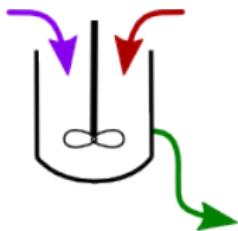


Introduction to Reactor Design

ChE 3K4



Kevin Dunn, 2013

kevin.dunn@mcmaster.ca

<http://learnche.mcmaster.ca/3K4>

Slide credits and notes

- ▶ These slides were created by Dr. Mhaskar.
- ▶ Minor modifications/additions by Kevin Dunn.

- ▶ Words in **purple** are definitions
- ▶ Words in **this colour** are hyperlinks
- ▶ Other colours are to emphasize points

- ▶ Version numbering: first page shows an integer version number, and refers to each revision; also includes the month and year for reference.
- ▶ File names: 2013-3K4-class-01B.pdf implies today, which is week 1 of the term, second class (1A, 1B, 1C, 2A, 2B etc)
- ▶ Also used on course website

What we are going to learn here

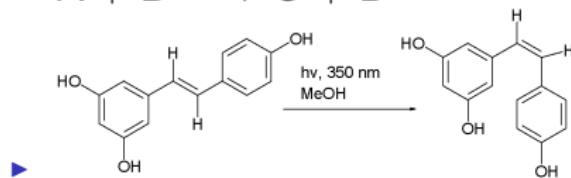
Review of chemistry and chemical engineering topics

- ▶ Rate of reaction
- ▶ Mole balances
- ▶ Batch reactors
- ▶ Continuous Tank Reactors (CSTRs)
- ▶ Tubular reactors
- ▶ Packed-bed reactors

Rate of reaction

- ▶ Chemical reactions are said to occur when species lose their identity, e.g. by decomposition, combination or isomerization.

- ▶ $A \rightarrow B + C$
- ▶ $A + B \rightarrow C + D$



[<http://en.wikipedia.org/wiki/Isomerization>]

- ▶ Rate of reaction is expressed as the rate of formation of products.

Rate of reaction

By definition:

r_j is defined as the rate of formation
of species j per unit volume

- ▶ formation \equiv generation
- ▶ Consider the reaction



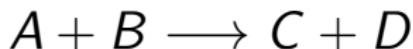
- ▶ r_A is the number of moles of species A **formed** per unit time per unit volume $\left[\frac{\text{mol}}{\text{s.L}} \right]$ or $\left[\frac{\text{mol}}{\text{s.m}^3} \right]$
- ▶ $r_A < 0$ in this case; yes, the sign is important for reaction rates

Rate of reaction

By definition:

r_j is defined as the rate of formation
of species j per unit volume

- disappeared \equiv consumed
- Consider the reaction



- $-r_A$ (now a positive quantity) is the number of moles of species A **disappearing** per unit time per unit volume $\left[\frac{\text{mol}}{\text{s.L}} \right]$ or $\left[\frac{\text{mol}}{\text{s.m}^3} \right]$
- $-r_A > 0$ in this case

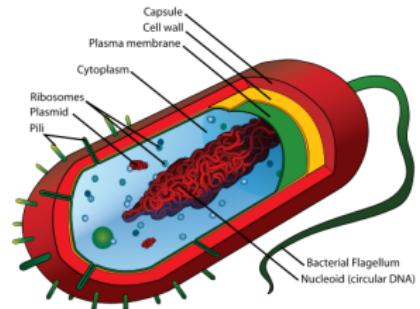
What affects $-r_A$?

- ▶ Reaction rate is an *intensive property* – function of concentration and temperature, but not size or configuration of reactor.
- ▶ Thermo recall: an *intensive property* does **not** depend on the size or scale of the system.
These are great properties to deal with: they apply whether we are dealing with



$25m \times 5m$

or



$\sim 1 \text{ to } 5 \mu\text{m}$

What affects $-r_A$?

- ▶ Generally:
 1. temperature, T
 2. concentration, C_j
 3. pressure (for gas systems we generally use pressure instead of concentration), P_j
 4. catalysts (we won't consider this for now)
- ▶ Rate law is an algebraic expression of the form

$$-r_A = \left(k_A(T) \right) \left(f(C_A, C_B, \dots) \right)$$

Analyzing $-r_A$ dependence

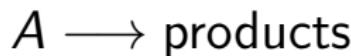
- ▶ A bank lends money at the rate of 5%. Does the interest depend on the amount borrowed?
- ▶ No, the interest rate is independent of the amount borrowed

Analyzing $-r_A$ dependence

- ▶ Does the “amount” of reaction depend on the volume, i.e. the size of the system, etc?
- ▶ No, the reaction rate is independent of the volume.
- ▶ The **number of moles** per unit volume determines concentration, which in turn determines the rate.
- ▶ So there is a dependence on the concentration, but not on the volume.

