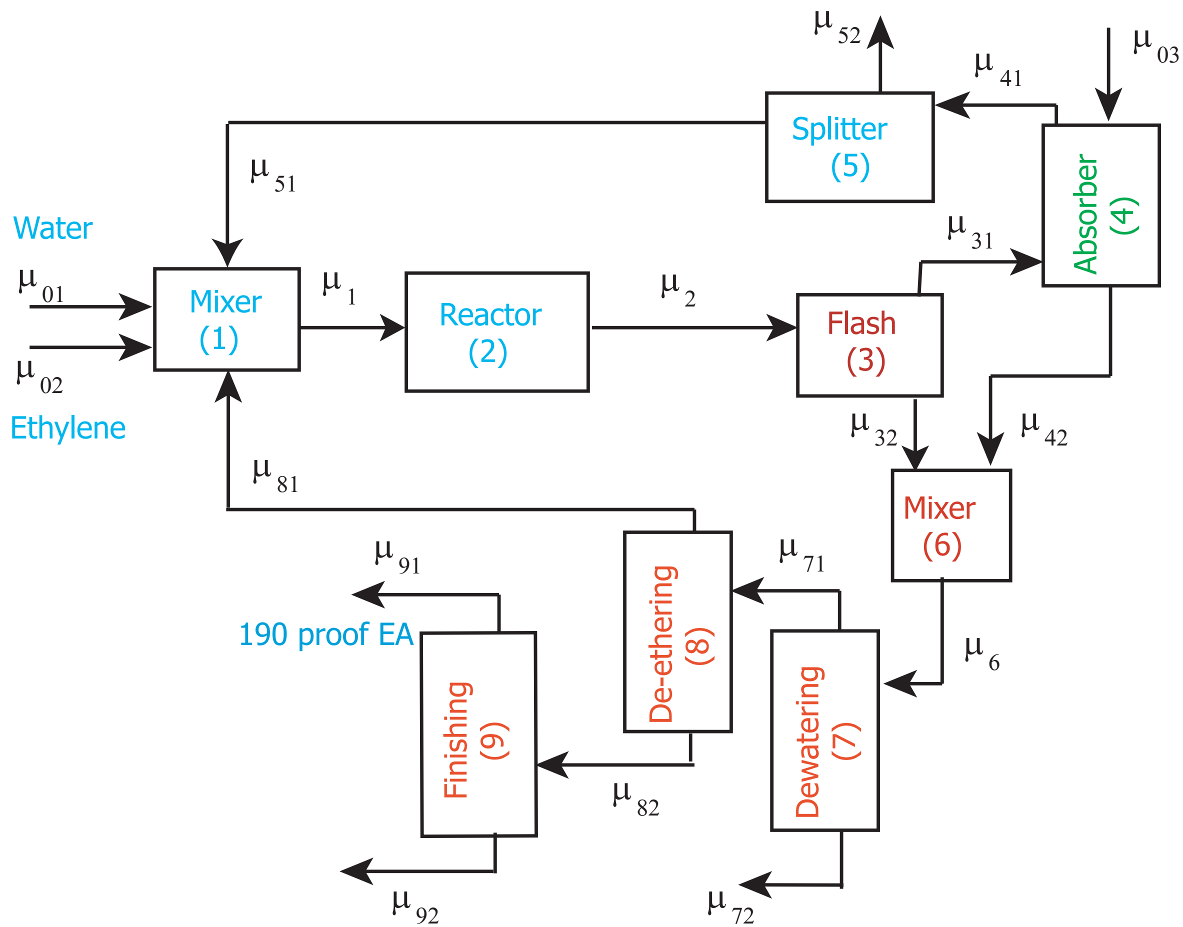


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Croton aldehyde is neglected in the mass balance.

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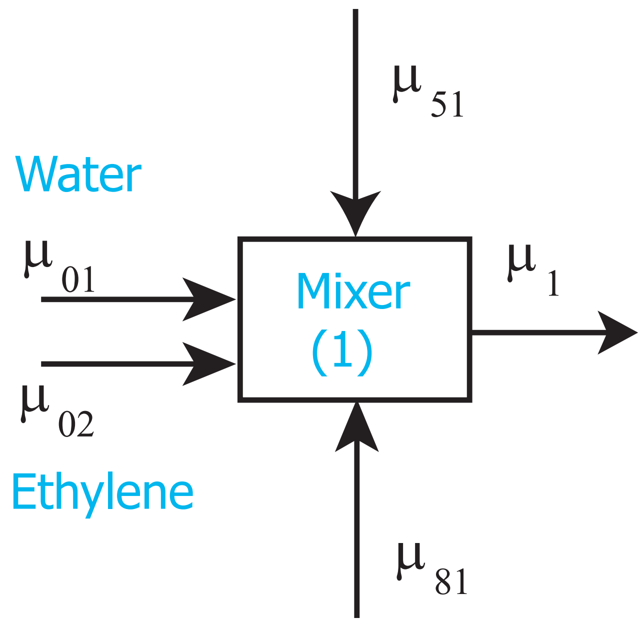

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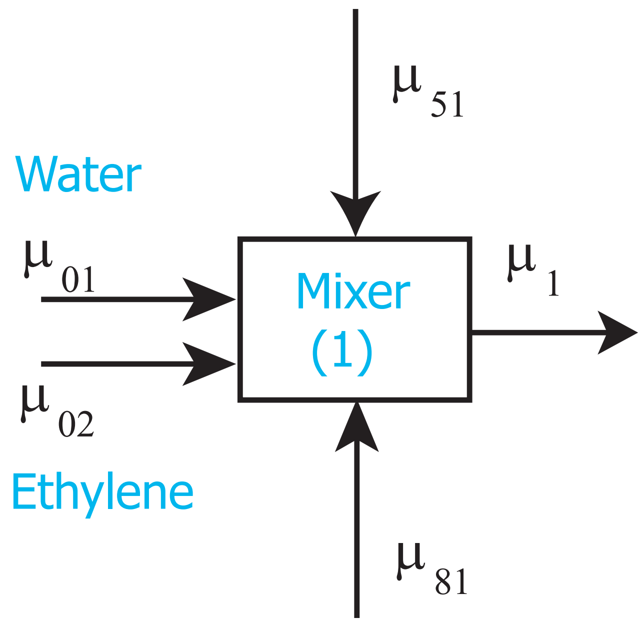


$$\mu_{01} + \mu_{02} + \mu_{51} + \mu_{81} = \mu_1$$

# Reactor

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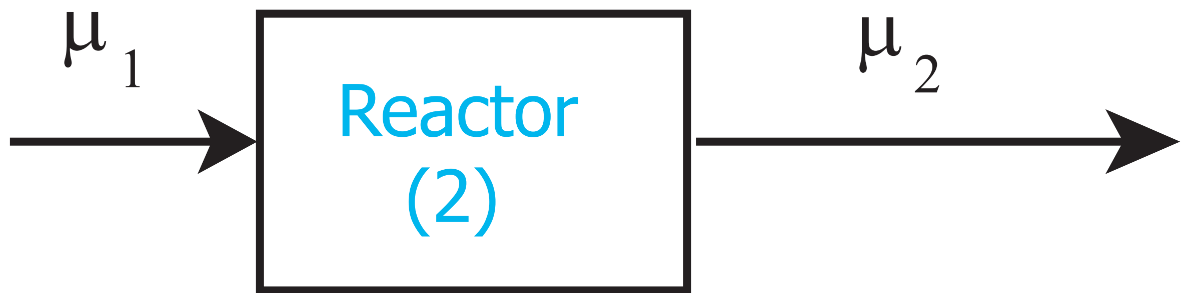

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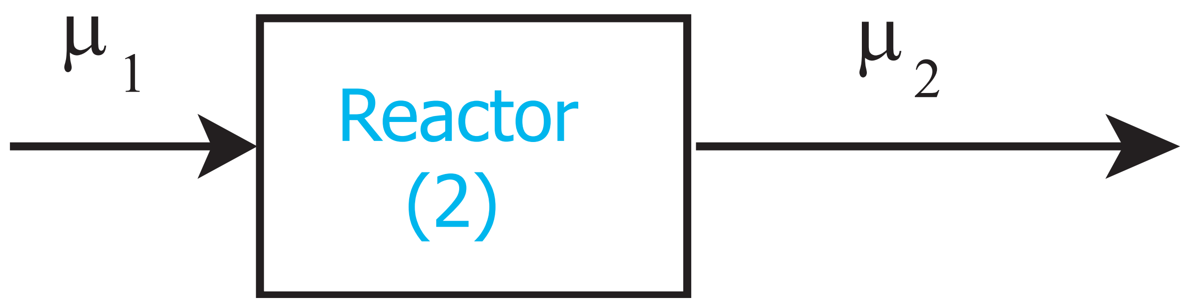


The following reactions are occurring:

$$EL + W \longrightarrow EA \qquad \eta_1 = 0.07 \quad (EL \; to \; EA)$$

$$PL + W \longrightarrow IPA \qquad \eta_2 = 0.007 \quad (PL \; to \; IPA)$$

$$2EA \rightleftharpoons DEE + W$$

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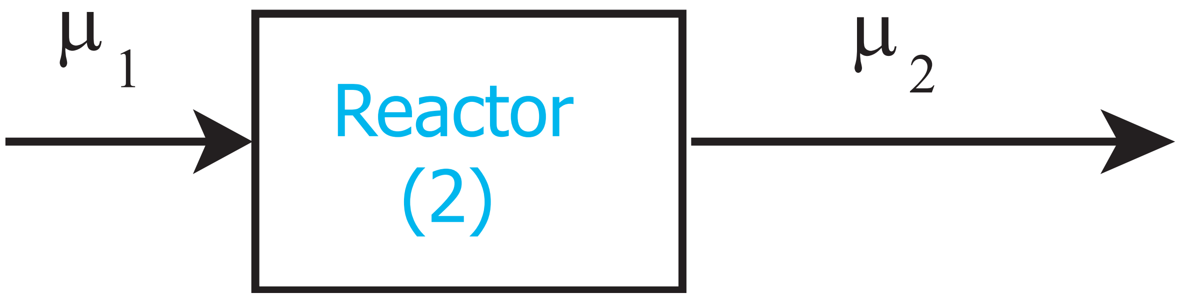


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Equilibrium can be maintained via recycle at $590\ K$ and $69\ bar$ according to:

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

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Limiting component is actually $W$!

