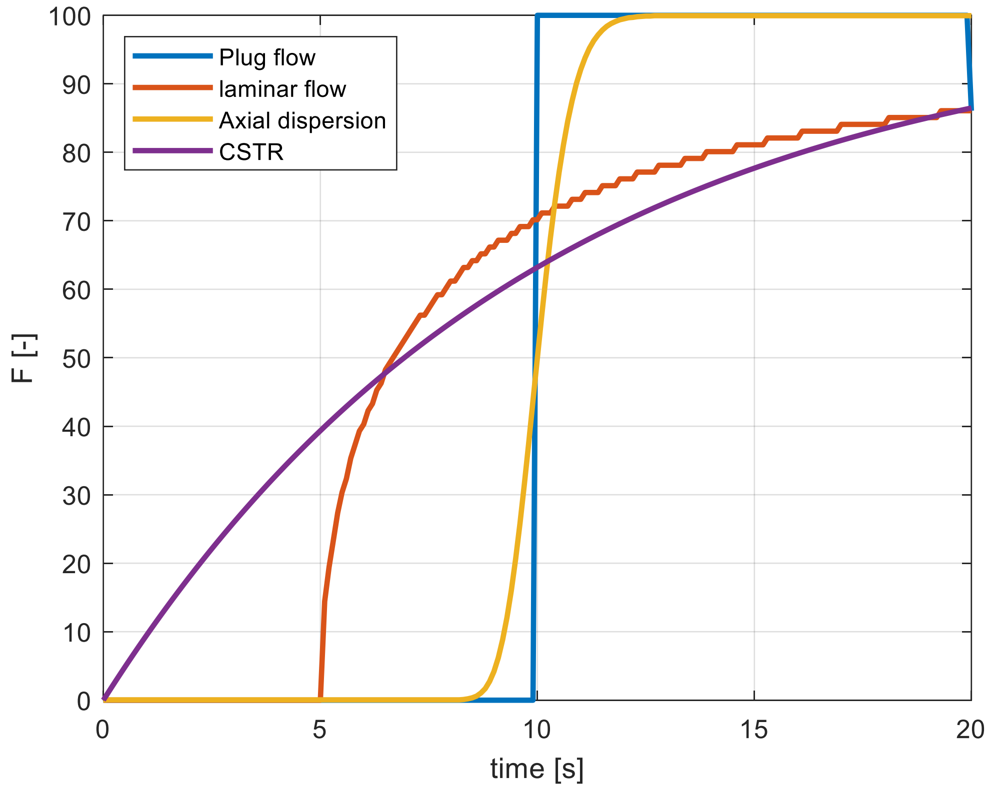
3. Mole balance

3.1 Flow patterns

F curves show how many particle have cumulatively left the reactor



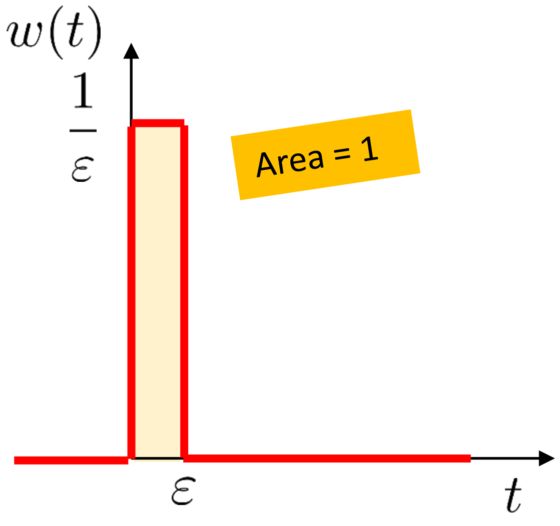
3. Mole balance

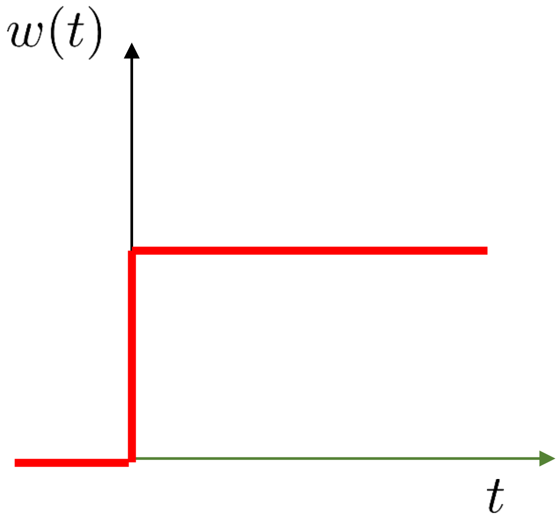
3.1 Flow patterns

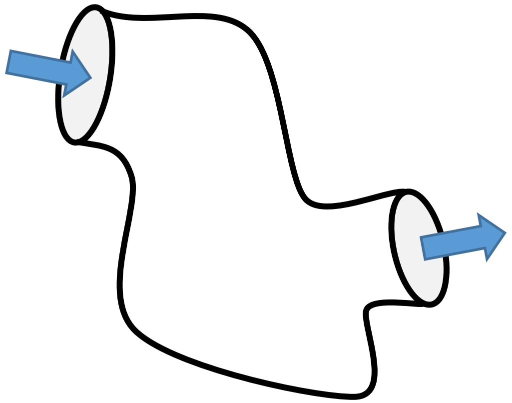
$$E(t) = \frac{dF(t)}{dt}$$

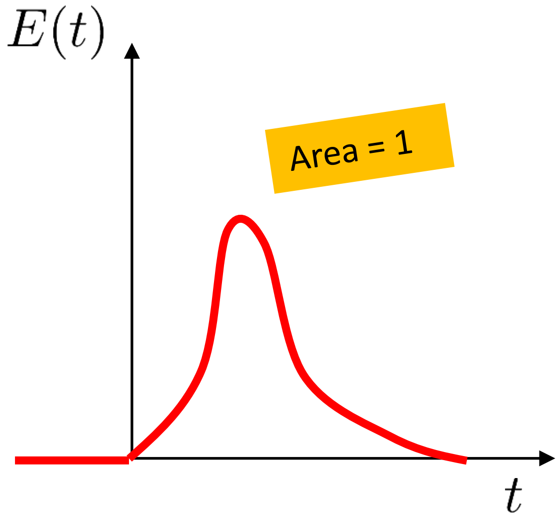
$$F(t) = \int_0^t E(t)dt$$

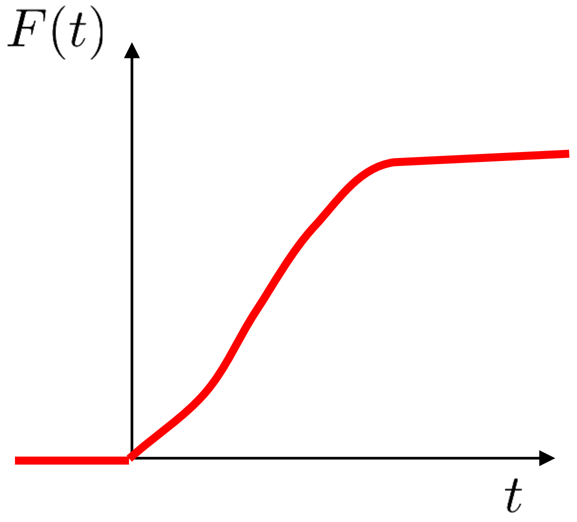
$$\int_0^\infty E(t)dt = 1$$







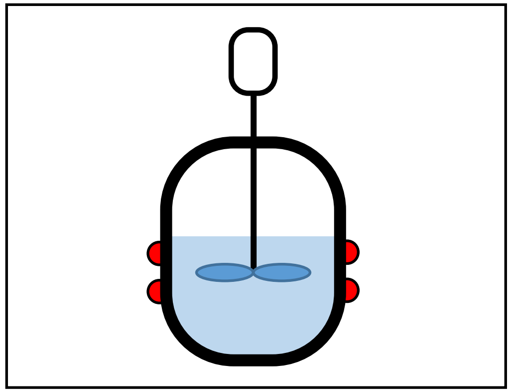




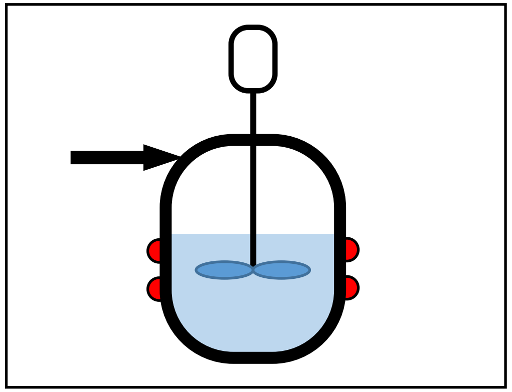
