Lecture #2.1

- Chemical industries involve at least one chemical reaction
- Chemical reactions take place in a REACTOR
- Reaction, Reactors and more Reactors!

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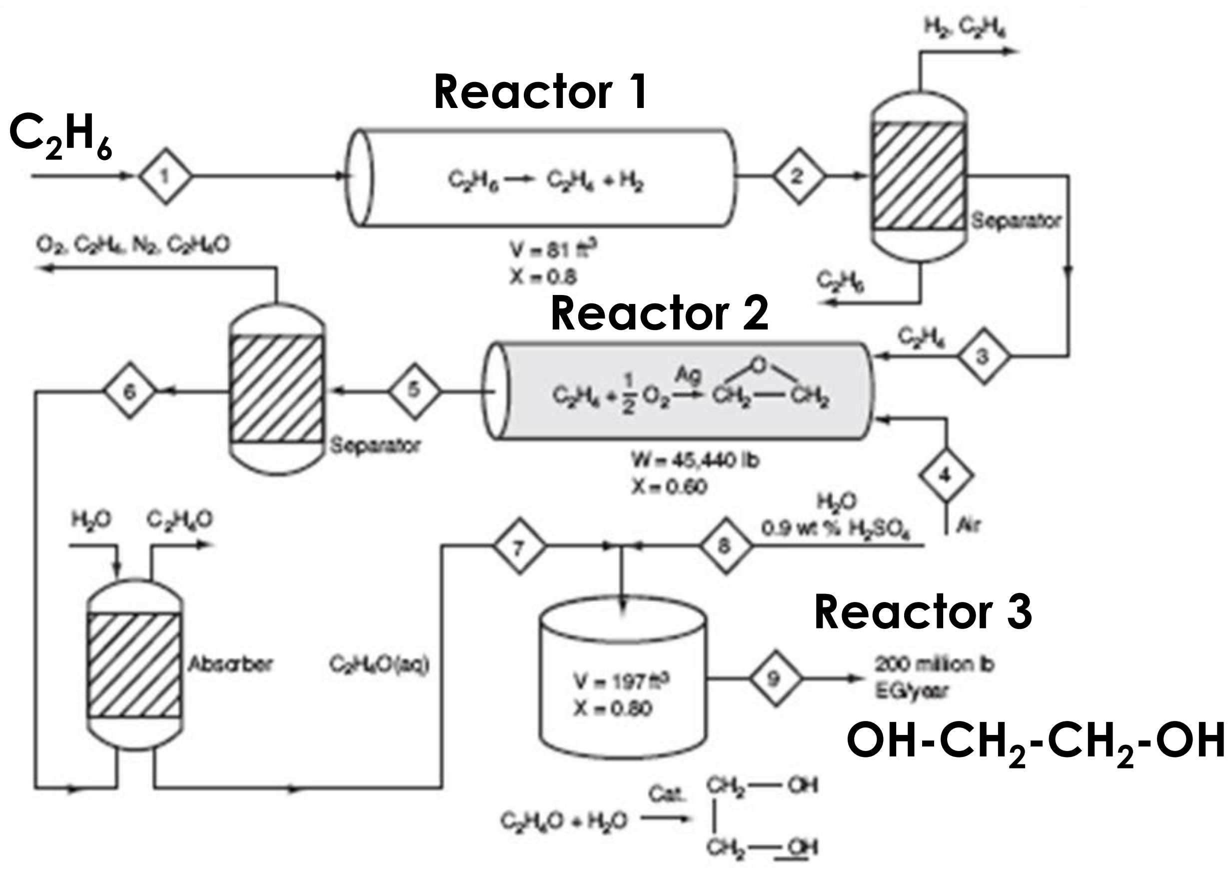


Process Flowsheet for Ethylene Glycol Manufacture

From "Elements of Chemical Reaction Engineering", 4th Editions, H.S. Fogler, For teaching purposes only.

