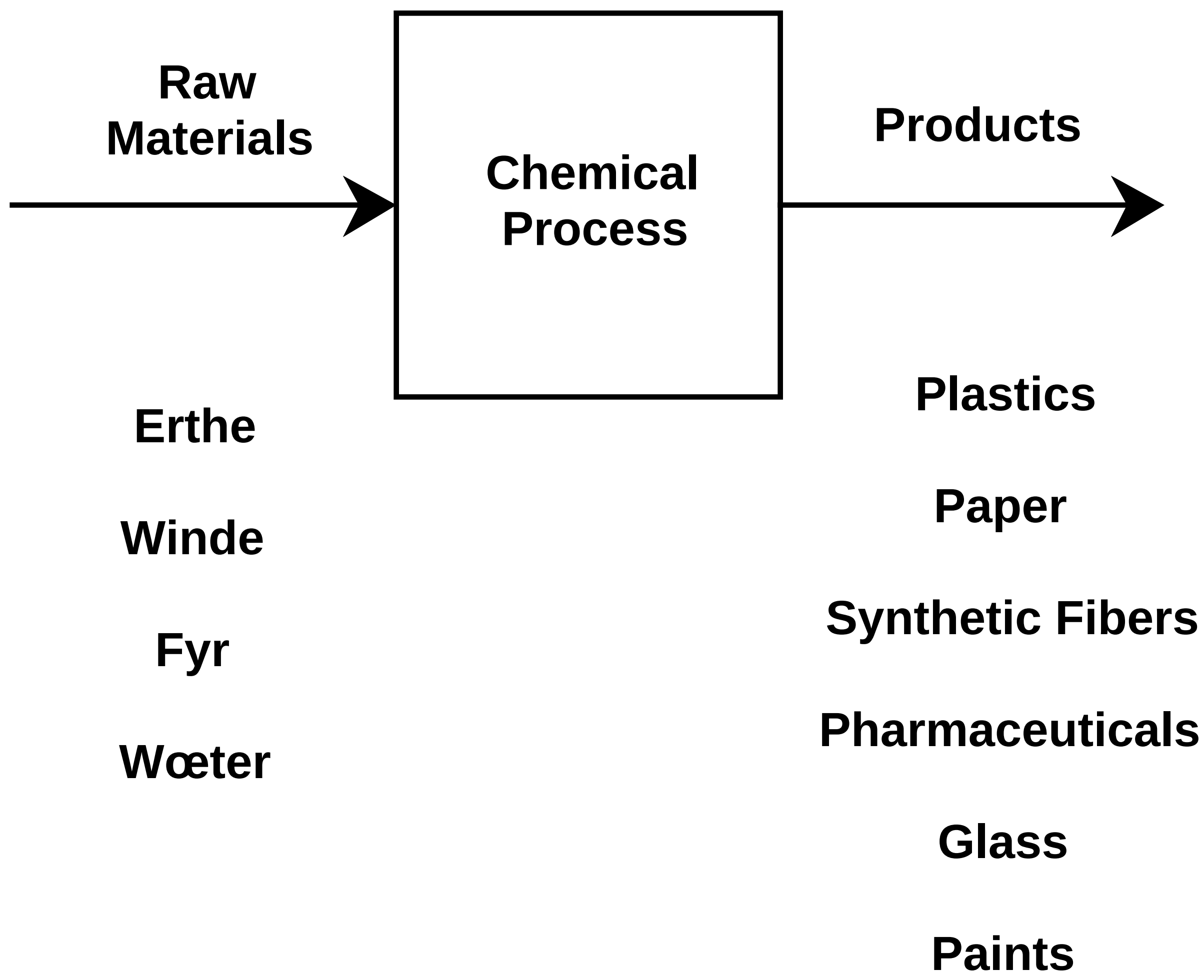