$$F(\infty) = 1$$

3. Mole balance

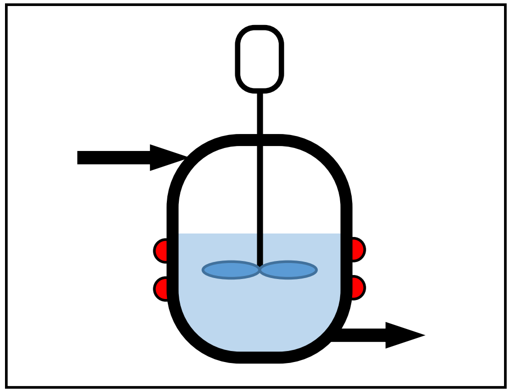
3.2 Ideal chemical reactors



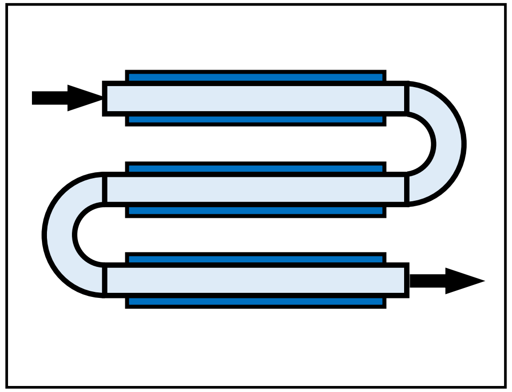
Batch Reactor (BR)



Semi Batch Reactor (SBR) or Fed Batch Reactor



Continuous Stirred Tank Reactor (CSTR) or Chemostat

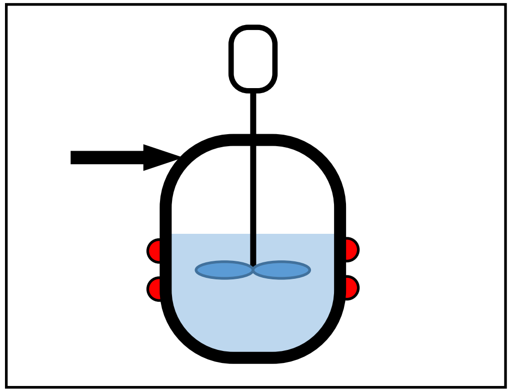


Plug Flow Reactor (PFR)

3. Mole balance

3.2 Ideal chemical reactors

Batch Reactor (BR)



Semi Batch Reactor (SBR) or Fed Batch Reactor

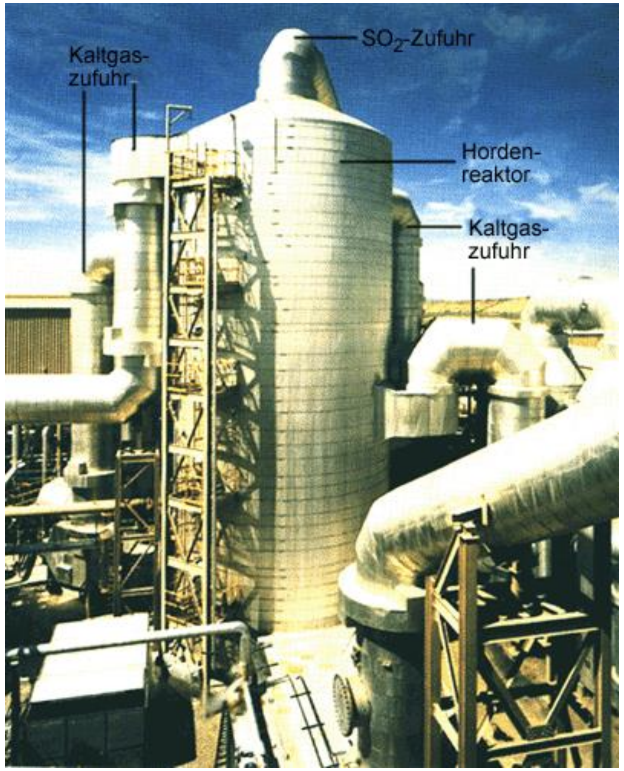
Continuous Stirred Tank Reactor (CSTR) or Chemostat