Briefly

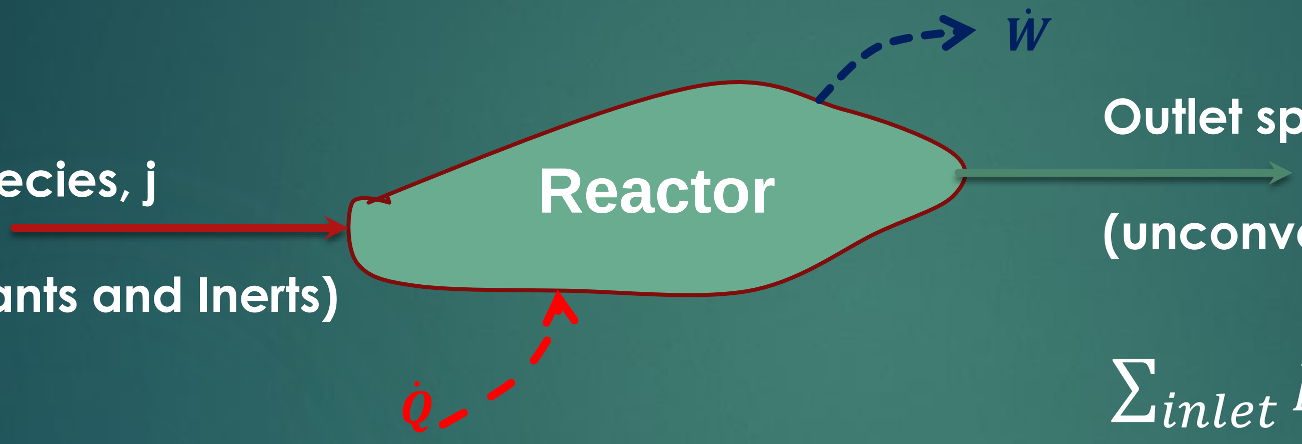
- Course policy
- Course content
- Reactions occur in primarily three ways
- Importance of Chemical Engineering Thermodynamics
- Reaction rate is independent of the reactor and is an algebraic function

ESO201A & CHE251A intro. us to mass, species, & energy balances in chemical processes

- For a control volume (Reactor) the three balances can be applied

Inlet species, j

(Reactants and Inerts)



Outlet species, j

(unconverted reactants, products and inerts)

In – Out + Generation = Accumulation

$$\sum_{inlet} \dot{M}_j - \sum_{outlet} \dot{M}_j = \frac{dM_{CV}}{dt}$$

$$\dot{M}_j \rightarrow \frac{\text{mass of species } j}{\text{time}}$$

$$(F_j)_{inlet} - (F_j)_{outlet} + G_j = \frac{d(Nj)_{CV}}{dt} \qquad F_j \rightarrow \frac{\text{moles of species 'j'}}{\text{time}} \qquad G_j \rightarrow \frac{\text{moles of 'j' generated}}{\text{time}}$$

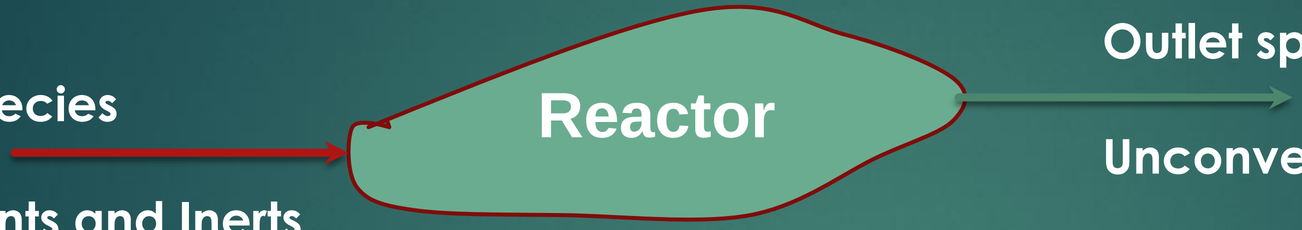
$$\sum_{inlet} \dot{E} - \sum_{outlet} \dot{E} + \dot{Q} - \dot{W} = \frac{dE_{CV}}{dt} \qquad \dot{E} \rightarrow \frac{\text{Energy (Enthalpy)}}{\text{time}} \qquad (Nj)_{CV} \rightarrow \text{moles of 'j' in CV}$$

From simple to complex for understanding

- Balance for species A (not showing heat and work)