# Flash Unit

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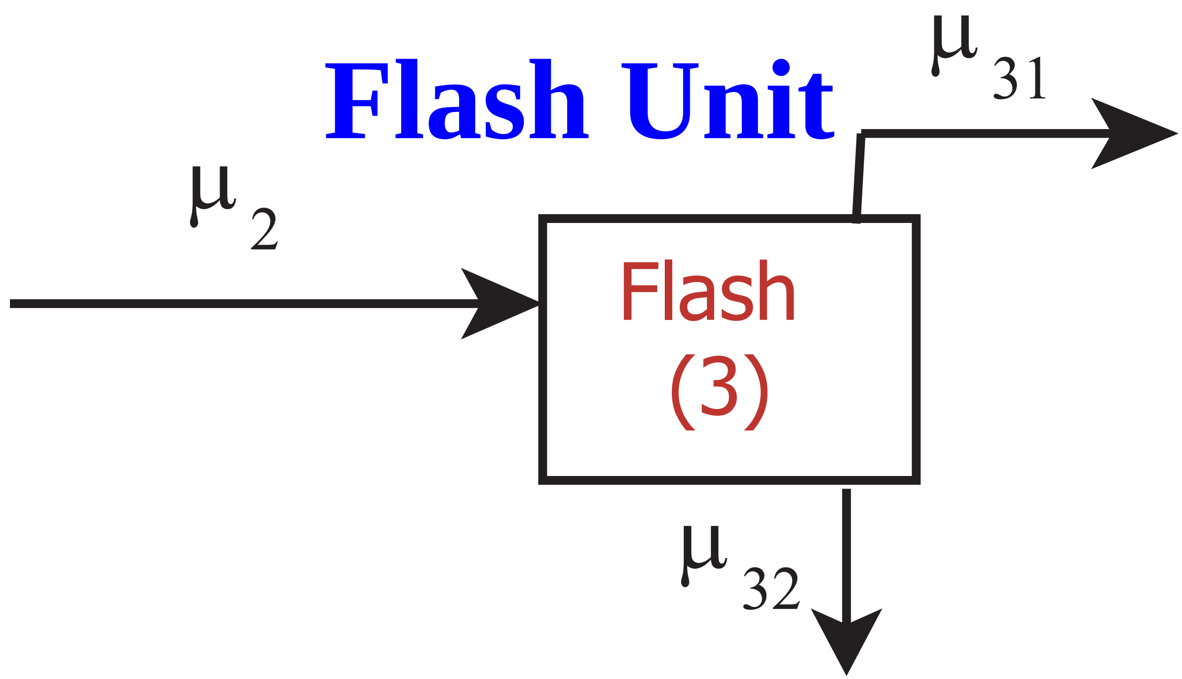

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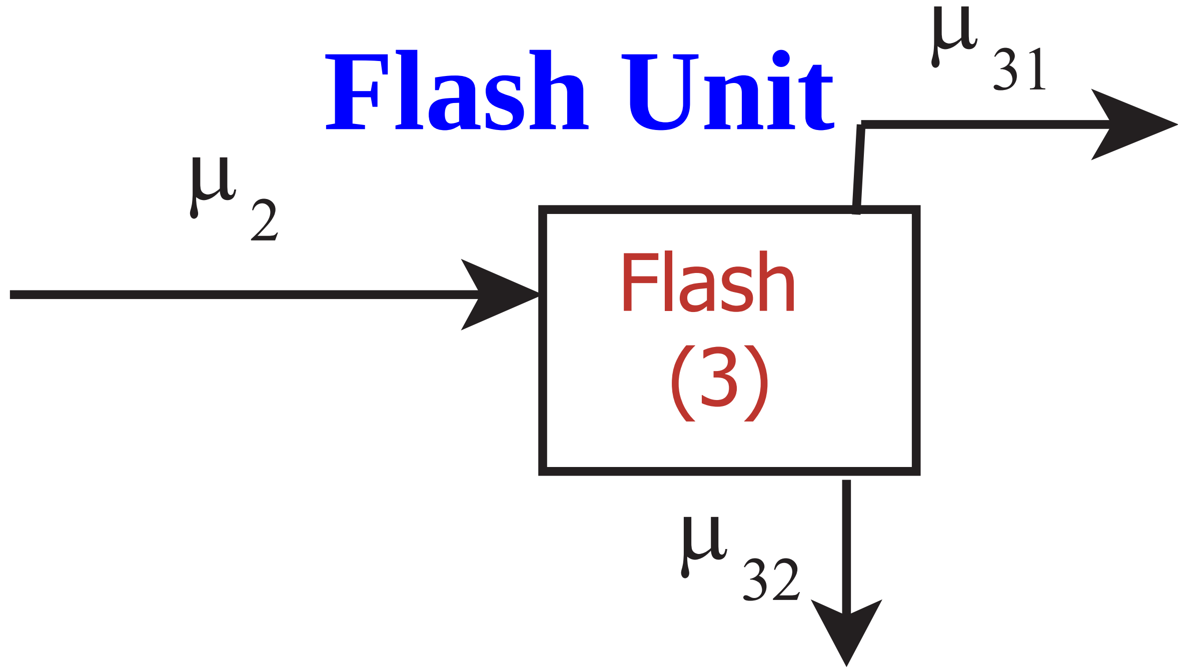


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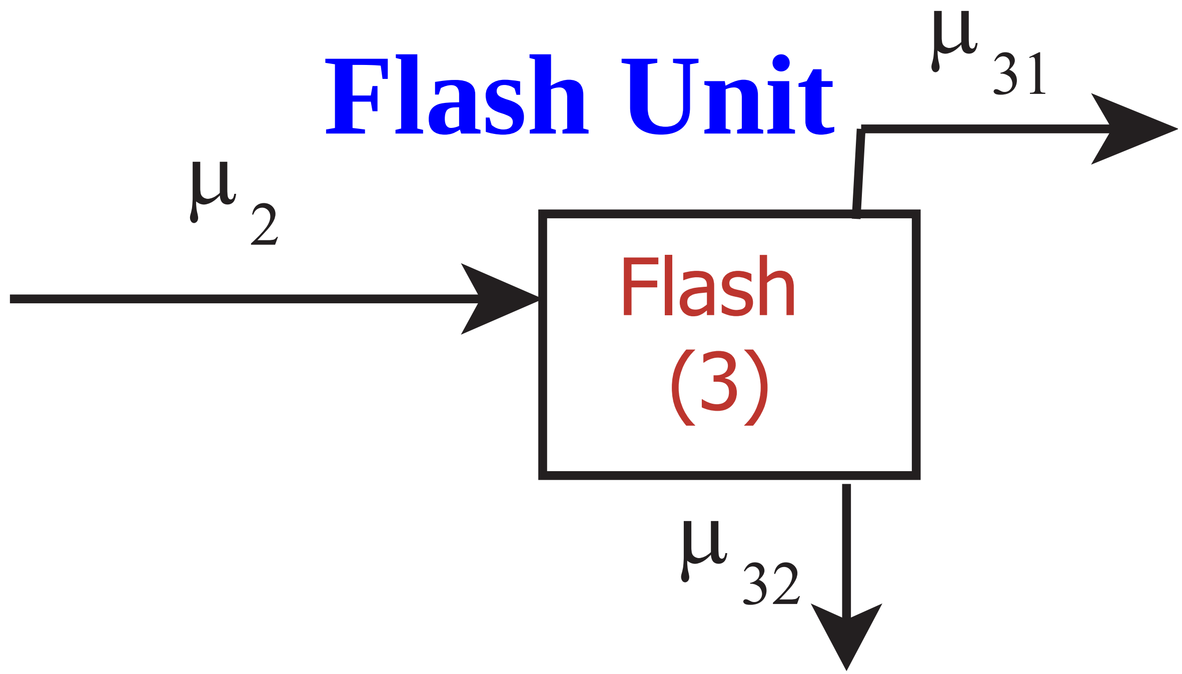


