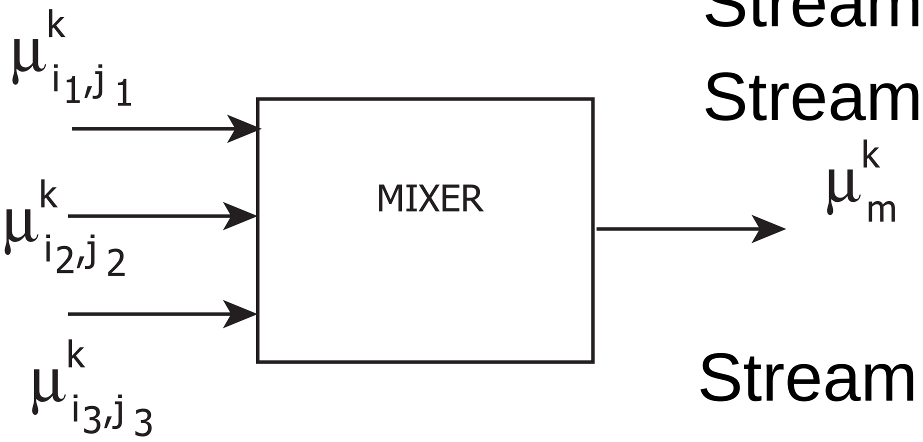
Mixer, Splitter, and Reactor

Process Model: Mixer

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



Stream j_1 is coming from unit i_1

Stream j_2 is coming from unit i_2

.

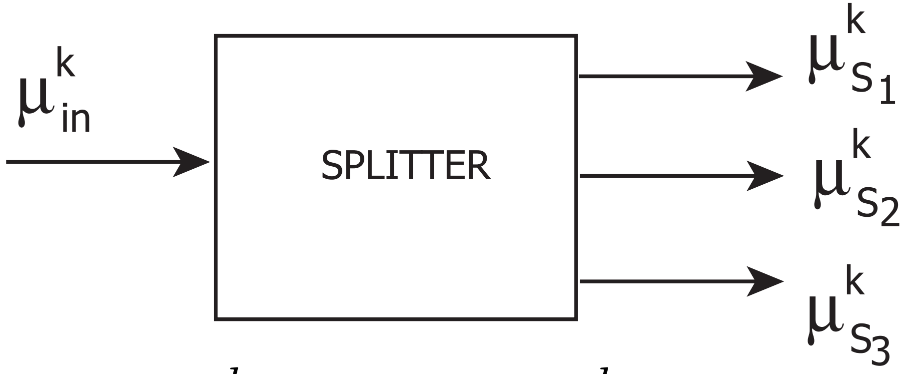
.

Stream j_n is coming from unit i_n

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

$$\boxed{\mu_m^k = \mu_{i_1,j_1}^k + \mu_{i_2,j_2}^k + \ldots + \mu_{i_n,j_n}^k}$$

Process Model: Splitter



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

Reactor

A reactor is a unit operation in which new chemical species are formed via chemical transformation.

There are three different types of reactor models

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

Specific Kinetic Reactor Model

- This model relates concentrations of species via specific reaction kinetics.
- 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

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

- The extent of reaction, η, for each reaction is specified by the user.
- 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

$$\begin{aligned} A + 2B &\longrightarrow C + 2D & \eta_1 = 0.6 \\ 2E + 7B &\longrightarrow 4C + 6D & \eta_2 = 0.8 \end{aligned}$$

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.

Stoichiometric Reactor Calculations

Step 1: Normalize all reactions w.r.t. limiting reactants.

$$
\begin{array}{lcll}
A + 2B & \longrightarrow & C + 2D & \eta_1 = 0.6 \\
E + \frac{7}{2}B & \longrightarrow & 2C + 3D & \eta_2 = 0.8
\end{array}
$$

Step 2: Generate stoichiomentric table using the convention:
Reactants have negative sign, inerts are zero and products have positive sign.

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

Stoichiometric Reactor Calculations

Step 3: Write down the mass balance for the limiting reactants.

$$
\begin{aligned}
\mu_R^A &= \mu_{in}^A - 0.6\mu_{in}^A = 0.4\mu_{in}^A \\
\mu_R^E &= \mu_{in}^E - 0.8\mu_{in}^E = 0.2\mu_{in}^E
\end{aligned}
$$

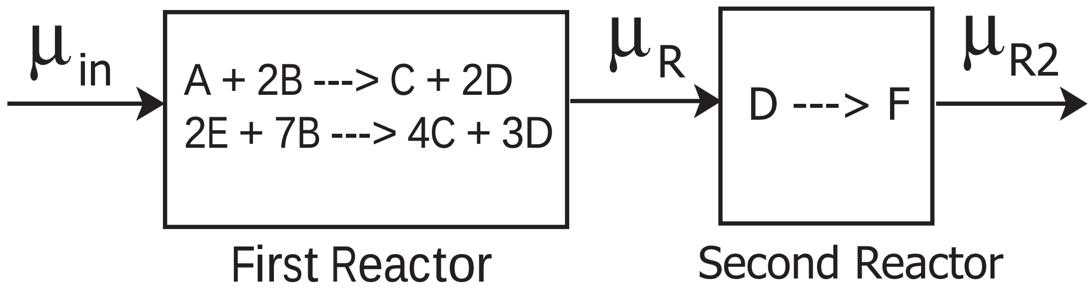
Step 4: Write down the mass balances for the remaining components based on stoichiometry.

$$
\begin{aligned}
\mu_R^B &= \mu_{in}^B - 2\left(0.6\mu_{in}^A\right) - \frac{7}{2}\left(0.8\mu_{in}^E\right) \\
\mu_R^C &= \mu_{in}^C + 0.6\mu_{in}^A + 2\left(0.8\mu_{in}^E\right) \\
\mu_R^D &= \mu_{in}^D + 2\left(0.6\mu_{in}^A\right) + 3\left(0.8\mu_{in}^E\right)
\end{aligned}
$$

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

Series reactions

$$
\begin{array}{lcll}
A + 2B & \longrightarrow & C + 2D & \eta_1 = 0.6 \\
2E + 7B & \longrightarrow & 4C + 6D & \eta_2 = 0.8 \\
D & \longrightarrow & F & \eta_3 = 0.7
\end{array}
$$



Balances for first reactor: Same as before

Balances for second reactor:

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