Plug Flow Reactor (PFR)

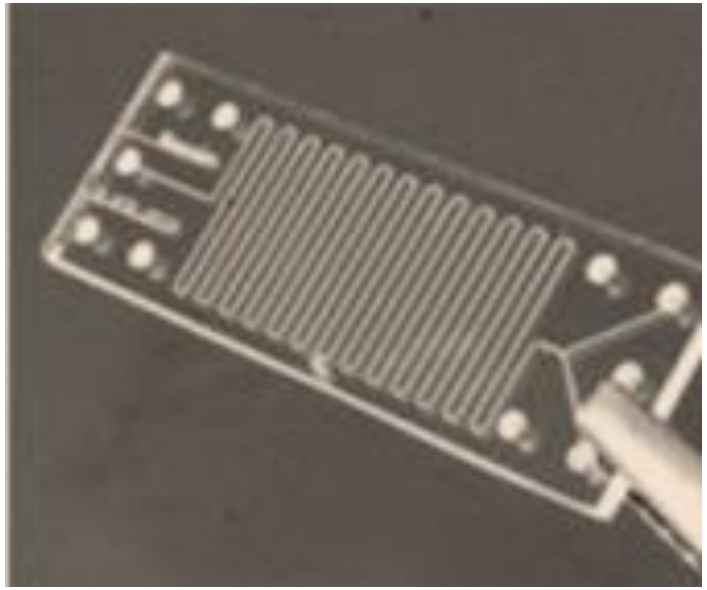
3. Mole balance

3.3 Real chemical reactors

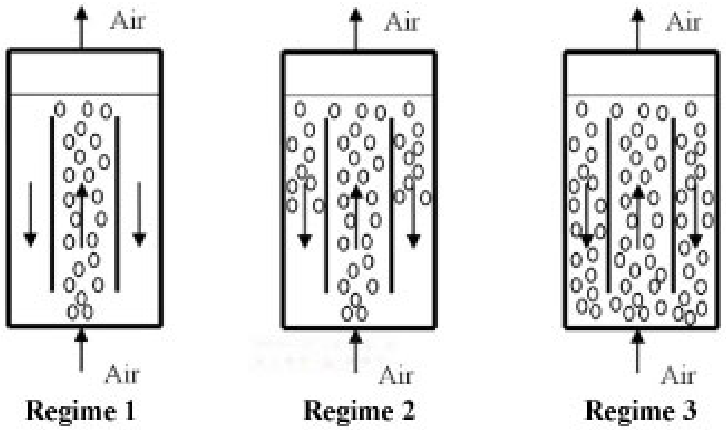
… might be very large



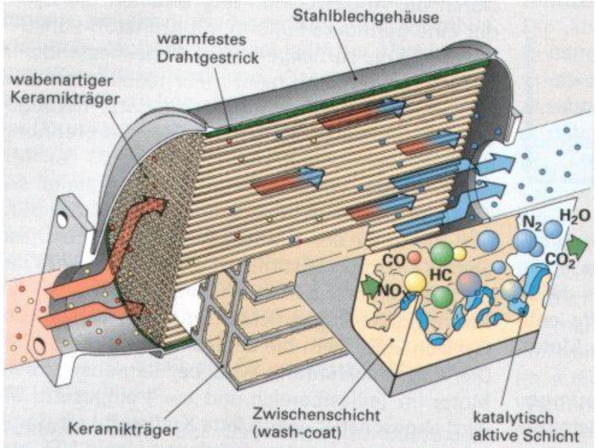
… or very small



… or involve multiple phases



G/L

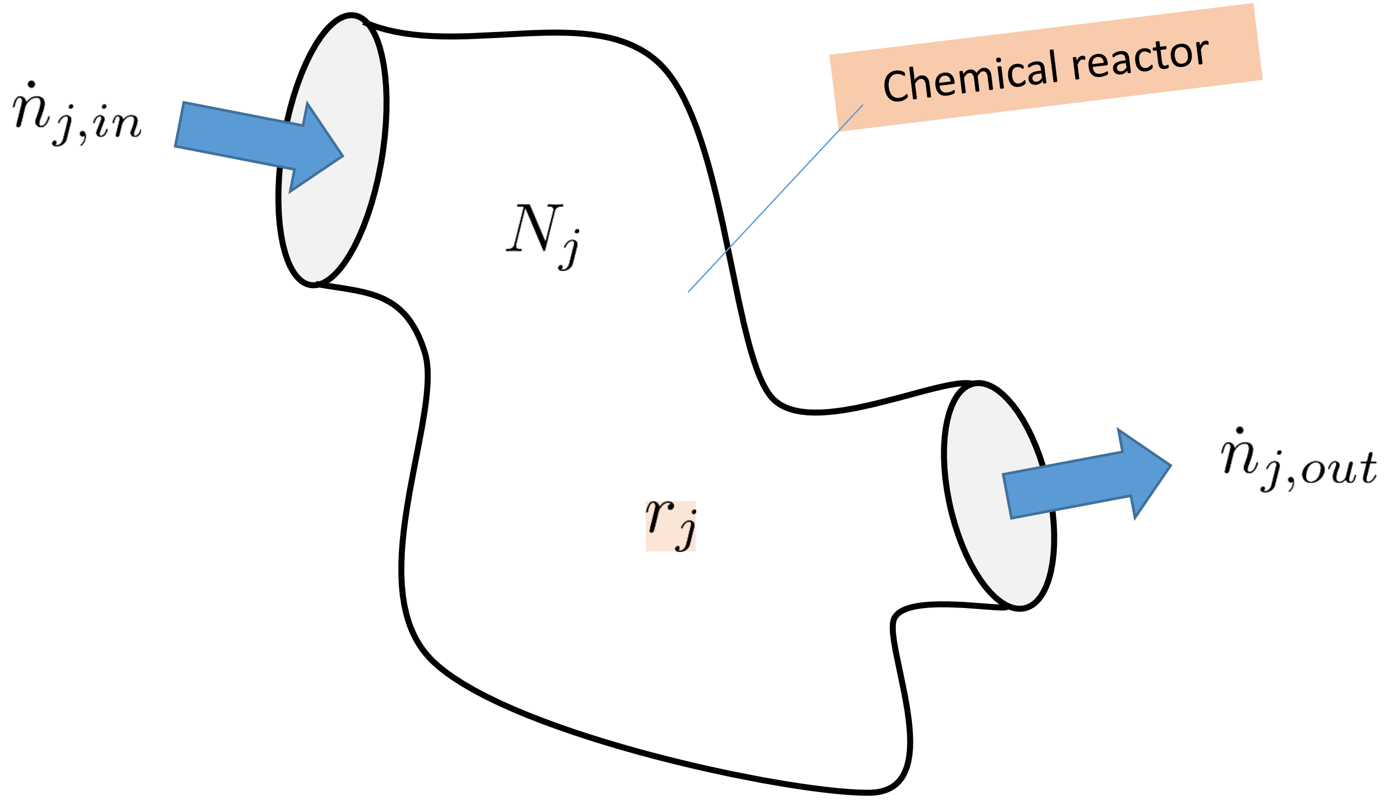


G/S

L/"S"