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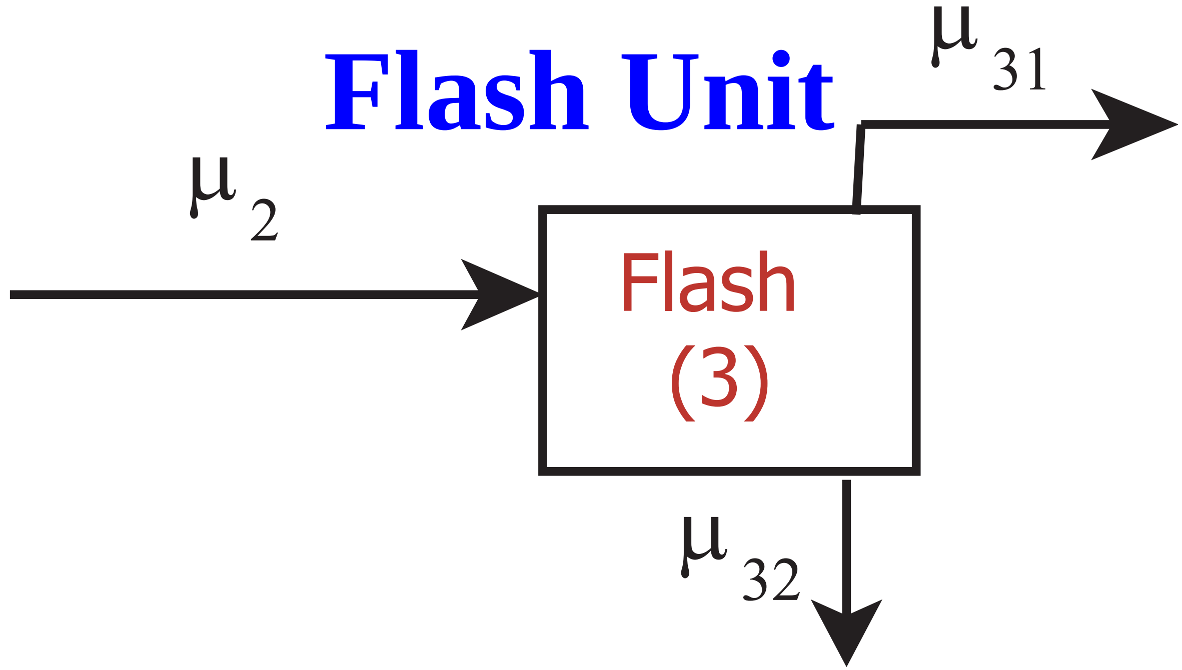


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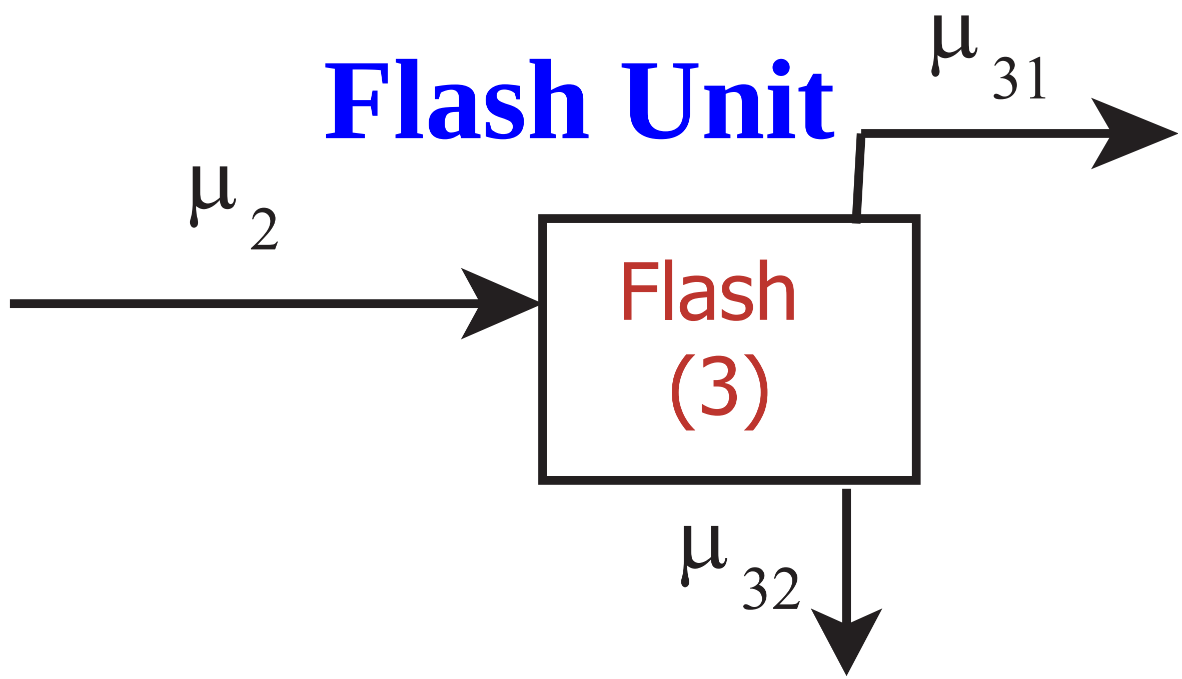


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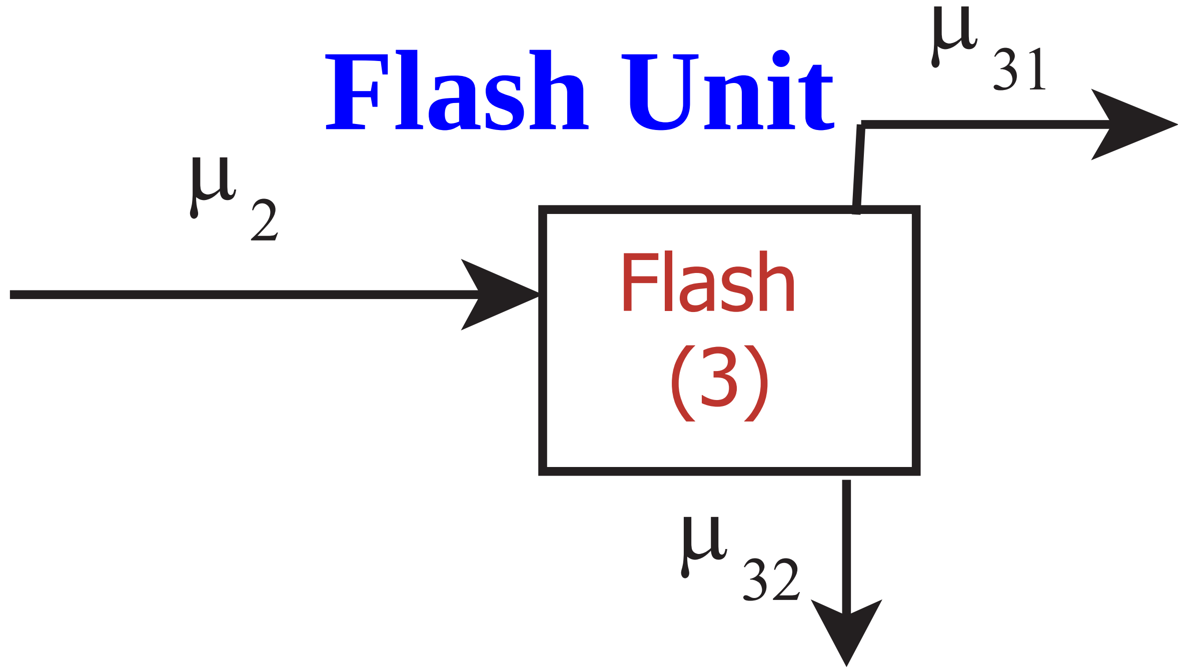


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Note that we ASSUMED a key component recovery.