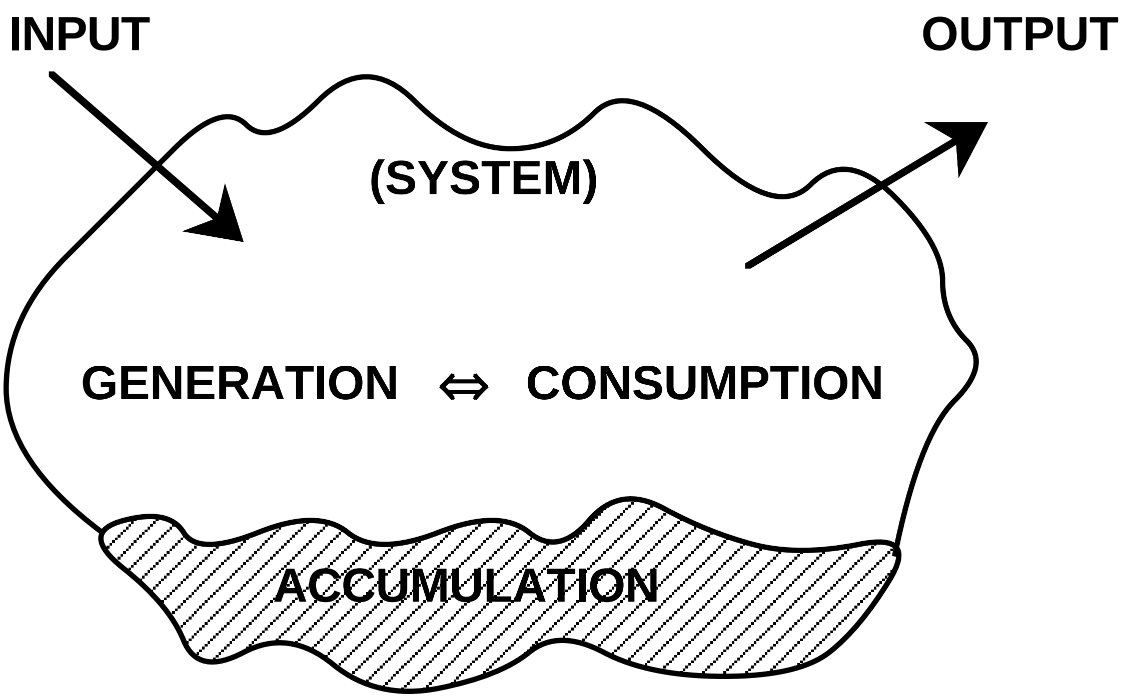
Chemical Process Systems



