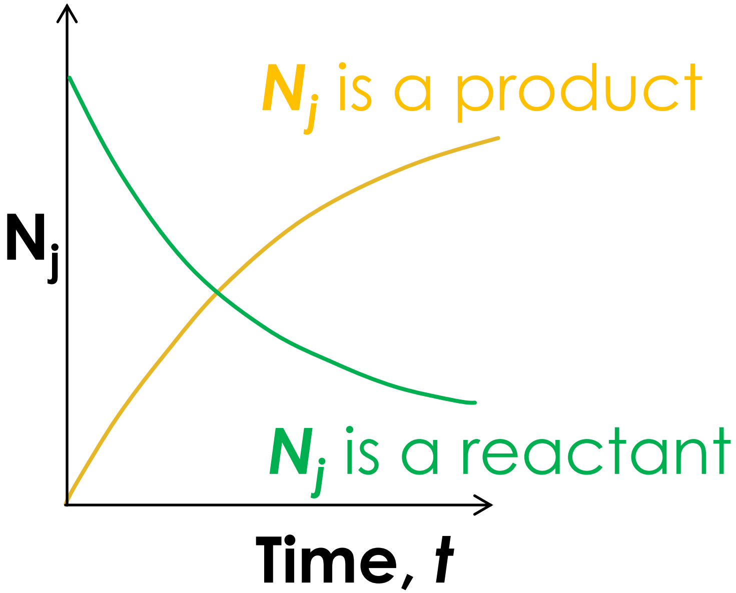
Build and Analyze reactors

$$(F_A)_{inlet} - (F_A)_{outlet} + G_A = \frac{d(N_A)_{CV}}{dt}$$

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



Lecture #2.2

- Mole balance of species j
- G_j term is important and is depends on the type of Reactor
- Mole balance equation applied to a BATCH REACTOR
- Apply mole balance to other type of reactors

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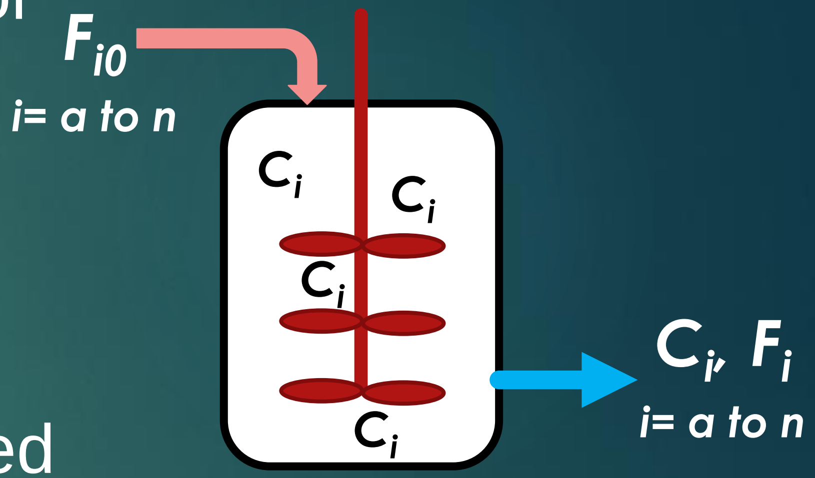
Mole balance equation can also be applied to flow reactors

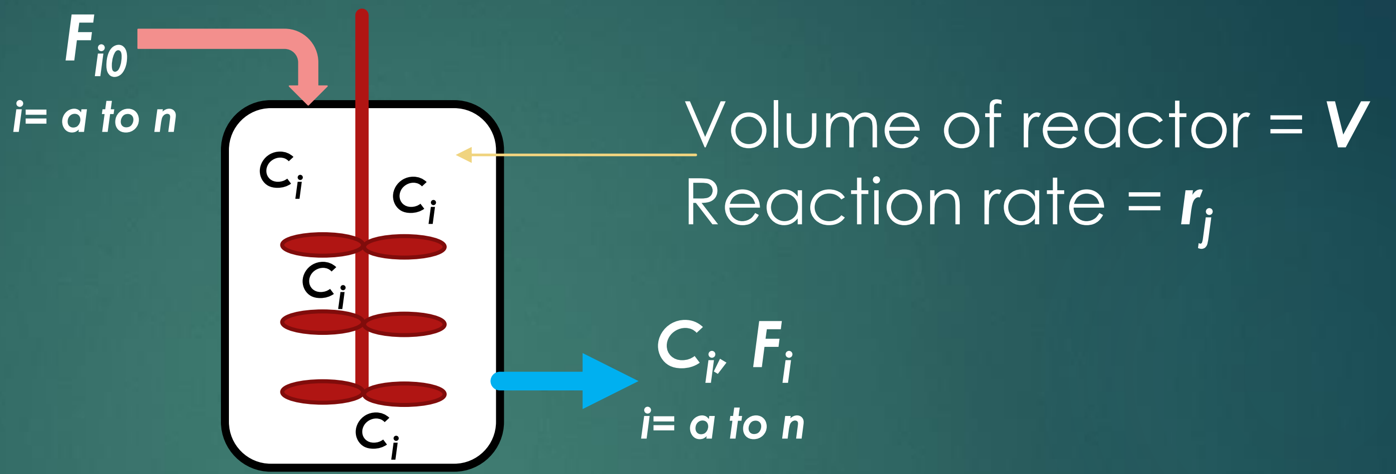
- Three types of “ideal” flow reactors are analyzed in the beginning
  - Continuous stirred tank reactor (CSTR)
  - Plug flow reactor (PFR)
  - Packed bed reactor (PBR)
- These ideal reactors are defined based on the flow properties inside the reactor
- CSTRs are assumed to be well-mixed, similar to BR
  - T, P and C_j are same everywhere in the tank and at the exit
- PFRs and PBRs have the concentration, $\boldsymbol{C_j}$, vary axially not radially