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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

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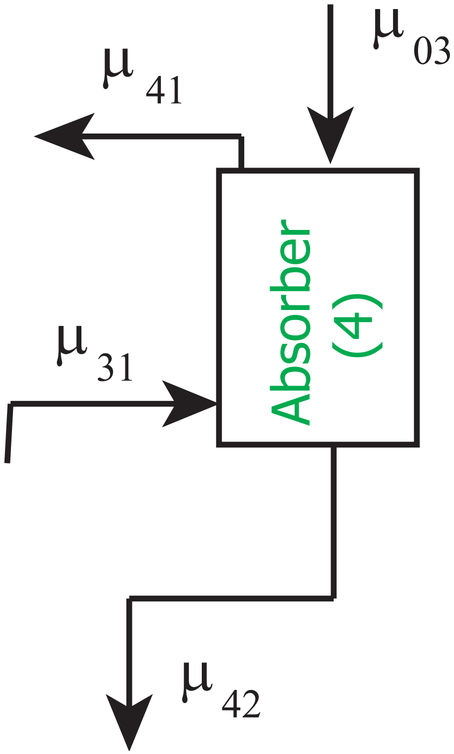

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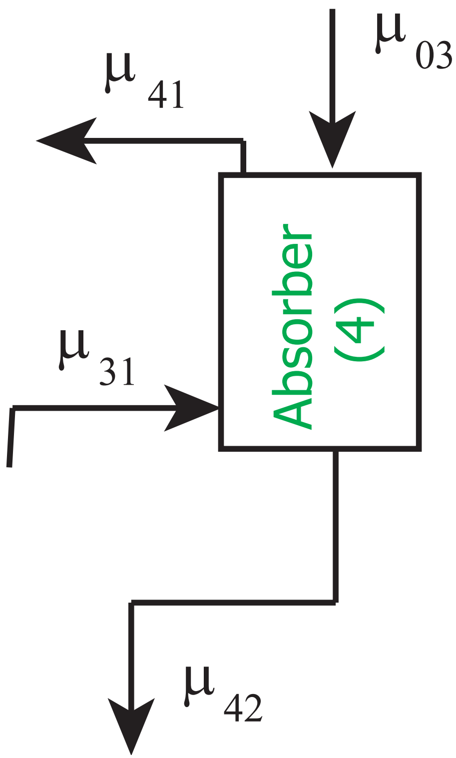


There are 4 degrees of freedom: $P$, $T$, key component recovery and liquid feed rate.

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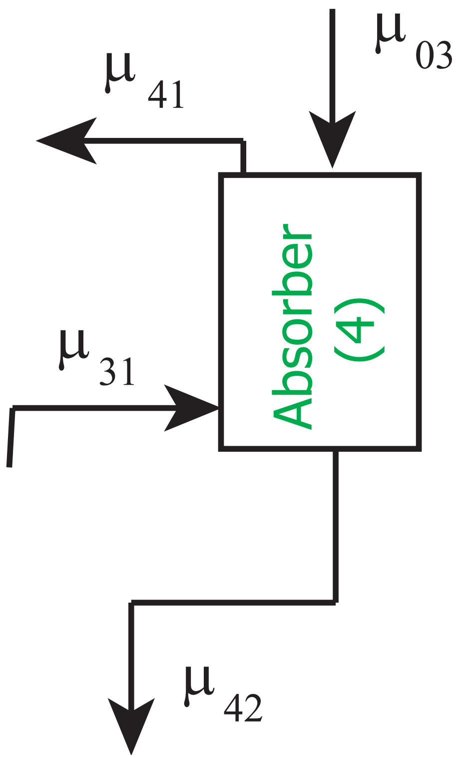


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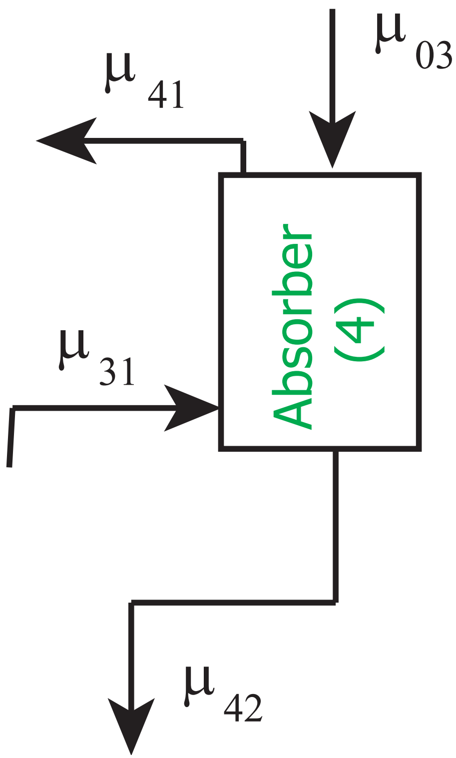


There are 4 degrees of freedom: $P$, $T$, key component recovery and liquid feed rate.

- 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.

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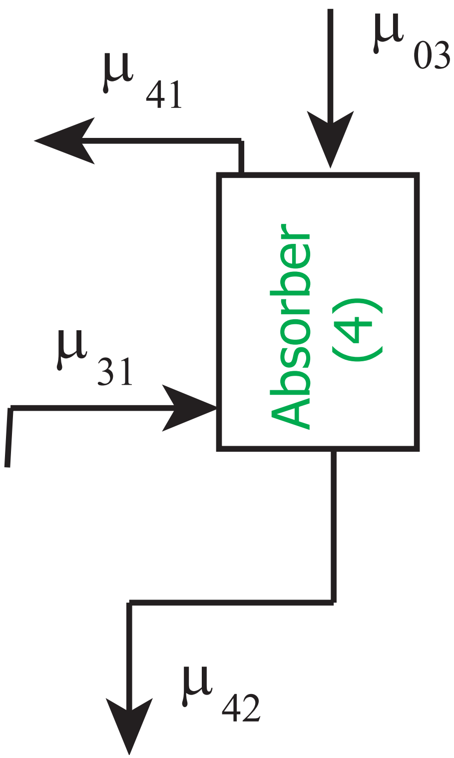


There are 4 degrees of freedom: $P$, $T$, key component recovery and liquid feed rate.

- 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% ($\xi_n = 0.99$)

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

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

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

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$$A_k = \frac{1.4}{\alpha_{k/EA}} = \frac{L}{VK_k} \quad \beta_N^k = \frac{1 - A_k^{N+1}}{1 - A_k} \qquad \beta_{N-1}^k = \frac{1 - A_k^N}{1 - A_k}$$

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$$v_1^k = \frac{v_{N+1}^k}{\beta_N^k} + \frac{\beta_{N-1}^k}{\beta_N^k} l_0^k \quad l_N^k = \left(1 - \frac{\beta_{N-1}^k}{\beta_N^k}\right) l_0^k + \left(1 - \frac{1}{\beta_N^k}\right) v_{N+1}^k$$

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Note that $\dfrac{\beta_{N-1}^k}{\beta_N^k} =$ fraction of $l_0$ in vapor $v_1$

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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

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A loss of 4.1% is acceptable.

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$$\begin{aligned} \mu_{41}(W) &= \frac{\mu_{31}(W)}{\beta_N^W} + \frac{\beta_{N-1}^W}{\beta_N^W}\mu_{03}(W) \\ &= 0.0019\mu_{31}(W) + 0.00092\mu_{31} \end{aligned}$$

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| $k$ | $\alpha_{k/n}$ | $A_k$ | $\beta_N$ | $\beta_{N-1}$ | $\mu_{41}(k)$ | $\mu_{42}(k)$ |
|---|---|---|---|---|---|---|
| $M$ | 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 | $0.24\mu_{31}(DEE)$ | $0.76\mu_{31}(DE$ |
| $EA$ | 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 | $0.0065\mu_{31}(IPA)$ | $0.993\mu_{31}(IP$ |

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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

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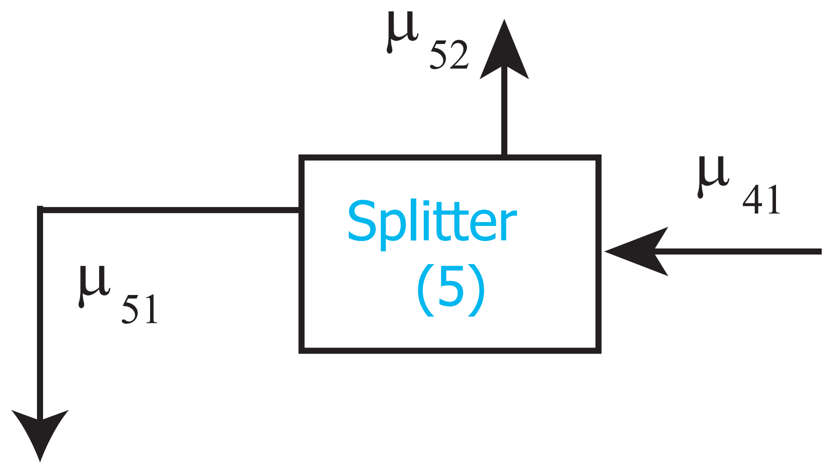

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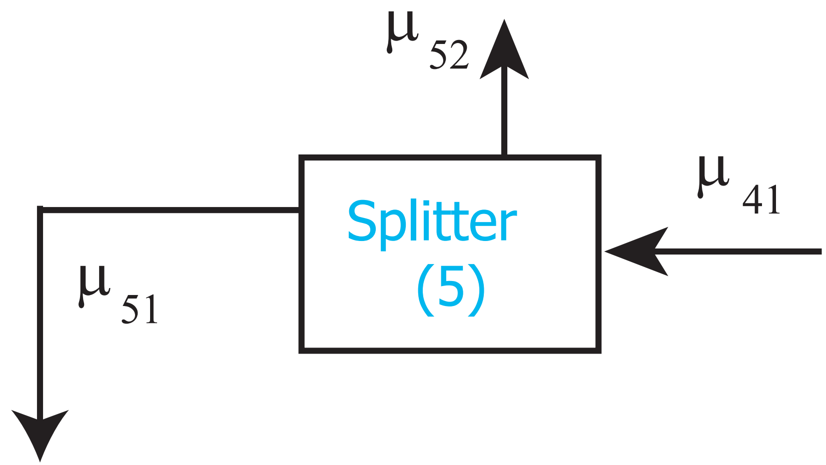


- We need to specify the purge rate $\xi$ to avoid accumulation of inerts.