Examples of reaction rate expressions

For



we might have

$$-r_A = kC_A$$

or

$$-r_A = kC_A^2$$

or

$$-r_A = k \frac{k_1 C_A}{1 + k_2 C_A}$$

and many others are possible.

The last equation is common in bioreactor systems.

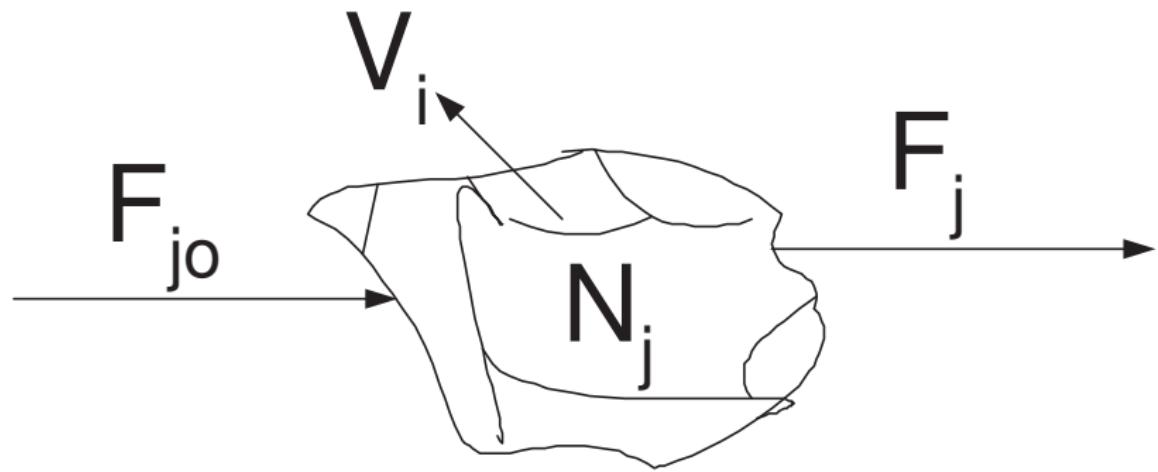
How do we obtain these rate expressions?

- ▶ Structure of the rate expression is guided by theory; trial and error testing
- ▶ We obtain the parameters from experiments (covered later)
 - ▶ e.g. $-r_A = kC_A^n$
 - ▶ determine k and n from experimental data

The general mole balance equation

We will use this over and over in the course. Let's understand this.

A mole balance on species j at any instant of time t , in an arbitrary system volume (V_i):



The general mole balance equation

A **mole balance** (not a mass balance) on species j at any instant of time t :

$$\text{In} + \text{Generated} - \text{Out} = \text{Accumulated}$$

$$\left[\begin{array}{l} \text{Rate of flow} \\ \text{of } j \text{ into} \\ \text{the system} \\ (\text{moles/time}) \end{array} \right] + \left[\begin{array}{l} \text{Rate of generation} \\ \text{of } j \text{ by chemical} \\ \text{reaction within} \\ \text{the system} \\ (\text{moles/time}) \end{array} \right] - \left[\begin{array}{l} \text{Rate of flow} \\ \text{of } j \text{ out of} \\ \text{the system} \\ (\text{moles/time}) \end{array} \right] = \left[\begin{array}{l} \text{Rate of} \\ \text{accumulation} \\ \text{of } j \text{ within} \\ \text{the system} \\ (\text{moles/time}) \end{array} \right]$$

$$F_{j0} + G_j - F_j = \frac{dN_j}{dt}$$

- ▶ $G_j = \frac{\text{moles}}{\text{time}} = r_j \cdot V = \frac{\text{moles}}{(\text{time})(\text{volume})} \cdot \text{volume}$
- ▶ Why don't we have a term for "consumed"?

The general mole balance equation

- ▶ We can subdivide the region into many subvolumes (M of them), and for each subvolume $i = 1, 2, \dots, M$:

$$\Delta G_{ji} = r_{ji} \Delta V_i$$

ΔG_{ji} is the rate of generation of j within subvolume i (chosen to be small enough so that all variables are constant, and therefore the reaction rate is the same in the subvolume)

The general mole balance equation

- ▶ Then

$$G_j = \sum_1^M \Delta G_{ji} = \sum_1^M r_{ji} \Delta V_i$$

an in the limit as $\Delta V_i \rightarrow 0$ and $M \rightarrow \infty$

$$G_j = \int_V r_j dV$$

giving

$$F_{j0} - F_j + \int_V r_j dV = \frac{dN_j}{dt} \quad (1-4)$$

The general mole balance equation

- ▶ **Note:** $\int_V r_j dV \leftarrow$ the r_j term is a function of V and cannot be taken out of the integral.
- ▶ Wait a minute: you said “Reaction rate is an **intensive property**” (slide 6), not a function of the volume/size/scale of the system