Continuous Stirred Tank Reactor (CSTR) used for continuous operations

- Also called Vat or Back-mixed or well-mixed reactor
- Often used for liquid phase reactions
- Normally operated at steady state
- Idealized CSTRs are assumed to be perfectly mixed
    - Temperature and concentrations same everywhere in the tank and at the exit
- Non ideal systems discussed later
- Relatively easy to maintain and good temperature control



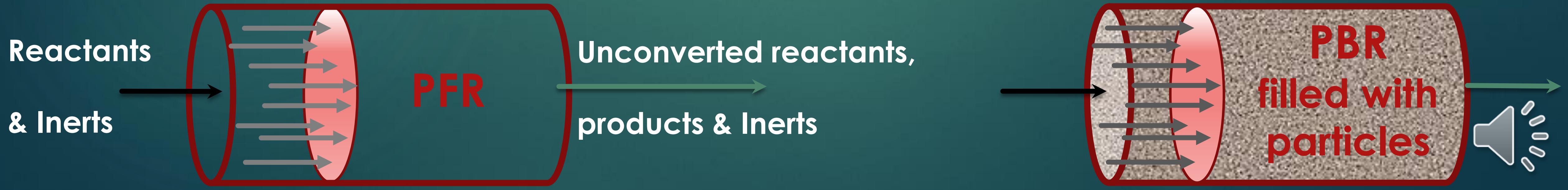
Mole balance for CSTR results in an algebraic expressions



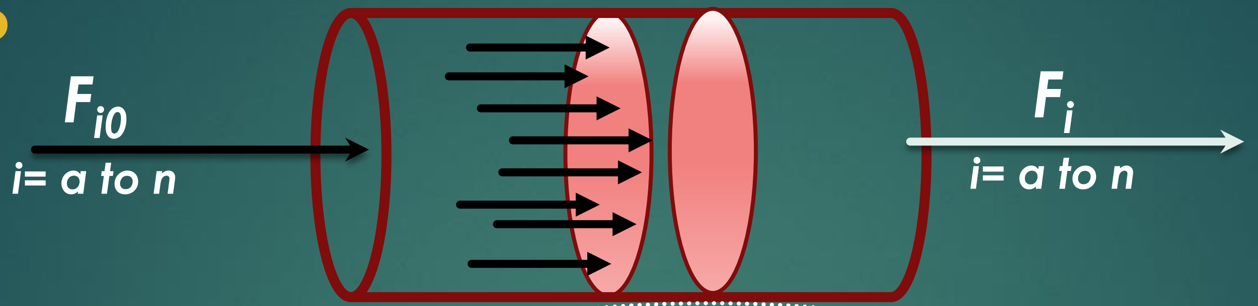
- Mole balance equation for j: $F_{j0} - F_j + \int r_j . dV = \frac{dN_j}{dt}$ = 0 at steady state
- Well-mixed: $\int r_j . dV = r_j . V$
- Therefore, the design eq^n is $$\boxed{V = \frac{F_{j0} - F_j}{-r_j}}$$
- ***V*** is the volume required to decrease molar flowrate of ***j*** from F_{j0} to F_j

PFRs and PBRs (idealized axial concentration gradients) have a variety of uses

- Flow is like a plug without radial variations → axial changes only
- Used mostly for gas-phase reactions
  - Difficult to control temperature (hot spot formation)
- PBR are used for heterogeneous catalytic reactions
  - Reaction rate based on mass of catalyst
  - Channeling/bypass (non-ideality) sometimes occurs



Mole balance for PFR/PBR results in differential equations



$(F_j)_V$ $(F_j)_{V+\Delta V}$ For PBR also $\Delta V \rightarrow \Delta W$ $(F_j)_W$ $(F_j)_{W+\Delta W}$

r_j r'_j

- At steady state: $\frac{dN_i}{dt} = 0$
- Mole balance for species ***j*** across **ΔV**: $(F_j)_V - (F_j)_{V+\Delta V} + r_j . \Delta V = 0$
- Taking the limits ***ΔV*** $\rightarrow$ **0** and doing the necessary changes
- The design eqn for PFR is: $\boldsymbol{\frac{dF_j}{dV} = r_j}$ and $\boldsymbol{V = \int_{F_{j0}}^{F_j} \frac{dF_i}{r_j}}$
- For PBR (we deal with ***W*** and ***W+ΔW***): $\boldsymbol{\frac{dF_j}{dW} = r'_j}$ and $\boldsymbol{W = \int_{F_{j0}}^{F_j} \frac{dF_i}{r'_j}}$

Design equations of PFR/PBR can be integrated to find *V* or *W*

- For PFR, $\frac{dF_j}{dV} = r_j$ can be integrated → $V = \int_{F_{j0}}^{F_j} \frac{dF_j}{r_j}$
- Where ***V*** is the volume required to decrease the molar flowrate from F_{j0} to F_j
- Similarly, for PBR $\frac{dF_j}{dW} = r'_j \rightarrow W = \int_{F_{j0}}^{F_j} \frac{dF_j}{r'_j}$
- Where ***W*** is the weight required to decrease the molar flowrate from F_{j0} to F_j