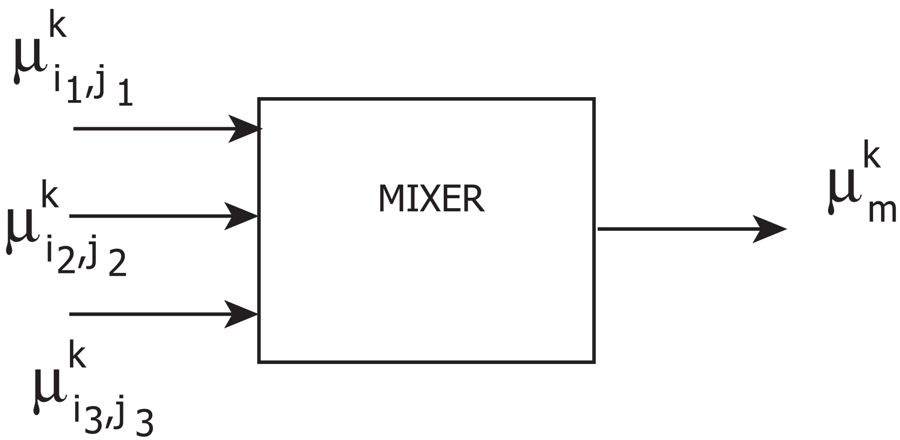
Mixer, Splitter, and Reactor

Process Model: Mixer

Consider a mixer that is mixing n streams, each of which has k components.



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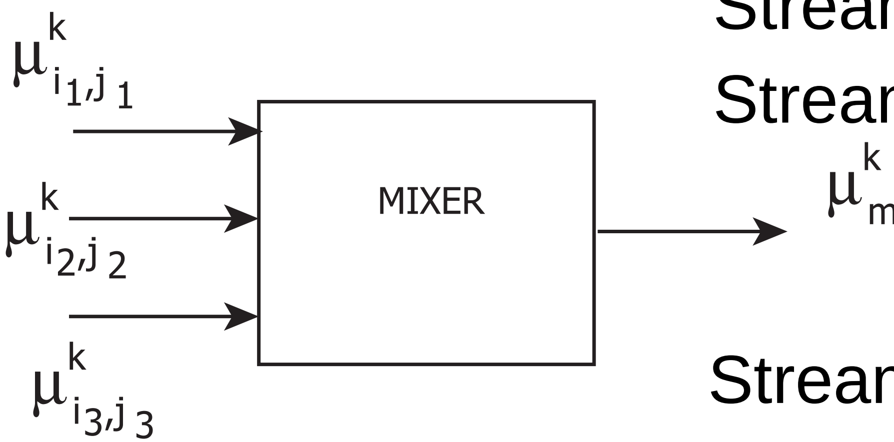

Stream j_1 is coming from unit i_1

Stream j_2 is coming from unit i_2

.

.

Stream j_n is coming from unit i_n

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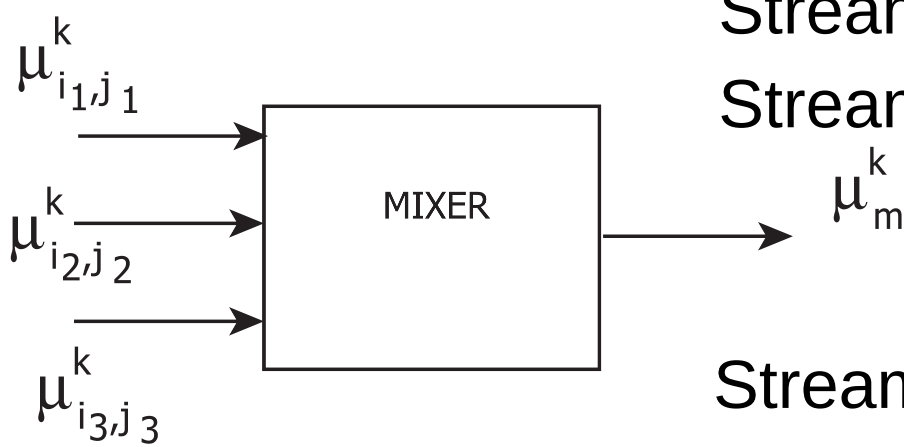