The general mole balance equation

- ▶ If all the system variables (temperature, pressure, concentration, etc.) are uniform throughout the volume, V , **only then** can the reaction rate be taken out:
- ▶ More correct to write: $r_j(V)$

$$G_j = \int_V r_j(V) dV = r_j \int_V dV = r_j \cdot V$$

$$\frac{\text{moles}}{\text{time}} = \frac{\text{moles}}{(\text{time})(\text{volume})} \cdot \text{volume}$$

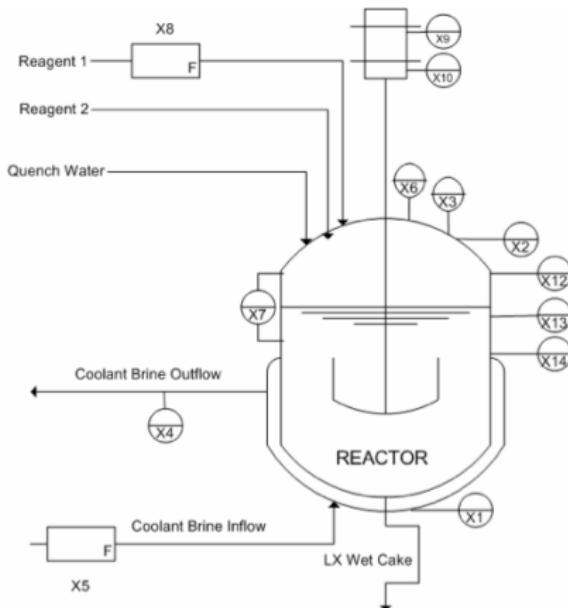
The general mole balance equation

- ▶ Now, let's apply the balance equation to various reactor types

Batch reactors

- ▶ No inflow or outflow.
- ▶ Charge reactors with reactants, then close up.
- ▶ What then?

Batch systems



[From Cecilia Rodrigues' M.A.Sc thesis, 2006, McMaster University, used with permission]



[Flickr: #2516220152]

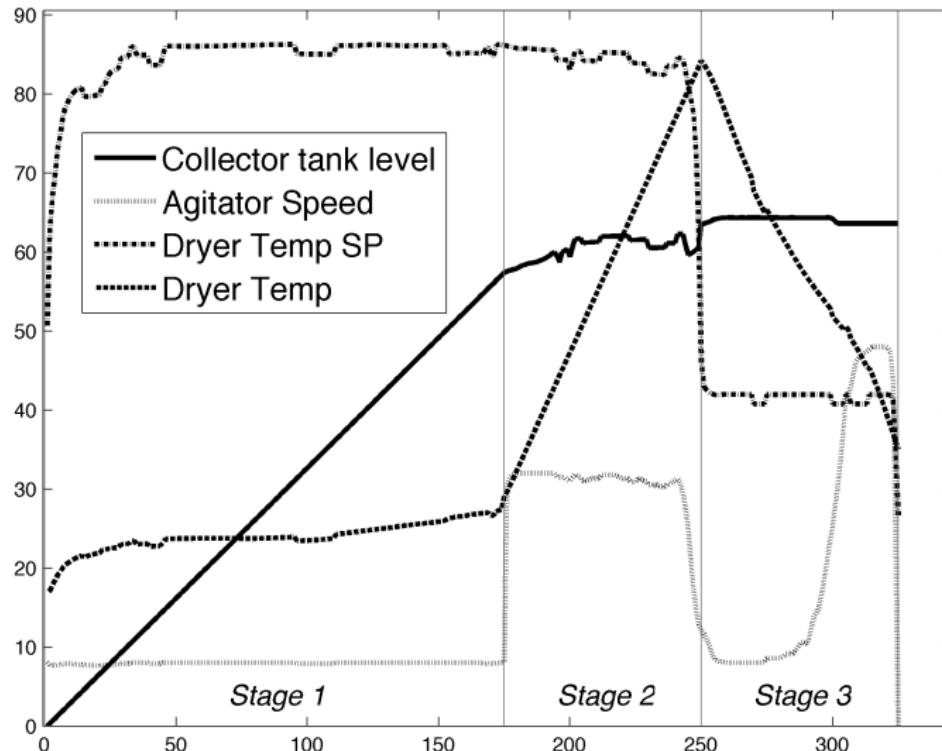
Batch systems

See illustration at

<http://woodmoorbeer.org/Pages/sierra.html>

Batch systems

Recorded values from a single batch



Batch reactors

Where are they used?