3. Mole balance

3.4 General mole balance

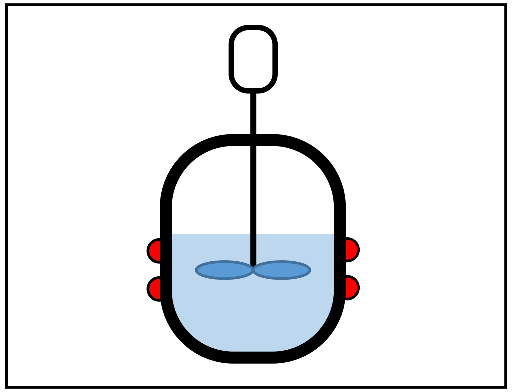


$$\frac{dN_j}{dt} = \dot{n}_{j,in} - \dot{n}_{j,out} + \int_V r_j \cdot dV$$

Change | Inflow / Outflow | Reaction

3. Mole balance

3.5 BR



Batch Reactor (BR)

Application

- for small-scale operation
- for testing new products
- for the manufacture of expensive products
- for processes that are difficult in continuous operation

Advantages

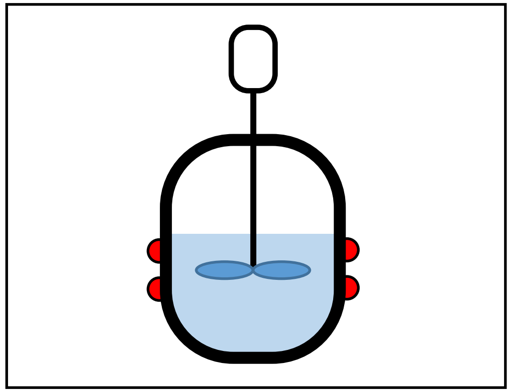
+ high conversions (long periods of time)
+ Versatile
+ Easy to clean

Disadvantages

- high labour costs per batch
- variability of products from batch to batch
- large scale production not feasible
- Long cleaning times (no production)

3. Mole balance

3.5 BR



Batch Reactor (BR)

General Mole Balance

$$\frac{dN_j}{dt} = \cancel{\dot{n}_{j,in}} - \cancel{\dot{n}_{j,out}} + \int_V r_j \cdot dV$$

$$\Rightarrow \quad \frac{dN_j}{dt} = + \int_V r_j \cdot dV$$

Assumption: Perfectly mixed, because of stirrer.

$$\Rightarrow \quad \boxed{\frac{dN_j}{dt} = r_j V}$$

Design Equation for BR (differential form)

3. Mole balance

3.5 BR

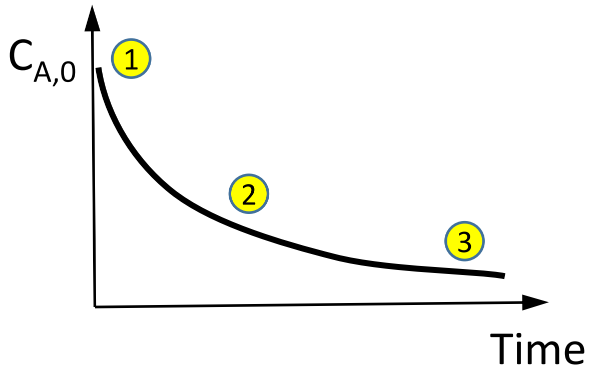
$$\frac{dN_A}{dt} = r_A \cdot V$$

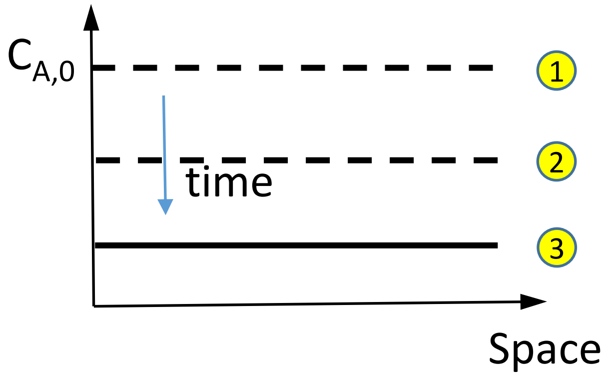
$$\Leftrightarrow \quad \frac{dN_A}{r_A \cdot V} = dt$$

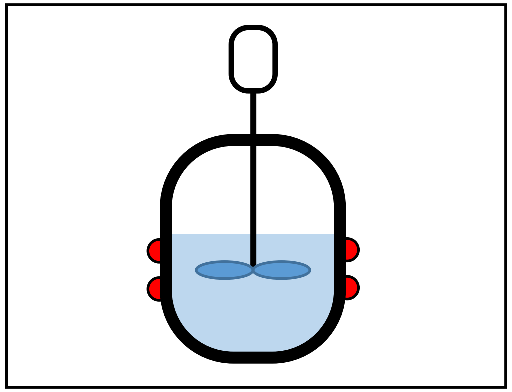
$$\Leftrightarrow \quad \int_{N_{A0}}^{N_{A1}} \frac{dN_A}{r_A \cdot V} = \int_0^{t_1} dt$$

$$\Leftrightarrow \quad \boxed{t_1 = \int_{N_{A0}}^{N_{A1}} \frac{dN_A}{r_A \cdot V}}$$

Design Equation for BR
(integral form)