- Large-scale, continuous
- Operated at steady state
- Need transient behavior for control

Chemical System Modeling

Conservation Laws



Input + Generation = Output + Consumption + Accumulation

Engineer's Guide to Chemistry

Mol – mass of material which has the same number of molecules as are present in 12 mass units of C^{12}.

g-mol (or mol) – 6.023×10^{23} molecules

kg-mol (or kmol) – 6.023×10^{26} molecules

lb-mol (or E94) – 2.732×10^{26} molecules

e.g. 1 mol CH_2O has mass (12 + 2 + 16) = 30 g

or 200 g CH_2O is 200/30 = 6.67 mol

Chemical Equations

$$a\mathrm{Fe_2O_3} + b\mathrm{CO} \rightarrow c\mathrm{Fe} + d\mathrm{CO_2}$$

Choose $a = 1$ (most complex molecule)

Then $c = 2$ to balance Fe

Also $b = \mathrm{d}$ to balance C

"Guess" b until O's balance. $b = d = 3$.

$$\mathrm{Fe_2O_3} + 3\mathrm{CO} \rightarrow 2\mathrm{Fe} + 3\mathrm{CO_2}$$

Elements of Chemical Processing Systems

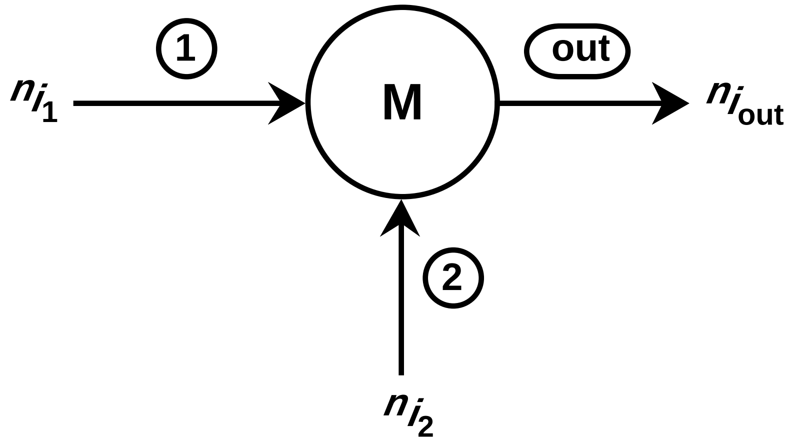
- Mixer

- Divider

- Separator

- Reactor

Mixer (Steady-state)



$$\text{Input} + \cancelto{0}{\text{Gen.}} = \text{Output} + \cancelto{0}{\text{Cons.}} + \cancelto{0}{\text{Accum.}}$$

For each component

$$n_{i_{\text{out}}} = n_{i_1} + n_{i_2}$$

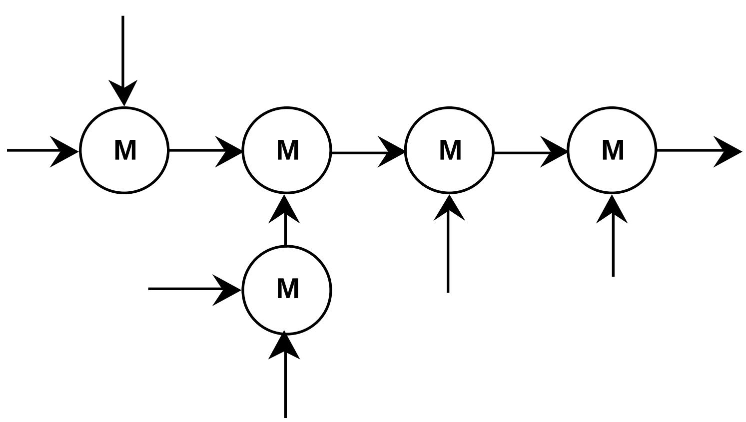
Total

$$n_{\text{out}} = n_1 + n_2 \text{ where } n = \sum n_i$$

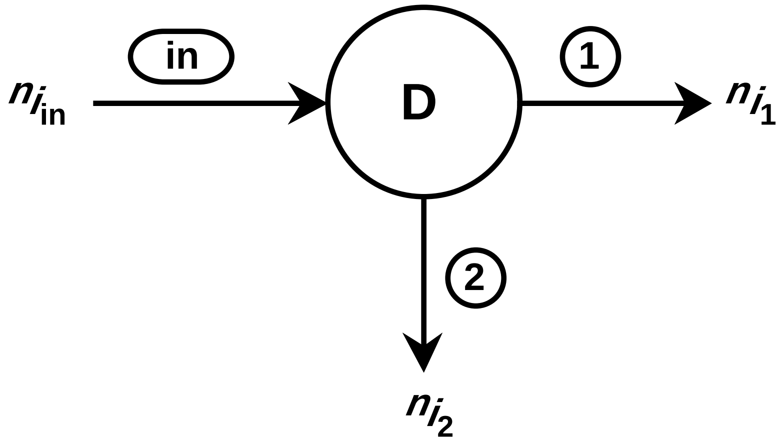
n_{i_1} is the number of moles of species i in stream 1.

n_1 is the total number of moles in stream 1.