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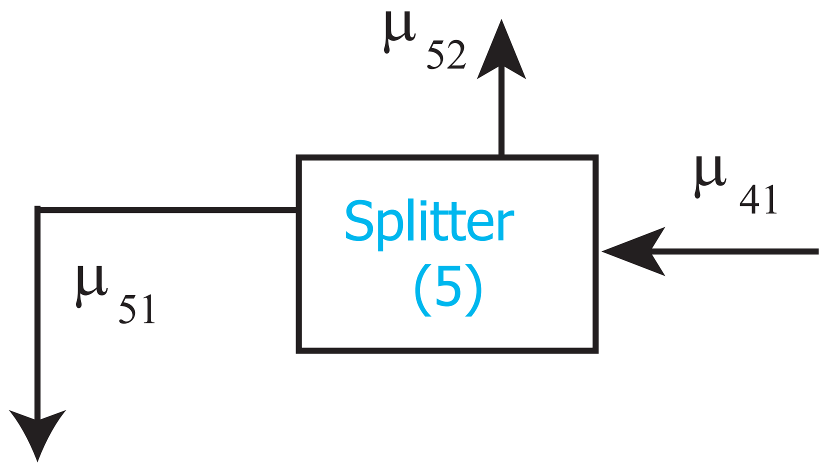


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- Specifically, methane entering the reactor should be less than 10%.

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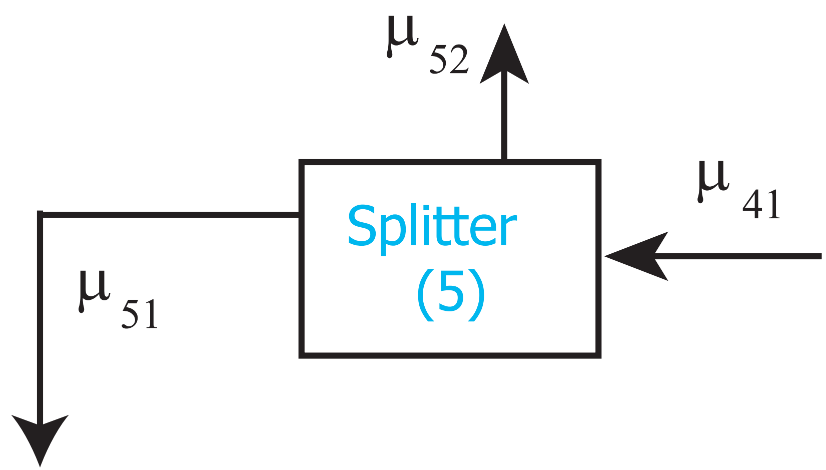


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- Specifically, methane entering the reactor should be less than 10%.

From mass balance:

$$\begin{aligned} \mu_{52} &= \xi\mu_{41} \\ \mu_{51} &= (1-\xi)\mu_{41} \end{aligned}$$

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

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$$\left[ \begin{array}{c} Mole\ fraction\ of\ M \\ entering\ reactor \end{array} \right] = \frac{\mu_1(M)}{\mu_1(M) + \mu_1(PL) + \mu_1(EL) + \mu_1(W)}$$

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EL Balance

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<u>EL Balance</u>

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

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

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Thus $\mu_1(EL) = (1-\xi)(0.979)(0.985)(0.93)\mu_1(EL) + 96$

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Thus $\mu_1(EL) = (1 - \xi)(0.979)(0.985)(0.93)\mu_1(EL) + 96$

This implies that $\mu_1(EL) = \dfrac{96}{0.1 + 0.9\xi}$

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

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PL Balance

$$\mu_1(PL) = \mu_{51}(PL) + 3$$
$$\mu_{51}(PL) = (1 - \xi)\mu_{41}(PL)$$
$$\mu_{41}(PL) = 0.901\mu_{31}(PL)$$
$$\mu_{31}(PL) = 0.932\mu_2(PL)$$
$$\mu_2(PL) = 0.993\mu_1(PL)$$

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

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Thus $\mu_1(PL) = (1 - \xi)(0.901)(0.932)(0.993)\mu_1(PL) + 3$

This implies that $\mu_1(PL) = \dfrac{3}{0.17 + 0.83\xi}$

# M Balance

$$\mu_1(M) = \mu_{51}(M) + 1$$
$$\mu_{51}(M) = (1 - \xi)\mu_{41}(M)$$
$$\mu_{41}(M) = \mu_{31}(M)$$
$$\mu_{31}(M) = 0.996\mu_2(M)$$
$$\mu_2(M) = 0.93\mu_1(M)$$

## M Balance

$$\mu_1(M) = \mu_{51}(M) + 1$$
$$\mu_{51}(M) = (1 - \xi)\mu_{41}(M)$$
$$\mu_{41}(M) = \mu_{31}(M)$$
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## M Balance

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## M Balance

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Thus $\mu_1(M) = (1-\xi)(0.996)\mu_1(M) + 1$

This implies that $\mu_1(M) = \dfrac{1}{0.004 + 0.996\xi}$

## W Balance

$$\mu_1(W) \quad = \quad 0.6\mu_1(EL)$$

## M Balance

$$\mu_1(M) = \mu_{51}(M) + 1$$
$$\mu_{51}(M) = (1-\xi)\mu_{41}(M)$$
$$\mu_{41}(M) = \mu_{31}(M)$$
$$\mu_{31}(M) = 0.996\mu_2(M)$$
$$\mu_2(M) = 0.93\mu_1(M)$$

Thus $\mu_1(M) = (1-\xi)(0.996)\mu_1(M) + 1$

This implies that $\mu_1(M) = \dfrac{1}{0.004 + 0.996\xi}$

## W Balance

$$\mu_1(W) \;=\; 0.6\mu_1(EL) \qquad \textit{Assumed earlier}$$

## M Balance

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Thus $\mu_1(M) = (1-\xi)(0.996)\mu_1(M) + 1$

This implies that $\mu_1(M) = \dfrac{1}{0.004 + 0.996\xi}$

## W Balance

$$\begin{aligned} \mu_1(W) &= 0.6\mu_1(EL) \qquad \textcolor{red}{\textit{Assumed earlier}} \\ &= \frac{53.6}{0.1 + 0.9\xi} \end{aligned}$$

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

$$\left[ \begin{array}{c} Mole\ fraction\ of\ M \\ entering\ reactor \end{array} \right] = \frac{\mu_1(M)}{\mu_1(M) + \mu_1(PL) + \mu_1(EL) + \mu_1(W)}$$

we have:

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

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we have:

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

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we have:

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

Solving for $\xi$ by trial and error, we get $\xi = 0.0019$.

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

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we have:

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

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

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

$$\left[\begin{array}{c} Mole\ fraction\ of\ M \\ entering\ reactor \end{array}\right] = \frac{\mu_1(M)}{\mu_1(M) + \mu_1(PL) + \mu_1(EL) + \mu_1(W)}$$

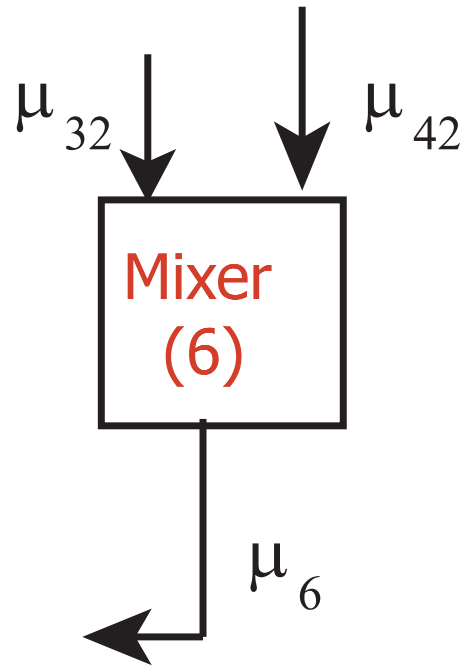
we have:

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

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

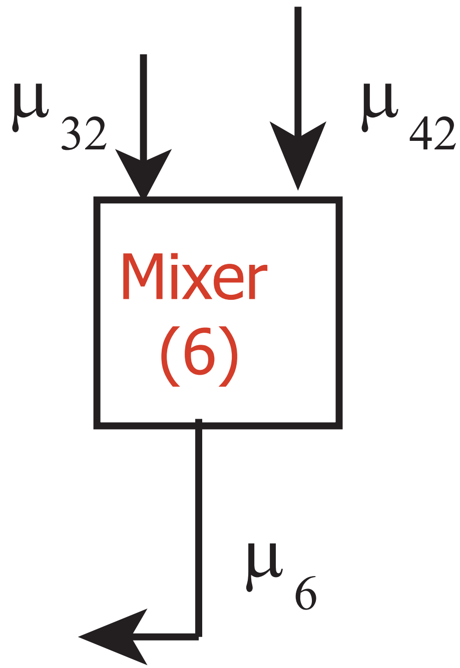
# Mixer

# Mixer




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

# Mixer

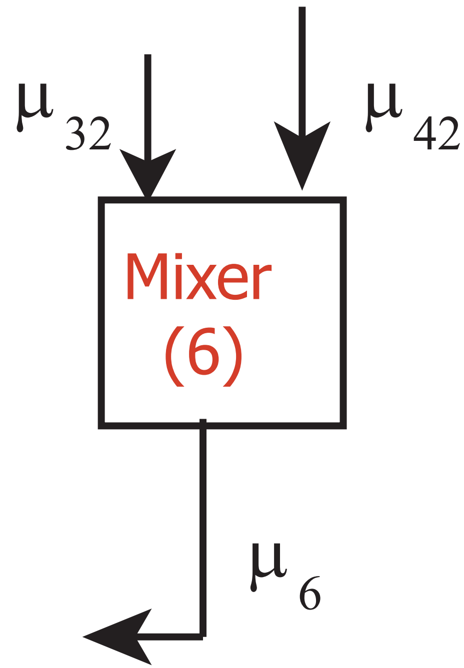



We can write down a mass balance for each component as follows:

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

where $k = M, EL, PL, DEE, EA, IPA, W$

# Mixer




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

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

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Note that we wrote component balances for $\mu_{32}(k)$ and $\mu_{42}(k)$ earlier.

# Dewatering Column

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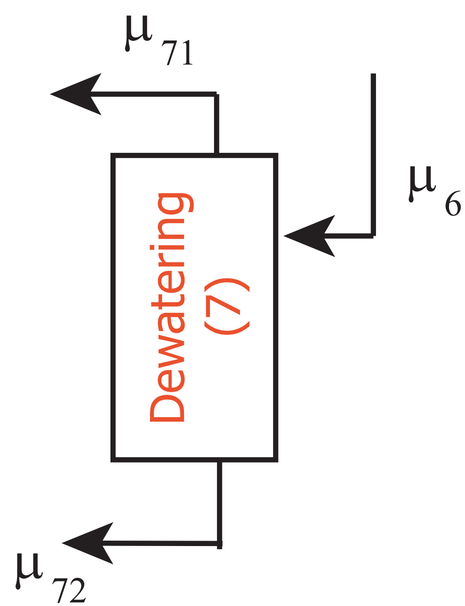

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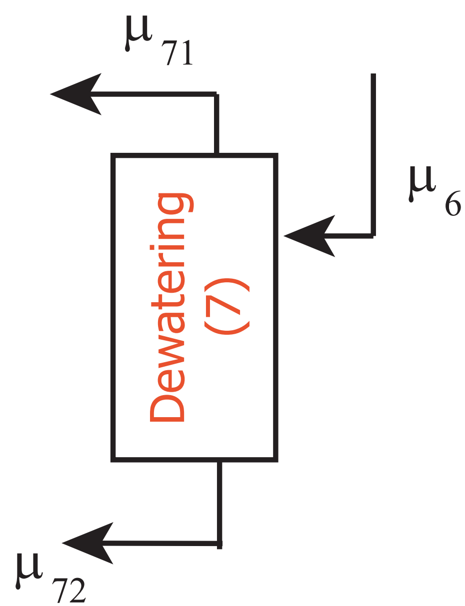
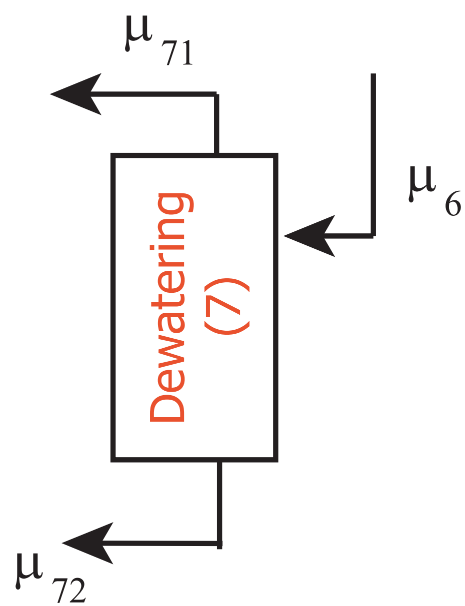



Specifications:

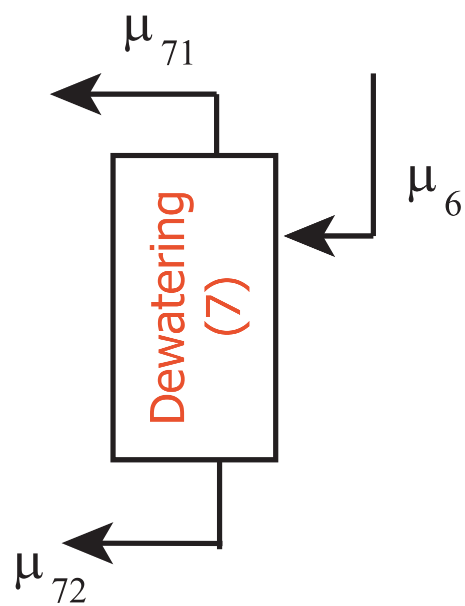
# Dewatering Column




Specifications:

- 90% of the water goes to the bottom product.

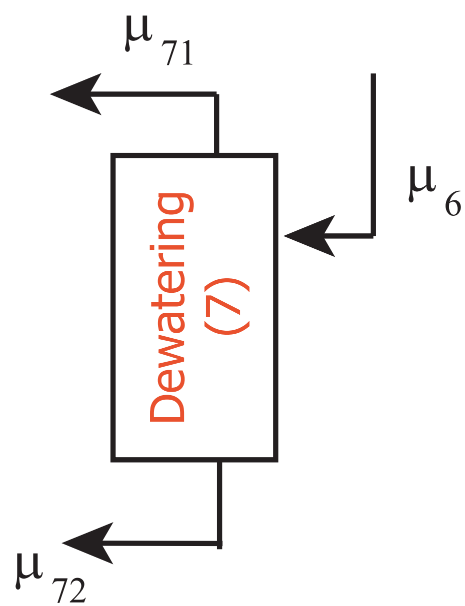
# Dewatering Column




Specifications:

- 90% of the water goes to the bottom product.
- 99.5% of the $EA$ goes as the top product.

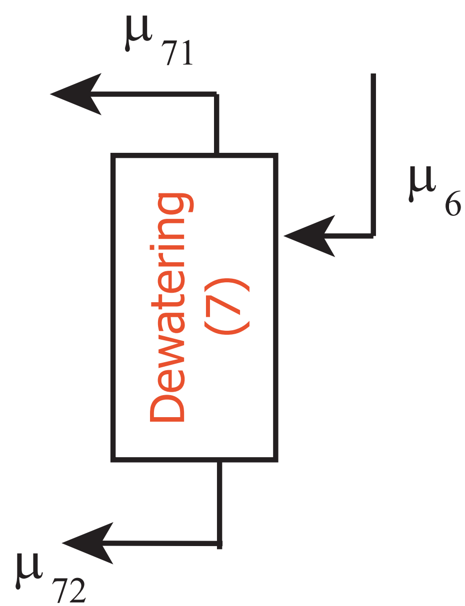
# Dewatering Column




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.

# 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:

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$$lk = EA$$

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

- $EL, PL,$ and $DEE$ are lighter than the light key.
- $IPA$ 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 $PL$.

$$\alpha_{EA/W} = \frac{P^0_{EA}}{P^0_W} = \frac{114}{47.1} = 2.43$$

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From Fenske Equation:

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

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$$\xi_{IPA} = \frac{\alpha^N_{IPA/W}\xi_W}{1+(\alpha^N_{IPA/W}-1)\xi_W} = 0.96$$

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Thus we have:

| $k$ | $M$ | $EL$ | $PL$ | $DEE$ | $EA$ | $IPA$ | $W$ |
|---|---|---|---|---|---|---|---|
| $\xi_k$ | | | | | | | |

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Thus we have:

| $k$ | $M$ | $EL$ | $PL$ | $DEE$ | $EA$ | $IPA$ | $W$ |
|---|---|---|---|---|---|---|---|
| $\xi_k$ | 1.0 | 1.0 | 1.0 | 1.0 | 0.995 | 0.96 | 0.1 |

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$$\xi_{IPA} = \frac{\alpha^N_{IPA/W}\xi_W}{1+(\alpha^N_{IPA/W}-1)\xi_W} = 0.96$$

Thus we have:

| $k$ | $M$ | $EL$ | $PL$ | $DEE$ | $EA$ | $IPA$ | $W$ |
|---|---|---|---|---|---|---|---|
| $\xi_k$ | 1.0 | 1.0 | 1.0 | 1.0 | 0.995 | 0.96 | 0.1 |

$\mu_{71}(k) = \xi_k \mu_6(k)$ and $\mu_{72}(k) = (1-\xi_k)\mu_6(k)$
where $k = M, EL, PL, DEE, EA, IPA, W$