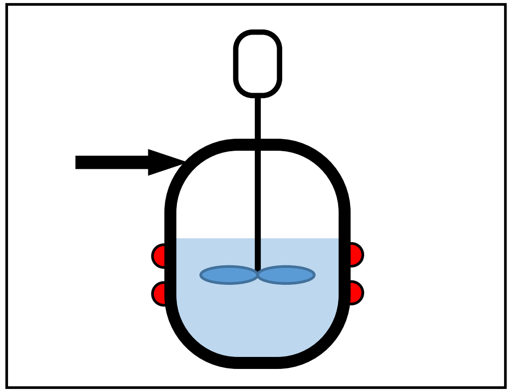




Batch Reactor
(BR)

3. Mole balance

3.6 SBR



Semi Batch Reactor (SBR) or Fed Batch Reactor

$$\frac{dN_j}{dt} = \dot{n}_{j,in} - \cancel{\dot{n}_{j,out}} + \int_V r_j \cdot dV$$

$$\Rightarrow \frac{dN_j}{dt} = \dot{n}_{j,in} + \int_V r_j \cdot dV$$

Assumption: Perfectly mixed, because of stirrer.

$$\Rightarrow \boxed{\frac{dN_j}{dt} = \dot{n}_{j,in} + r_j V}$$

Design Equation for SBR (differential form)

3. Mole balance

3.7 CSTR

Application

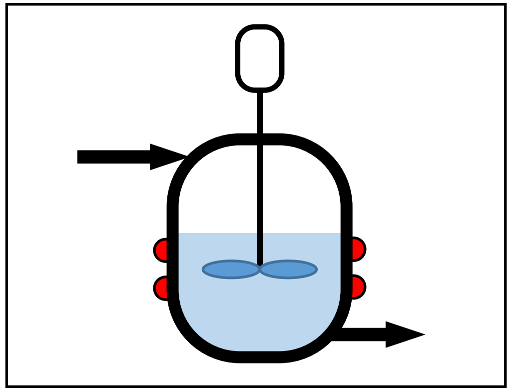
- Commonly used in industrial processes
- Used primarily for liquid phase reactions.

Advantages

\+ Good temperature control is easily maintained
\+ Cost effective construction
\+ Large capacity
\+ Interior of reactor is easily accessed

Disadvantages

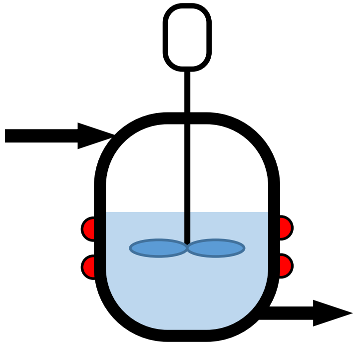
\- Conversion of reactant to product per volume is small compared to other flow reactors



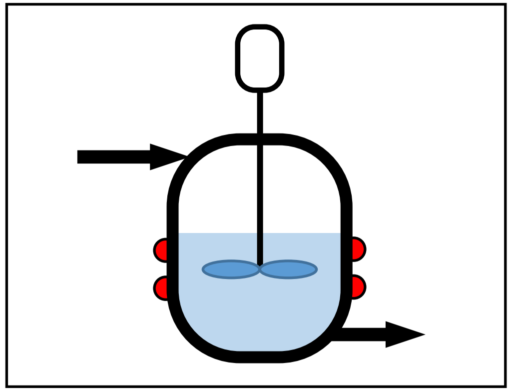
Continuous Stirred Tank Reactor (CSTR) or Chemostat

3. Mole balance

3.7 CSTR



Conditions in the exit stream (e.g. conc. & temp.) are identical to those in the tank!



Continuous Stirred Tank Reactor (CSTR) or Chemostat

$$\frac{dN_j}{dt} = \dot{n}_{j,in} - \dot{n}_{j,out} + G_j$$

Assumptions:

- Steady state &
- perfectly mixed

$$\Longrightarrow \qquad 0 = \dot{n}_{j,in} - \dot{n}_{j,out} + r_j V$$

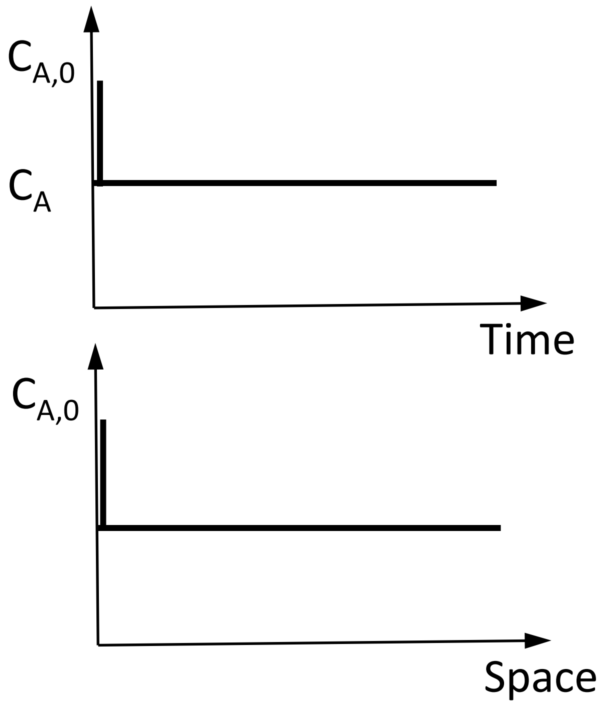
3. Mole balance

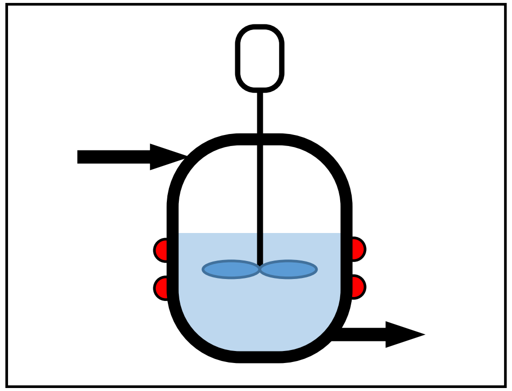
3.7 CSTR

$$0 = \dot{n}_{j,in} - \dot{n}_{j,out} + r_j V$$

$$\Leftrightarrow \quad \boxed{V = \frac{\dot{n}_{j,in} - \dot{n}_{j,out}}{-r_j}}$$

Design Equation for CSTR (algebraic form)





Continuous Stirred Tank Reactor (CSTR) or Chemostat

Molar flow rate

$$\dot{n}_j = C_j \, \dot{V} \qquad \left[\frac{mol}{s} = \frac{mol}{m^3}\frac{m^3}{s}\right]$$