Multiple streams



Divider (Steady state)



$$n_{i_1} + n_{i_2} = n_{i_{\mathrm{in}}}$$

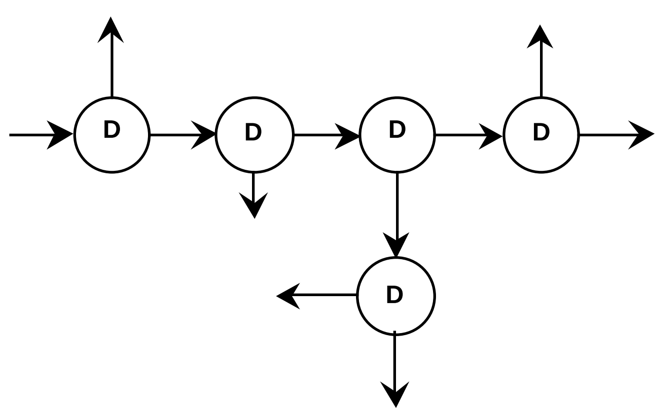
$$n_1 + n_2 = n_{\mathrm{in}}$$

also

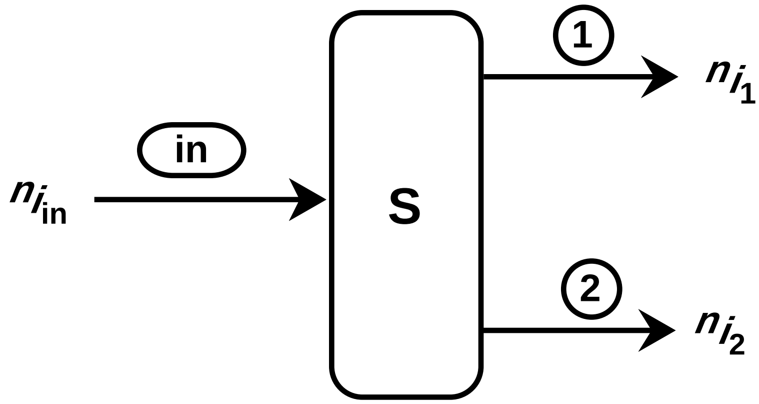
$$x_{i_1} = x_{i_2} = x_{i_{\mathrm{in}}} \qquad x_{i_s} = \frac{n_{i_s}}{n_s}$$

x_{i_1} is the *mole fraction* of species i in stream 1.

Multiple Streams



Separator (Steady state)



Specify *split fraction*

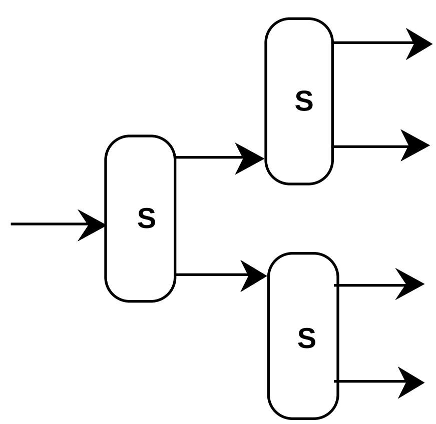
$$t_{i_s} = \frac{n_{i_s}}{n_{i_{in}}}$$

t_{i_1} is the split fraction of species i with respect to stream 1.