# De-ethering Column

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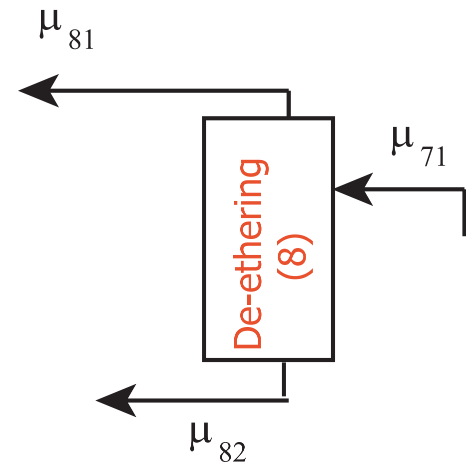
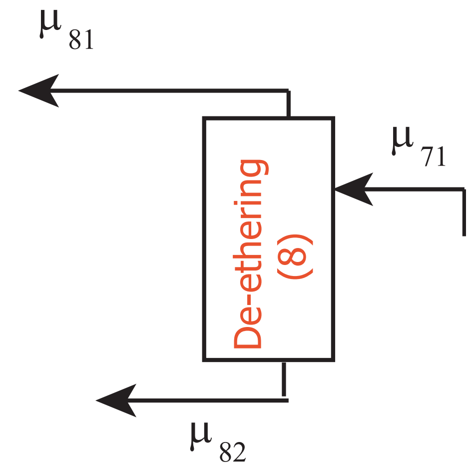


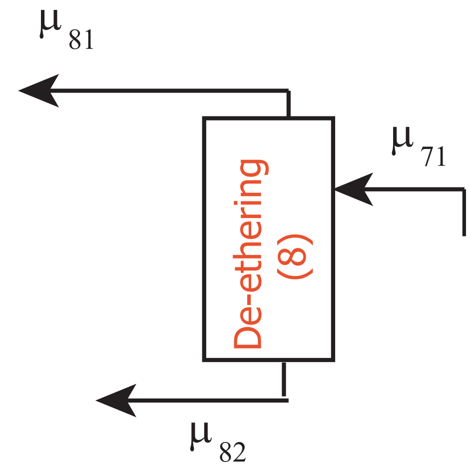
# De-ethering Column

- $DEE$ is removed overhead and recycled.



# De-ethering Column

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



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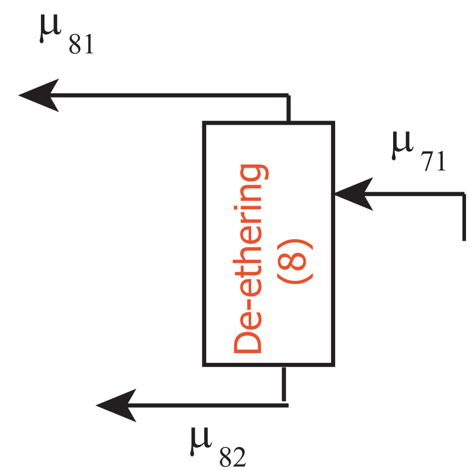
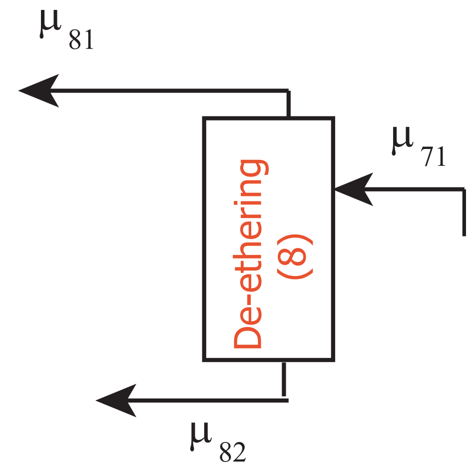



- $DEE$ is removed overhead and recycled.
- Specify $\xi_{DEE} = 0.995$ (light key) and $\xi_{EA} = 0.005$ (heavy key).
- $M,\ EL$ and $PL$ are lighter than the light key. $IPA$ and $W$ are heavier than the heavy key.

# De-ethering Column

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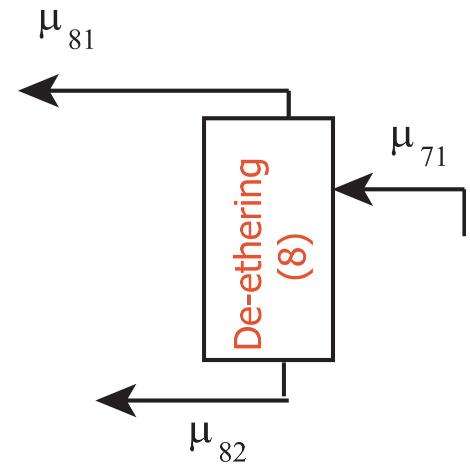
- $M,\ EL$ and $PL$ are lighter than the light key. $IPA$ and $W$ are heavier than the heavy key. There are no distributed components.

# De-ethering Column




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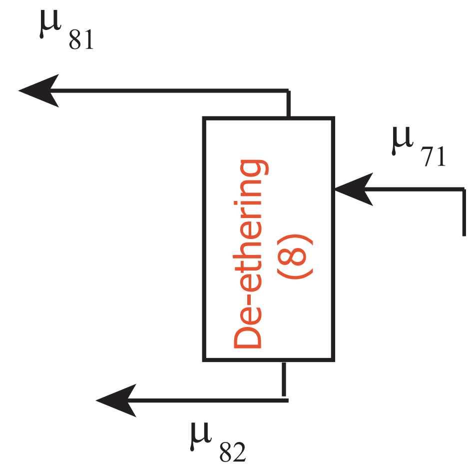
Thus we have:

| $k$ | $M$ | $EL$ | $PL$ | $DEE$ | $EA$ | $IPA$ | $W$ |
|---|---|---|---|---|---|---|---|
| $\xi_k$ | | | | | | | |

# De-ethering Column

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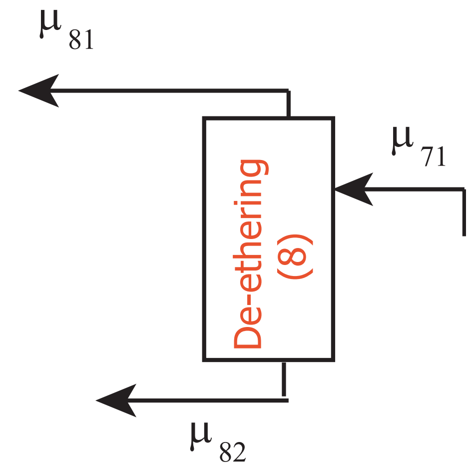
Thus we have:

| $k$ | $M$ | $EL$ | $PL$ | $DEE$ | $EA$ | $IPA$ | $W$ |
|---|---|---|---|---|---|---|---|
| $\xi_k$ | $1.0$ | $1.0$ | $1.0$ | $0.995$ | $0.005$ | $0.0$ | $0.0$ |

# De-ethering Column

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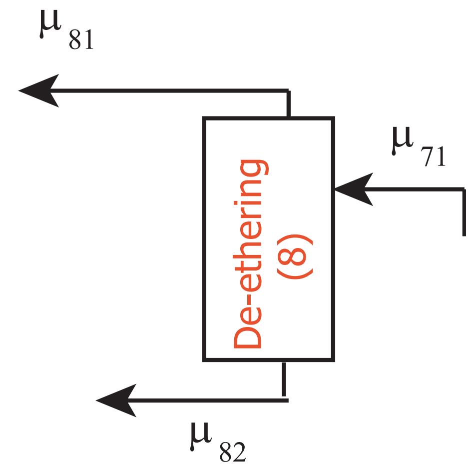
Thus we have:

| $k$ | $M$ | $EL$ | $PL$ | $DEE$ | $EA$ | $IPA$ | $W$ |
|---|---|---|---|---|---|---|---|
| $\xi_k$ | $1.0$ | $1.0$ | $1.0$ | $0.995$ | $0.005$ | $0.0$ | $0.0$ |

$$\mu_{81}(k) = \xi_k \mu_{71}(k)$$

# De-ethering Column




- $DEE$ is removed overhead and recycled.
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- $M,\ EL$ 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:

| $k$ | $M$ | $EL$ | $PL$ | $DEE$ | $EA$ | $IPA$ | $W$ |
|---|---|---|---|---|---|---|---|
| $\xi_k$ | 1.0 | 1.0 | 1.0 | 0.995 | 0.005 | 0.0 | 0.0 |

$\mu_{81}(k) = \xi_k \mu_{71}(k)$
$\mu_{82}(k) = (1 - \xi_k)\mu_{71}(k)$
where $k = M, EL, PL, DEE, EA, IPA, W$