Concentration *Volumetric flow*

$$\Rightarrow \quad \boxed{V = \frac{C_{j,in}\dot{V}_{in} - C_{j,out}\dot{V}_{out}}{-r_j}}$$

3. Mole balance

3.7 CSTR

Graphical solution

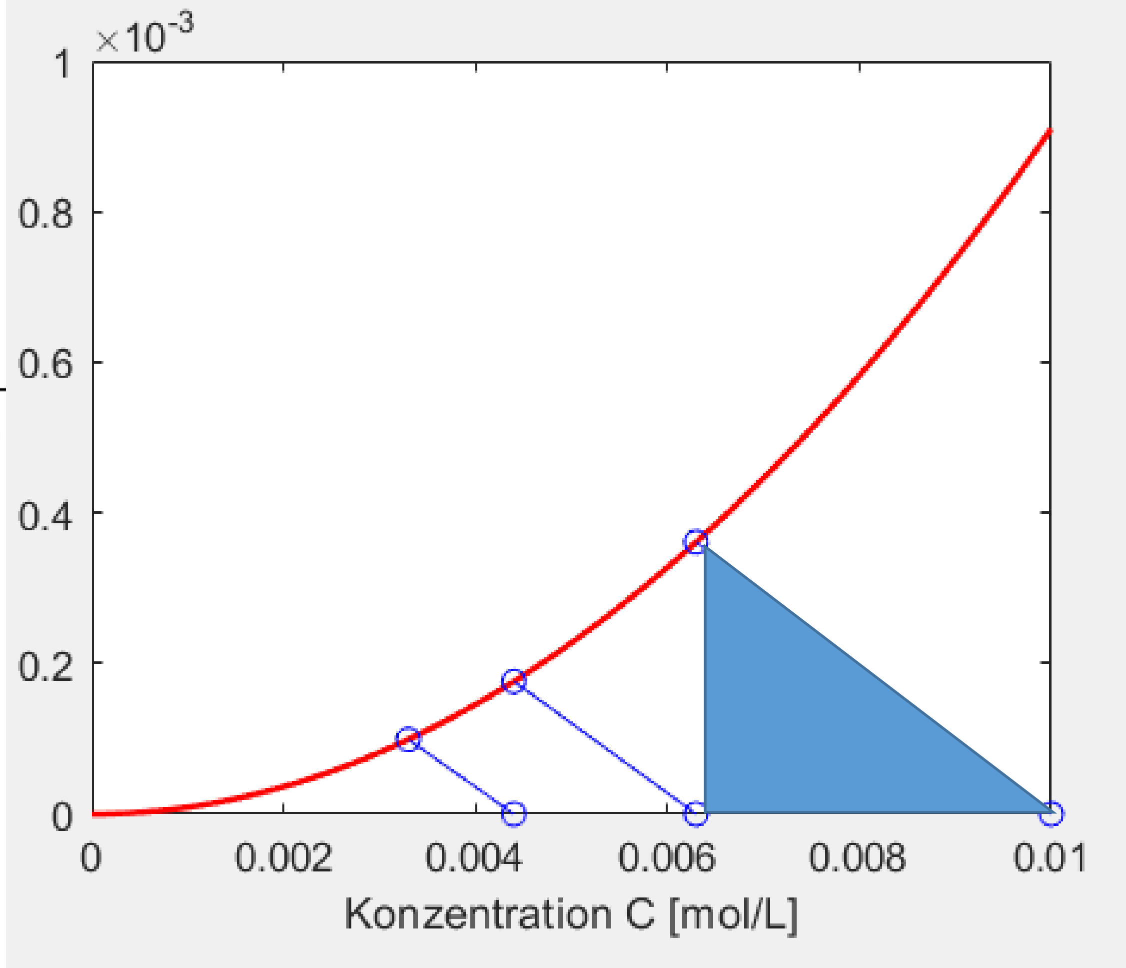
$$V = \frac{\dot{V}(C_{j,in} - C_{j,out})}{-r_j}$$

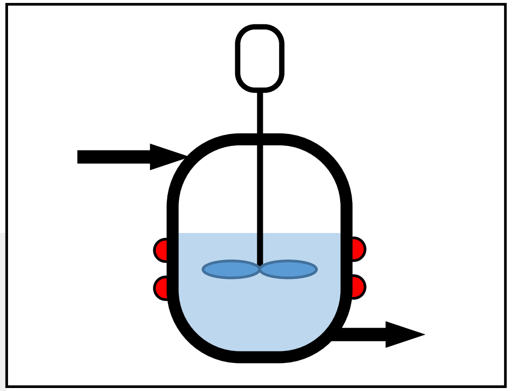
$$-\frac{\dot{V}}{V} = -\frac{1}{\tau} = \frac{r_j}{(C_{j,in} - C_{j,out})}$$

Slope

$$r_j \qquad \frac{1}{\tau}$$

$$C_{j,out} - C_{j,in}$$

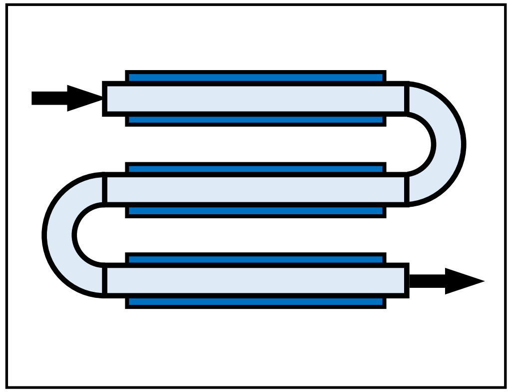




Continuous Stirred Tank Reactor (CSTR) or Chemostat

3. Mole balance

3.8 PFR



Plug Flow Reactor (PFR)

- Another type of reactor commonly used in industry is the tubular reactor.
- Tubular reactors are used most often for gas-phase reactions.