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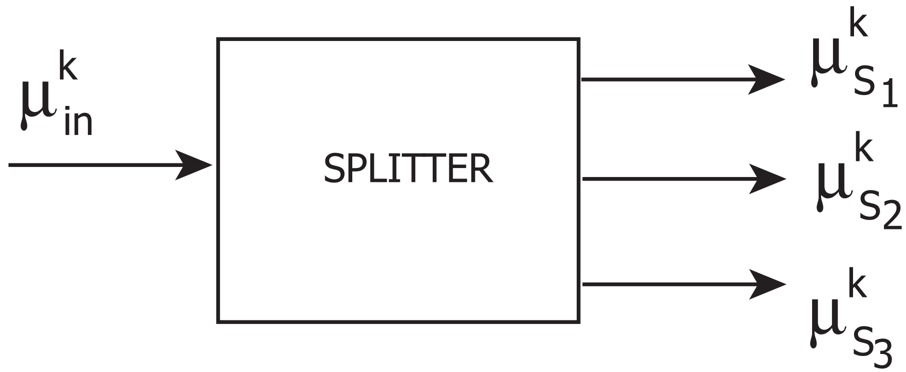
Then, the mixer balance for component k is given by:

$$\mu^k_m = \mu^k_{i_1,j_1} + \mu^k_{i_2,j_2} + ... + \mu^k_{i_n,j_n}$$

Process Model: Splitter



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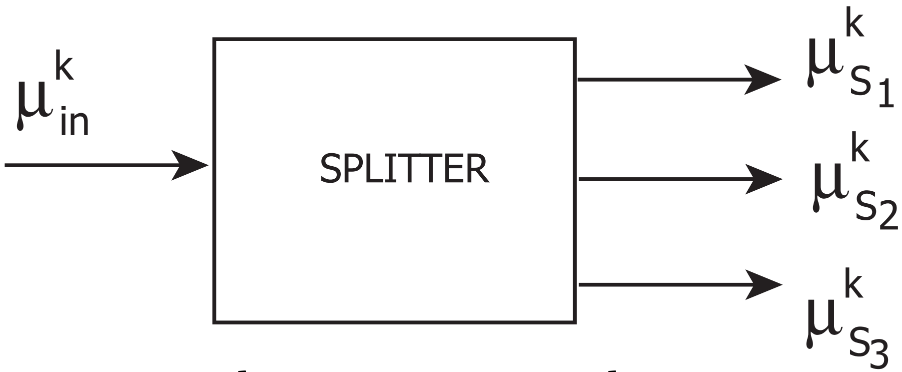
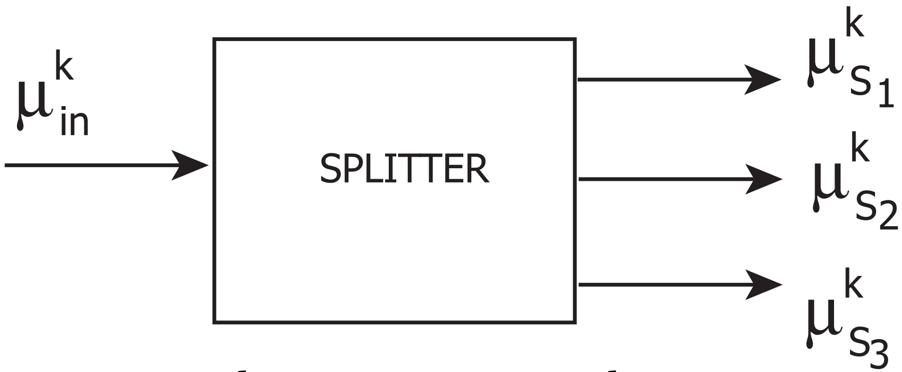


$$\mu^k_{S_1} = \xi_1 \mu^k_{in}$$
$$\mu^k_{S_2} = \xi_2 \mu^k_{in}$$

$$\vdots$$

$$\mu^k_{S_{n-1}} = \xi_{n-1} \mu^k_{in}$$

Process Model: Splitter



$$
\begin{aligned}
\mu_{S_1}^k &= \xi_1 \mu_{in}^k \\
\mu_{S_2}^k &= \xi_2 \mu_{in}^k \\
&. \\
&. \\
\mu_{S_{n-1}}^k &= \xi_{n-1} \mu_{in}^k \\
\mu_{S_n}^k &= \left[1 - (\xi_1 + \xi_2 + ... + \xi_{n-1})\right] \mu_{in}^k
\end{aligned}
$$