# Final Azeotropic Separation

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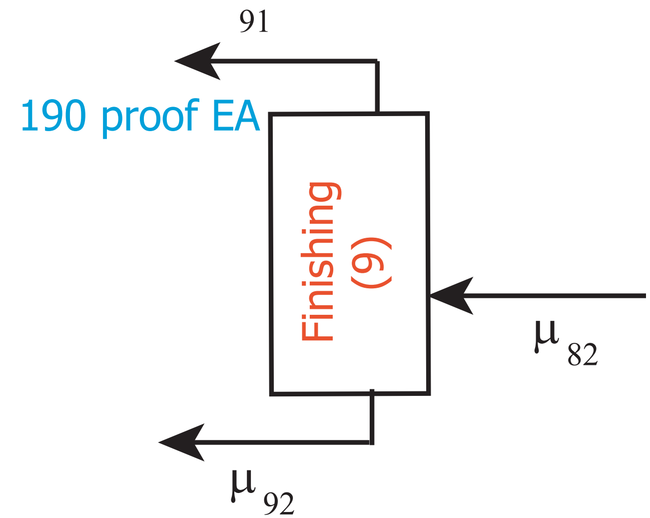
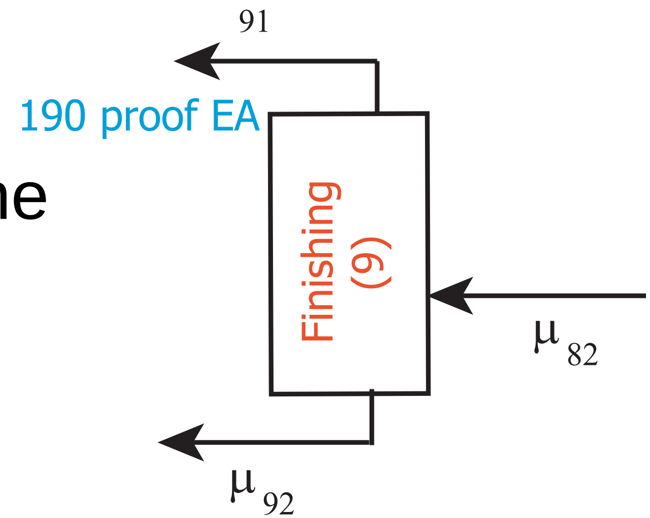


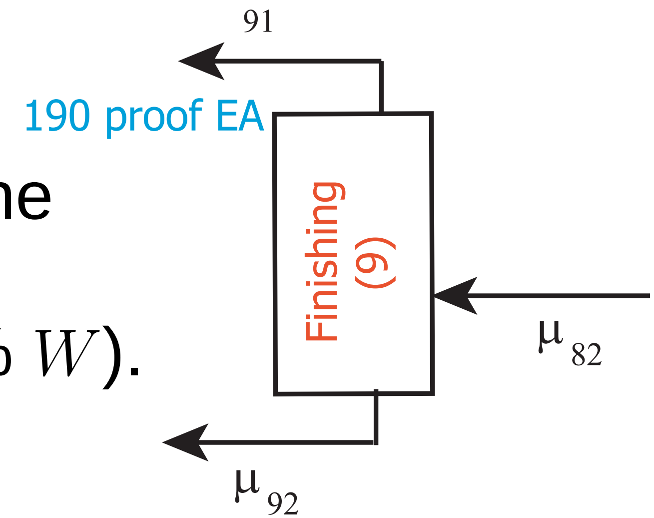
# Final Azeotropic Separation

- This last column is used to obtain the ethanol product at the azeotropic composition



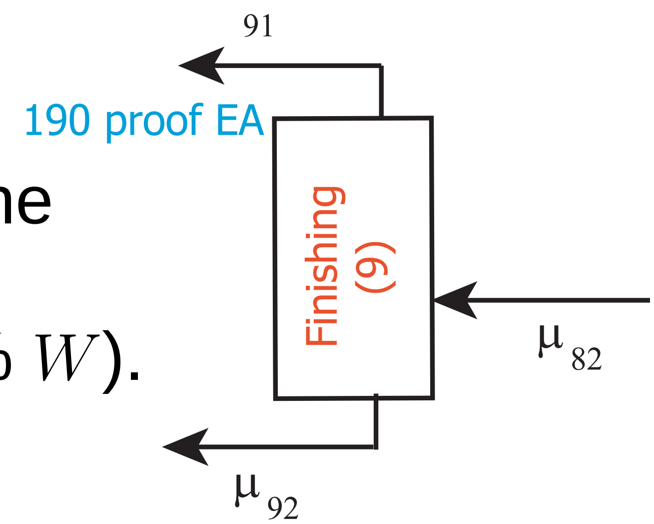
# Final Azeotropic Separation

- This last column is used to obtain the ethanol product at the azeotropic composition (85.5% $EA$ and 14.5% $W$).



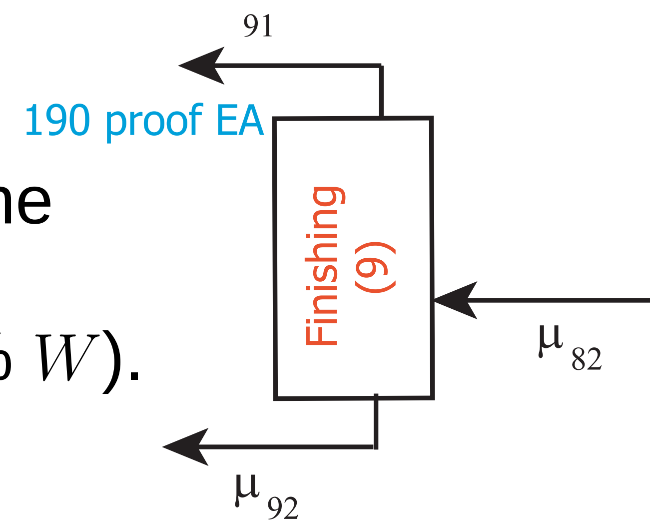
# Final Azeotropic Separation

- This last column is used to obtain the ethanol product at the azeotropic composition (85.5% $EA$ and 14.5% $W$).
- Specify $\xi_{az} = 0.995$



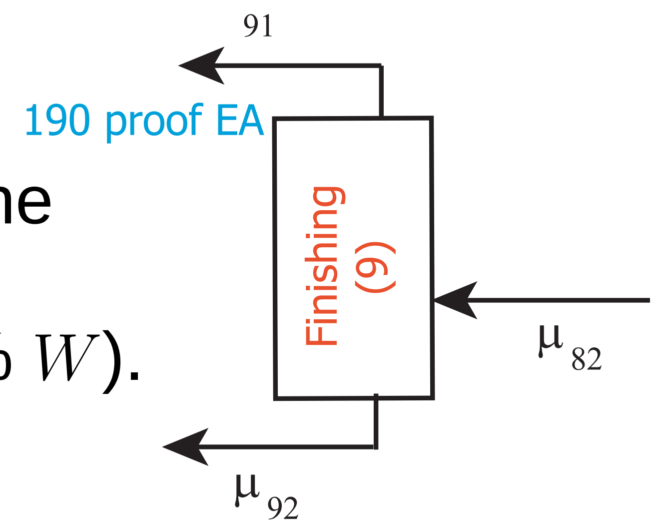
# Final Azeotropic Separation

- This last column is used to obtain the ethanol product at the azeotropic composition (85.5% $EA$ and 14.5% $W$).
- Specify $\xi_{az} = 0.995$
  No more than 0.1% $IPA$.



# Final Azeotropic Separation

- This last column is used to obtain the ethanol product at the azeotropic composition (85.5% $EA$ and 14.5% $W$).
- Specify $\xi_{az} = 0.995$
  No more than 0.1% $IPA$.
- To follow these specifications, it is necessary to know the molar flow rate $\mu_{82}$.



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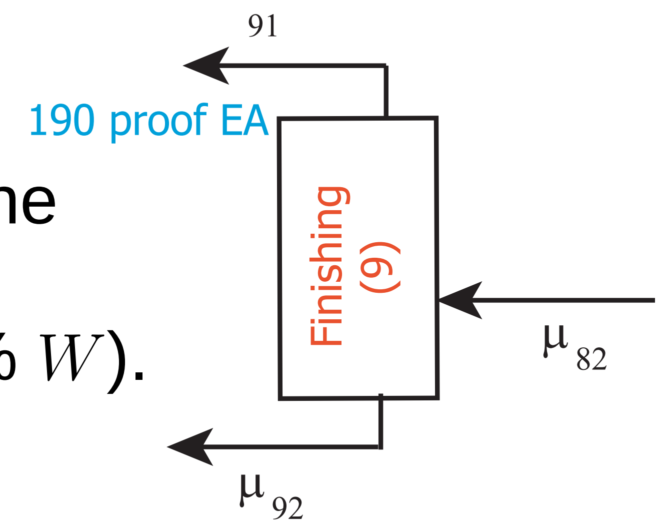


- This last column is used to obtain the ethanol product at the azeotropic composition (85.5% $EA$ and 14.5% $W$).
- Specify $\xi_{az} = 0.995$
  No more than 0.1% $IPA$.
- To follow these specifications, it is necessary to know the molar flow rate $\mu_{82}$.
- Once $\mu_{82}$ is known, a simple mass balance can be used to calculate $\mu_{91}$ and $\mu_{22}$.