- ▶ small scale products (low volumes)
- ▶ usually extremely high value product:
medicines, speciality chemicals
- ▶ hard-to-make products
- ▶ multiple steps in the “recipe”

Batch reactors

- ▶ Typically perfectly mixed, so $\int_V r_j(V) dV$ can be replaced by $r_j \cdot V$
- ▶ The mole balance: start with the general equation, then simplify:

$$F_{j0} - F_j + \int_V r_j(V) dV = \frac{dN_j}{dt}$$

$$\cancel{F_{j0}}^0 - \cancel{F_j}^0 + r_j \cdot V = \frac{dN_j}{dt}$$

Batch reactors

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

Note: V is *not* assumed to be constant here. It could be a function of time or of the extent of reaction (and indirectly a function of time).

So for batch reactors:

$$\frac{dN_j(t)}{dt} = r_j(t) \cdot V(t)$$

Batch example problem



with $-r_A = kC_A$ and $k = 0.23\text{min}^{-1}$ in a constant volume batch reactor.

We are also given the inlet concentration and volume: $C_{A0} = 2\text{mol/L}$, $V = 10\text{L}$.

How long does it take to reduce the concentration of A in reactor to 10% of its initial value (i.e. a 90% conversion)?

Batch example problem

Batch example problem

Continuous-Stirred Tank Reactor

- ▶ CSTR's: are assumed to be well mixed
- ▶ System properties constant throughout reactor.
- ▶ This implies the product concentrations, temperatures, and other **intensive** properties *leaving the tank* are the same as that *within* tank.

Continuous-Stirred Tank Reactor (CSTR)



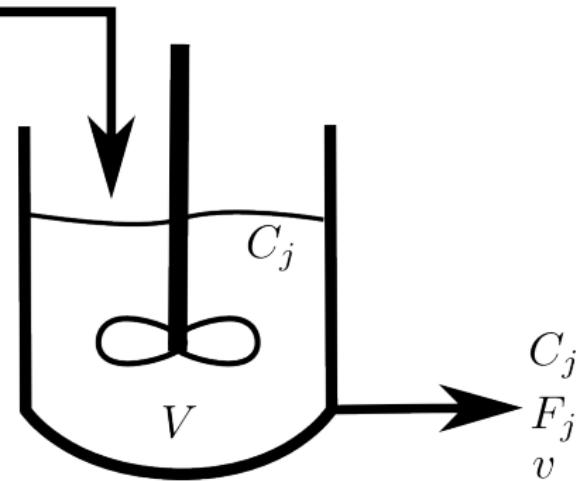
[Flickr #6240399099]

Continuous-Stirred Tank Reactor

- ▶ Where are CSTRs used? When we want entire system to be operated:
 - ▶ at the same concentration
 - ▶ at the same temperature
- ▶ where we require good agitation to contact the reactants
- ▶ e.g. emulsion polymerization
- ▶ a catalyst is suspended in a liquid product
- ▶ leaching gold from crush ore (rock); crushed particles $\sim 50\mu m$ with gold particles exposed
- ▶ Leaching: $4\text{Au} + 8\text{NaCN} + \text{O}_2 + 2\text{H}_2\text{O} \longrightarrow 4\text{Na}[\text{Au}(\text{CN})_2] + 4\text{NaOH}$

Continuous-Stirred Tank Reactor (CSTR)

C_{j0}
 F_{j0}
 v_0



- ▶ At any given time, t
- ▶ F : molar flow rate
- ▶ C : concentration
- ▶ v : volumetric flow
- ▶ subscript j , j^{th} species
- ▶ subscript 0, inlet stream

C_j : Concentration of species j in the reactor of liquid volume V

- ▶ V is **not** the total physical reactor volume

Continuous-Stirred Tank Reactor (CSTR)

- ▶ General mole balance equation:

$$F_{j0} - F_j + \int_V r_j(V) dV = \frac{dN_j}{dt}$$

- ▶ $\frac{dN_j}{dt} = 0$, (often analyzed at steady state, **but not necessarily**).
- ▶ No spatial variation with reactors

$$\Rightarrow \int_V r_j(V) dV = r_j V \Rightarrow V = \boxed{V = \frac{F_{j0} - F_j}{-r_j}}$$

Continuous-Stirred Tank Reactor (CSTR)

- ▶ Note: Can relate to concentration via

$$F_j = C_j v$$
$$\frac{\text{moles}}{\text{time}} = \frac{\text{moles}}{\text{vol}} \cdot \frac{\text{vol}}{\text{time}}$$

$$V = \frac{v_0 C_{A0} - v C_A}{-r_A} \quad (1-9)$$