Reactor

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- Specific Kinetic Model
- Equilibrium-based Reactor Model
- Stoichiometric Reactor Model

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- The reaction kinetics are typically determined via laboratory experiments.
- The type of reactor is taken into consideration in the model.
  For instance, in a CSTR, the reactor model may be written as:

  $$F.C - F.C_0 = V.r(C,T)$$

  where r is the reaction rate

Equilibrium-based Reactor Model

Equilibrium-based Reactor Model

The equilibrium constant K is related to the free energy ΔG and temperature T as follows:

$$K = exp\left(-\frac{\Delta G}{RT}\right)$$

Stoichiometric Reactor Model

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- The reaction stoichiometry is used to determine the molar flowrate of each species at steady state.
- The molar flow rates can be used to determine reactor size.

Stoichiometric Reactor Calculations

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$$
\begin{aligned}
A + 2B &\longrightarrow C + 2D & \eta_1 &= 0.6 \\
2E + 7B &\longrightarrow 4C + 6D & \eta_2 &= 0.8
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It is given that A is the limiting reactant for the first reaction (with 60% conversion) and E is the limiting reactant for the second reaction (with 80% conversion).

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It is given that A is the limiting reactant for the first reaction (with 60% conversion) and E is the limiting reactant for the second reaction (with 80% conversion).

If the molar flowrate of each species coming into the reactor is known, compute the molar flowrate of each species going out of the reactor.

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r	A	B	E	C	D
1	-1	-2	0	1	2
2	0	-7/2	-1	2	3

Stoichiometric Reactor Calculations

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\mu_R^A &= \mu_{in}^A - 0.6\mu_{in}^A &= 0.4\mu_{in}^A \\
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\mu_R^B = \mu_{in}^B - 2\left(0.6\mu_{in}^A\right) - \frac{7}{2}\left(0.8\mu_{in}^E\right)
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$$\mu_R^C = \mu_{in}^C + 0.6\mu_{in}^A + 2\left(0.8\mu_{in}^E\right)$$

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\mu_R^D &= \mu_{in}^D + 2\left(0.6\mu_{in}^A\right) + 3\left(0.8\mu_{in}^E\right)
\end{aligned}$$

Note that in Steps 3 and 4, all equations are linear.

Series reactions

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\begin{array}{llll}
A + 2B & \longrightarrow & C + 2D & \eta_1 = 0.6 \\
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D & \longrightarrow & F & \eta_3 = 0.7
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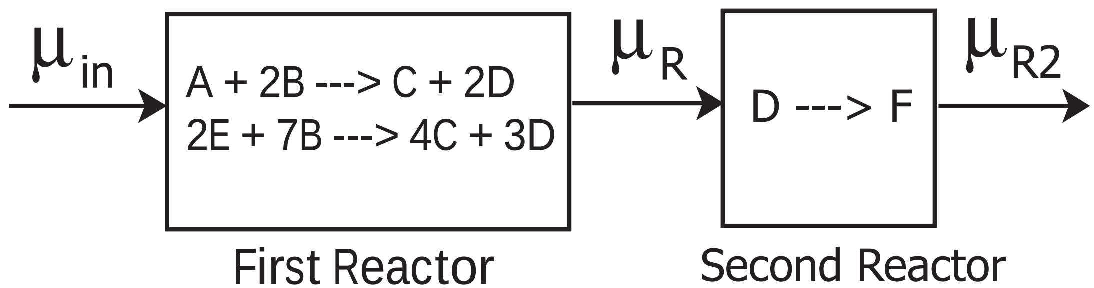

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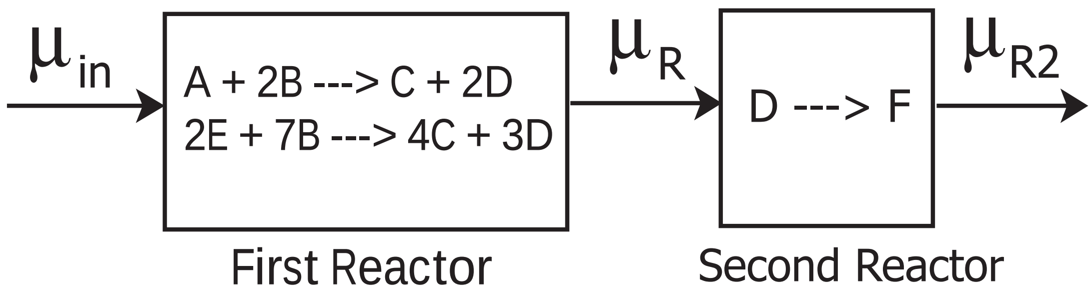