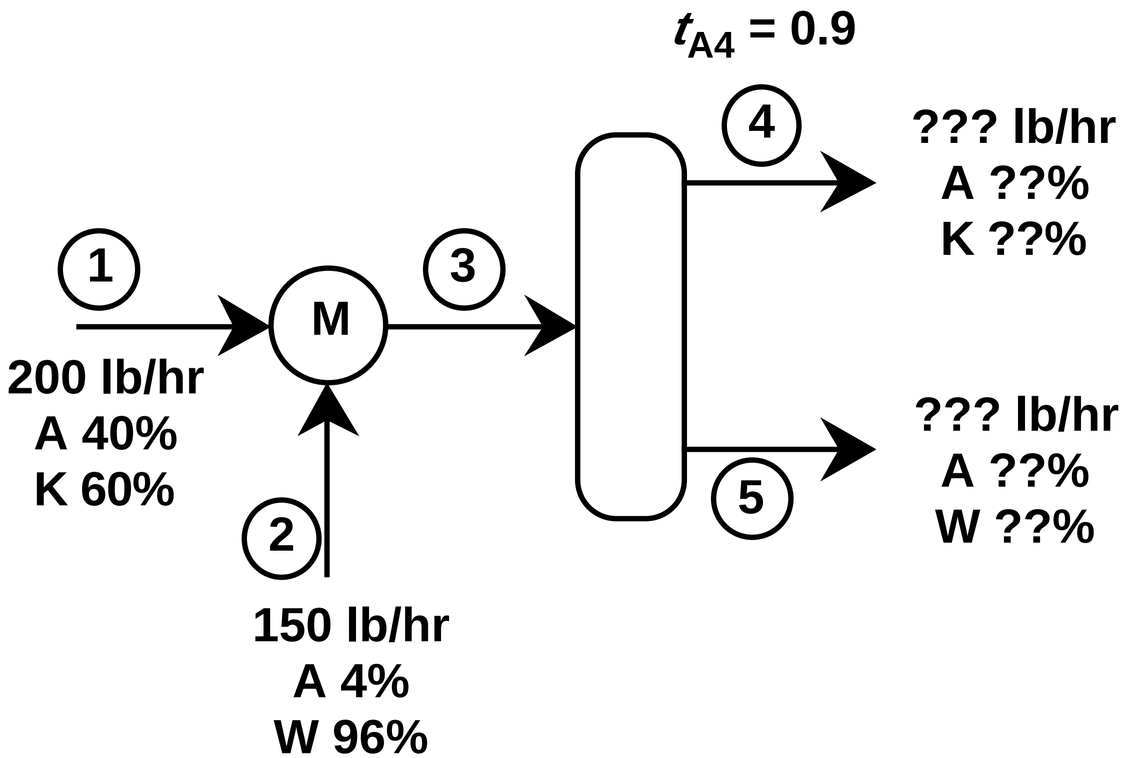
$$n_{i_1} = t_{i_1} n_{i_{in}}$$

$$n_{i_2} = (1 - t_{i_1}) n_{i_{in}}$$

Multiple streams



Steady State Example



Material Balances

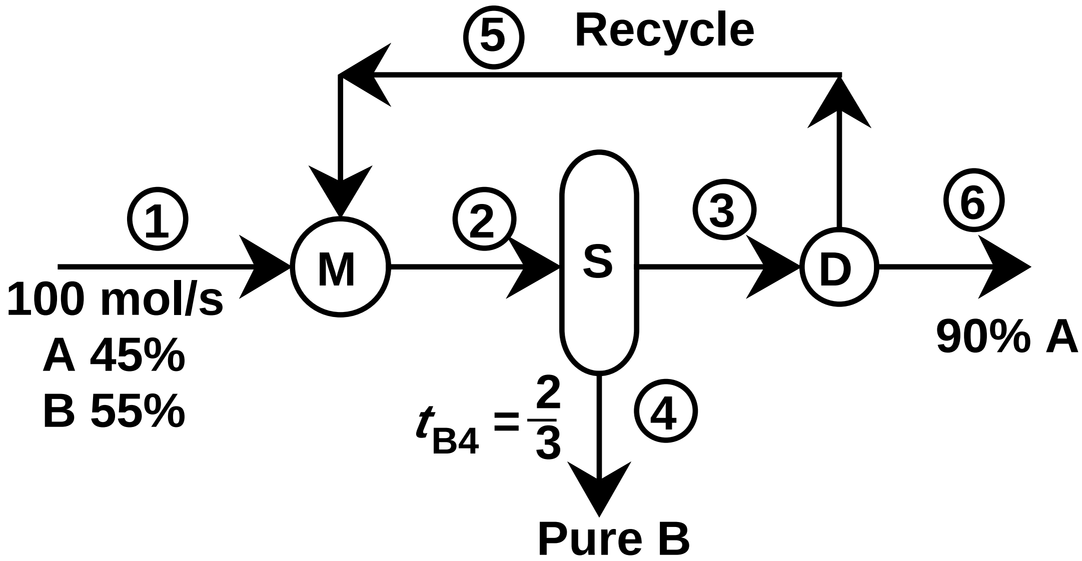
Mixer

$n_{A3} = (0.4)(200) + (0.04)(150) = 86$ lb/hr
$n_{K3} = (0.6)(200) = 120$ lb/hr
$n_{W3} = (0.96)(150) = 144$ lb/hr

Separator

$n_{A4} = (0.9)(86) = 77.4$ lb/hr
$n_{A5} = (0.1)(86) = 8.6$ lb/hr
$n_{K4} = n_{K3} = 120$ lb/hr
$n_{W5} = n_{W3} = 144$ lb/hr

Example (Steady State with Recycle



Mixer

$$n_{A2} = 45 + 0.9\, n_5 \tag{1}$$

$$n_{B2} = 55 + 0.1\, n_5 \tag{2}$$

Separator

$$n_{A3} = n_{A2} \tag{3}$$

$$n_{B3} = \frac{n_{B2}}{3} \tag{4}$$

$$n_{B4} = n_4 = \frac{2}{3} n_{B2} \tag{5}$$

Divider

$$n_{A3} = 0.9\, n_6 + 0.9\, n_5 \tag{6}$$

$$n_{B3} = 0.1\, n_6 + 0.1\, n_5 \tag{7}$$