Advantages

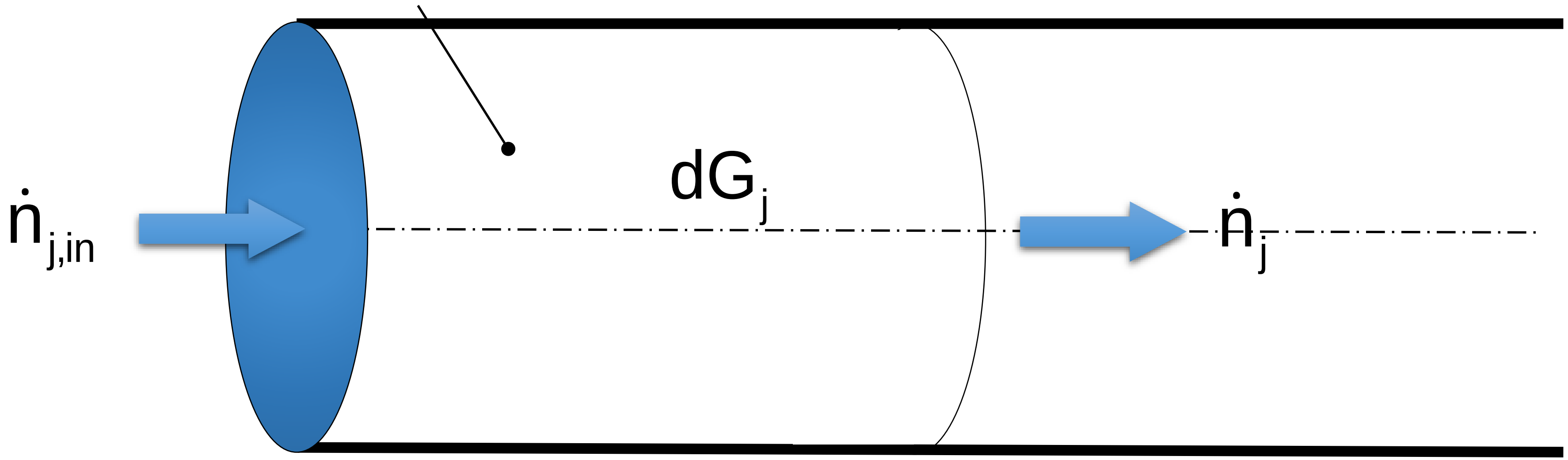
+ Simple maintenance
+ High conversion rate per reactor volume.
+ Mechanically simple
+ Unvarying product quality
+ Good for studying rapid reactions
+ Efficient use of reactor volume
+ Large capacity processing

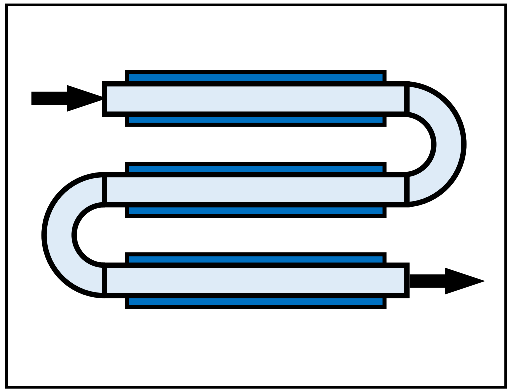
Disadvantages

- Difficult temperature control
- Exothermic reactions may lead to hot spots
- Difficult controlling due to temperature and composition variations

3. Mole balance

3.8 PFR





Plug Flow Reactor (PFR)

$$\frac{dN_j}{dt} = \dot{n}_{j,in} - \dot{n}_j + \int_V r_j \cdot dV$$

$$0 = \frac{d}{dV}(\dot{n}_{j,in} - \dot{n}_j) + \frac{d}{dV}\int_V r_j \cdot dV$$

Design Equation for PFR (differential form)

$$\boxed{\frac{d\dot{n}_j}{dV} = r_j}$$

3. Mole balance

3.8 PFR

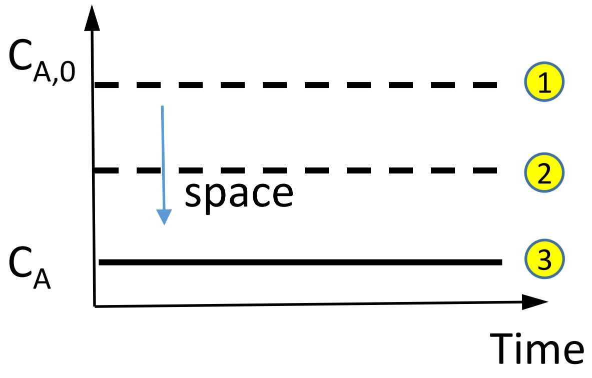
$$\frac{d\dot{n}_A}{dV} = r_A$$

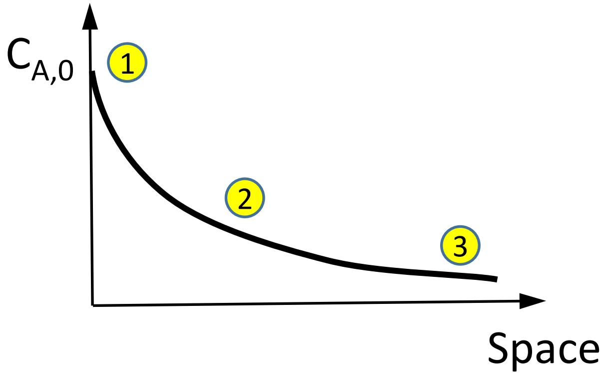
$$\frac{d\dot{n}_A}{r_A} = dV$$

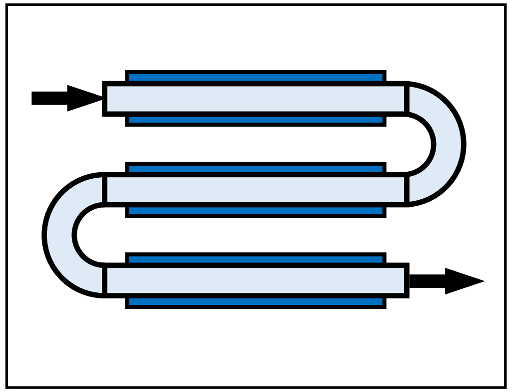
$$\int_0^{V_1} dV = \int_{\dot{n}_{A,0}}^{\dot{n}_{A,1}} \frac{d\dot{n}_A}{r_A}$$

$$\boxed{V_1 = \int_{\dot{n}_{A,0}}^{\dot{n}_{A,1}} \frac{d\dot{n}_A}{r_A}}$$

Design Equation for PFR (integral form)