Inlet species

Reactants and Inerts



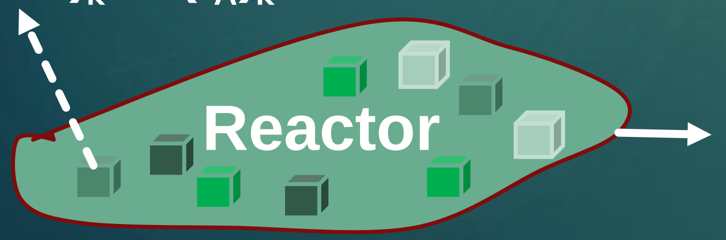
Outlet species

Unconverted reactants, products and Inerts

$$(F_A)_{inlet} - (F_A)_{outlet} + G_A = \frac{d(N_A)_{CV}}{dt} = 0 \quad \textbf{for steady state}$$

$$F_A \rightarrow \frac{moles\ of\ A}{time} \qquad G_A \rightarrow \frac{moles\ of\ A\ generated}{time} \qquad (N_A)_{CV} \rightarrow moles\ of\ A\ in\ CV$$

$(\Delta V)_k \leftrightarrow (r_A)_k$

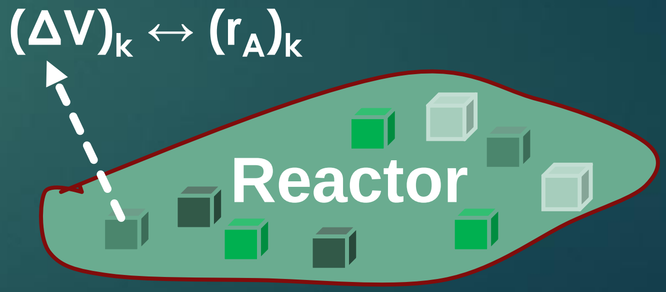


Rate of Generation, G_A, is summed over all volume elements $(\Delta V)_k$

$$\rightarrow G_A = \sum_{k=1}^{n} g_A = \sum_{k=1}^{n} (r_A)_k . (\Delta V)_k$$

Ideal reactors are defined based on variations of rates in Reactor

- For a well-mixed reactor, all $(r_A)_k$ are the same (rate of reaction is the same through out the reactor → T, P, Conc., Cat same throughout)
  - "Ideal" BATCH REACTOR and "Ideal" Continuous Stirred Tank Reactor (CSTR)
  - BATCH Reactor does not have any inlet or outlet flow and a CSTR is a ideal flow reactor
  - Then, $$G_A = \sum_{k=1}^{n} (r_A)_k . (\Delta V)_k = r_A . V$$



- Else, $$G_A = \sum_{k=1}^{n} (r_A)_k . (\Delta V)_k = \int r_A . dV$$

A general mole balance equation for species *j* in a reactor is useful for analysis

$$F_{j0} - F_j + \int r_j . dV = \frac{dN_j}{dt}$$

In – Out + Generation = Accumulation ← for species j

where, F_{j0} → inlet molar flow rate of *j*, $\frac{moles\ of\ j}{time}$

F_j → outlet molar flow rate of *j*, $\frac{moles\ of\ j}{time}$

r_j → rate of formation of *j* (applicable if *j* is reactant or product), $\frac{moles\ of\ j\ formed}{volume.time}$

N_j → moles of A in Reactor at time '*t*', $moles\ of\ j$

- **The general mole balance eq^n can be applied to different Reactors**

Batch Reactor (BR) is a closed system

Batch Reactors used for

- Testing new process that are under R&D
- Manufacture of expensive products
- Processes difficult to make continuous (Biochemical reactions, pharmaceuticals, paints, some polymerization reactions)

- Disadvantages
  - High labor
  - Variability of product
  - Difficulty for large scale operation
- Semi-batch used for gas-liquid reactions

Mole balance for species *j*

$$F_{j0} - F_j + \int r_j . dV = \frac{dN_j}{dt}$$

$$F_{j0} = 0 = F_j$$

Well-mixed $\rightarrow \int r_j . dV = r_j . V$

V is the volume of the **BR**, which may or may not change with ***t***

Thus, the **design eq^n** is

$$\boxed{\frac{dN_j}{dt} = r_j . V}$$

For semi batch reactor

$$F_{j0} \ or \ F_j \neq 0$$

Time taken to achieve a certain amount of product can be determined

- Design equation can be integrated $$\frac{dN_j}{dt} = r_j.V$$

- With $N_j = N_{j0}$ at $t = 0$ and $N_j = N_{j\_required}$ at $t = t_{required}$

- $$t_{required} = \int_{N_{j0}}^{N_{j\_required}} \frac{dN_j}{r_j.V}$$

- This is the time required to change the number of moles of ***j*** from $\boldsymbol{N_{j0}}$ to $\boldsymbol{N_{j\_required}}$

- NOTE: we have assumed $V \neq f(t)$