Set of linear algebraic equations. Solve using linear algebra or substitution.

Combine (1), (3), and (6)

$$45 + 0.9\, n_5 = 0.9\, n_6 + 0.9\, n_5$$

$$\Rightarrow \; n_6 = \frac{45}{0.9} = 50 \text{ mol/s}$$

Combine (2), (4), (7)

$$55 + 0.1\, n_5 = 3\,(0.1\, n_6 + 0.1\, n_5)$$

$$= 15 + 0.3\, n_5$$

$$\Rightarrow \; n_5 = \frac{40}{0.2} = 200 \text{ mol/s}$$

Also

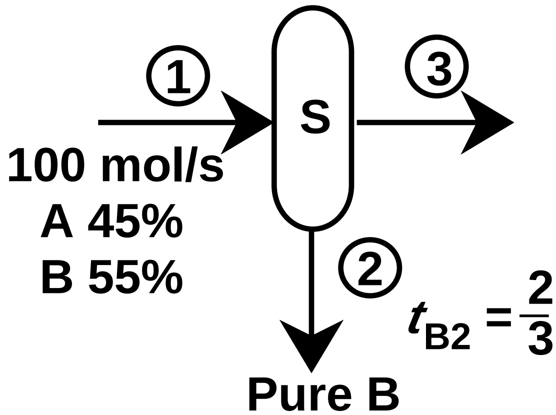
$$n_{A2} = n_{A3} = 45 + 0.9\,(200) = 225 \text{ mol/s}$$

$$n_{B2} = 55 + 0.1\,(200) = 75 \text{ mol/s}$$

$$n_{B3} = \frac{75}{3} = 25 \text{ mol/s}$$

$$n_{B4} = \frac{2}{3}(75) = 50 \text{ mol/s}$$

Note Without Recycle



$$n_{A3} = n_{A1} = 45 \text{ mol/s}$$

$$n_{B3} = \frac{n_{B1}}{3} = \frac{55}{3} = 18.3 \text{ mol/s}$$

$$x_{A3} = \frac{n_{A3}}{n_3} = \frac{45}{45 + 18.3} = 0.71 = 71\% \text{ vs. } 90\%$$