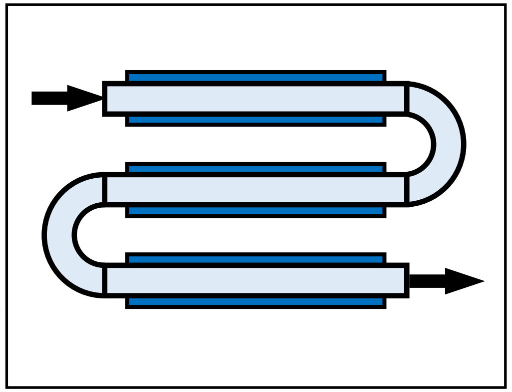


Plug Flow Reactor (PFR)

3. Mole balance

3.8 PFR

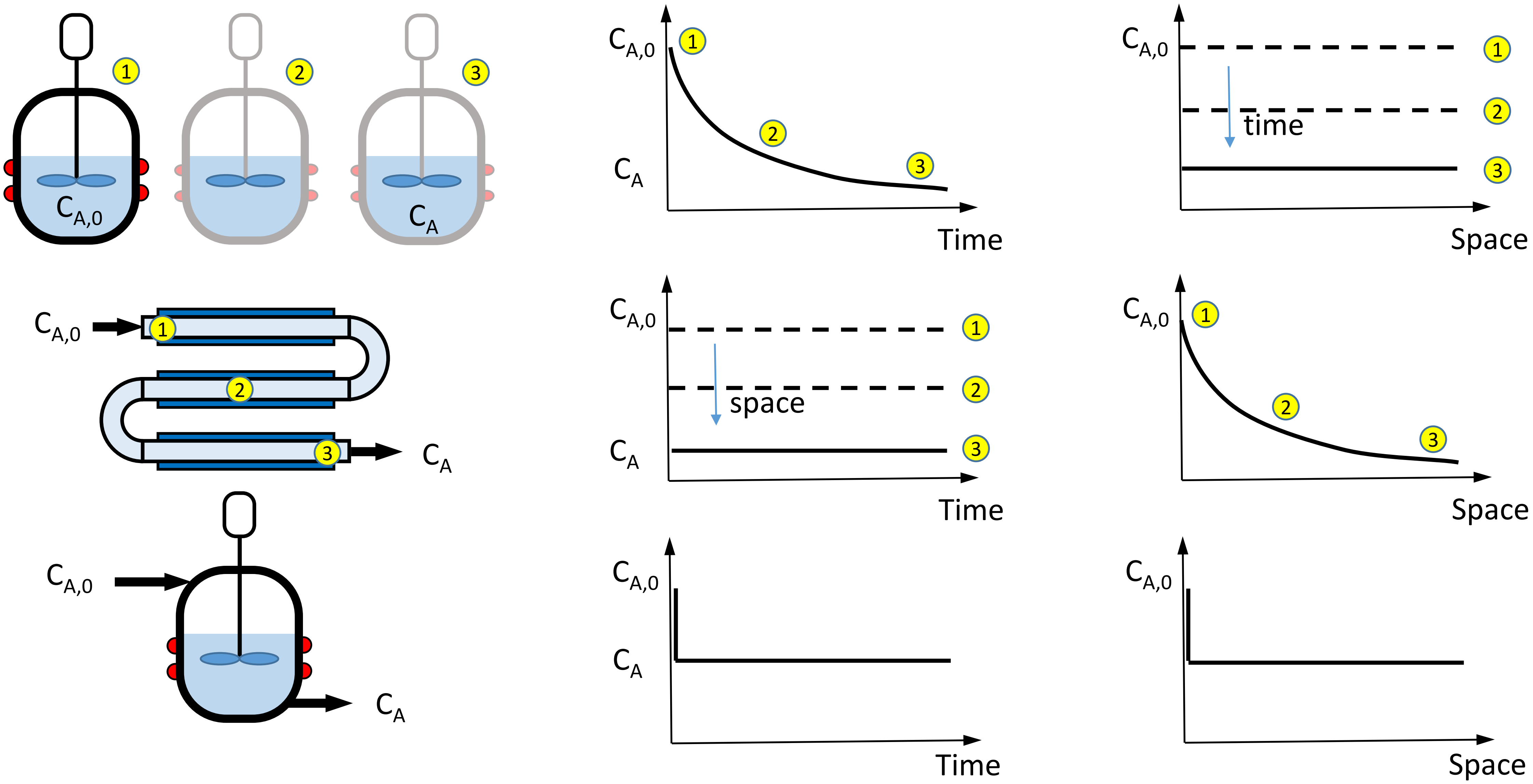
https://youtu.be/MgKWshe6YaU



Plug Flow Reactor (PFR)

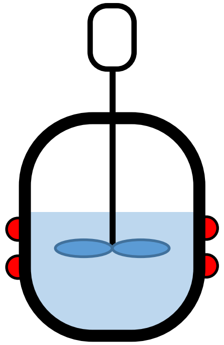
3. Mole balance

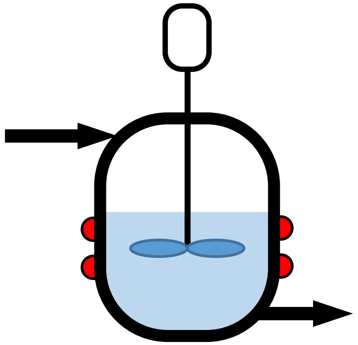
3.9 Space and time dependence



3. Mole balance

3.10 Design equations





Reactor	Differential form	Algebraic form	Integral form
BR	$\frac{dN_j}{dt} = r_j \cdot V$	-	$t = \int_{N_{A1}}^{N_{A0}} \frac{dN_A}{-r_A V}$
PFR	$\frac{d\dot{n}_j}{dV} = r_j$	-	$V = \int_{\dot{n}_{A1}}^{\dot{n}_{A0}} \frac{d\dot{n}_A}{-r_A}$
CSTR	-	$V = \frac{\dot{n}_{j0} - \dot{n}_j}{-r_j}$	-

3. Mole balance

Comprehension questions

1. Explain the four terms in a general mole balance!
2. What means continuous and discontinuous w.r.t. operation on an ideal reactor?
3. What means perfectly mixed? How does the generation term simplify under this condition?
4. Which reactor do you suggest for a fast reaction?
5. Which reactor do you suggest for a gas phase reaction?
6. For some reactors the temperature is hard to control? Discuss if a CSTR or PFR tend to hot spots for exothermic reactions.
7. Why is a PFR mechanically simpler?
8. Which reactors lead to high cleaning costs and downtime?
9. A PFR and a PBR are very similar. What is the main difference?