Balances for first reactor:

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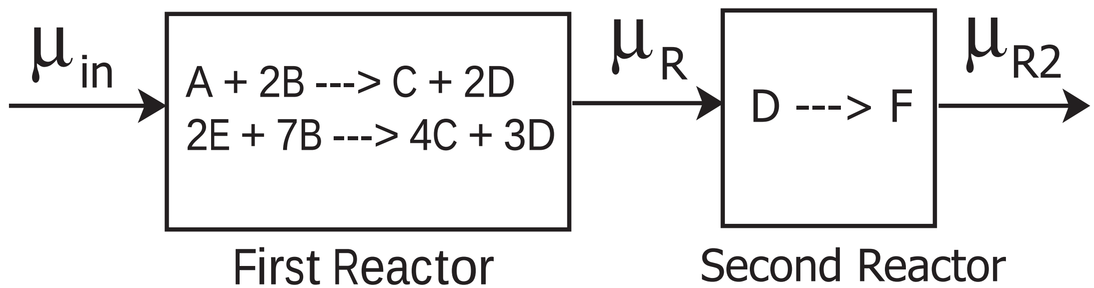

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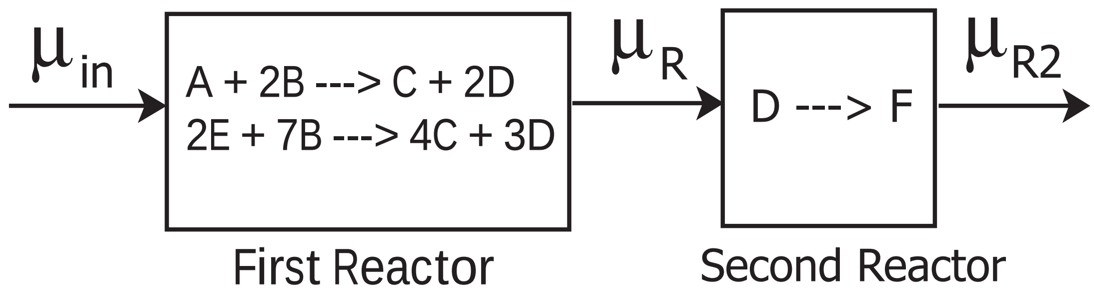

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Balances for second reactor:

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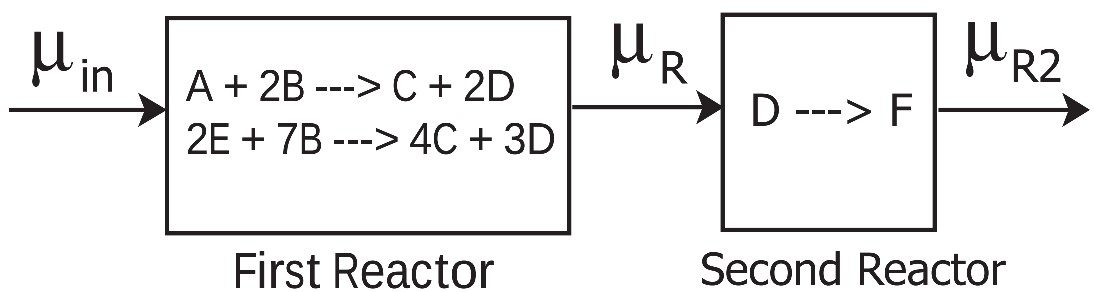
$$



Balances for first reactor: Same as before

Balances for second reactor:

$$
\begin{aligned}
\mu_{R2}^{D} &= \mu_{R}^{D} - 0.7\mu_{R}^{D} = 0.3\mu_{R}^{D} \\
\mu_{R2}^{F} &= \mu_{R}^{F} + 0.7\mu_{R}^{D}
\end{aligned}
$$