Welcome to
ChE 344
Reaction Engineering and Design

Lecture 1: Thurs, Jan 6, 2022

Course Introduction, Polymath, Wolfram, Mole Balances, and Ideal Reactors

Reading for today’s lecture: Chapter 1

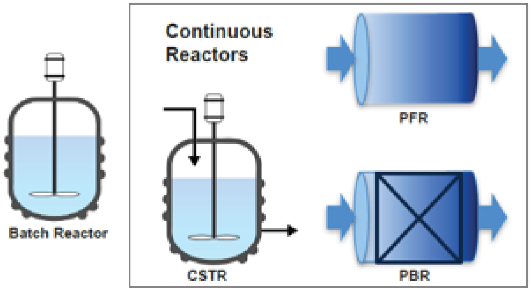
Homework 1 will be posted on Canvas next week, due

<u>Fri Jan 21 by 11:59pm</u>

Reading for Lecture 2: Chapter 2

Lecture 1: Introduction and Moles Balances
Related Text: Syllabus, Chapter 1

Main Reactor Types

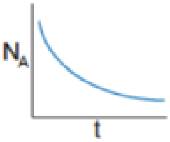
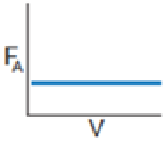
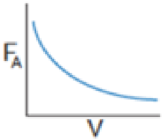


$$F_j = C_j v$$

General mole balance

$$F_{j0} - F_j + \int_0^V r_j dV = \frac{dN_j}{dt}$$

Mole balances (aka Design Equations) for reactor types (actually covered in Lecture 2, here for space purposes)

Reactor	Assumptions	Mole balance	Reactant profile
Batch	Spatially uniform, no inlet/outlet streams	$r_j V = \frac{dN_j}{dt}$	
CSTR	Spatially uniform, steady state	$V = \frac{F_j - F_{j0}}{r_j}$	
PFR	No radial variation, steady state	$r_j = \frac{dF_j}{dV}$	
Modifications for solid catalyst loading*			
PBR	Same as PFR, plus uniform catalyst	$r_j' = \frac{dF_j}{dW}$	
Fluidized CSTR**	Same as CSTR, plus uniform catalyst	$W = \frac{F_j - F_{j0}}{r_j'}$	

*$W = \rho_b V$. $r_j' \rho_b = r_j$.

**Not covered specifically in class, but same concept as PFR/PBR relationship.

Textbook

Elements of Chemical Reaction Engineering, 6th edition
By Professor H. Scott Fogler

Some of you may have your copy already

ebook or hardcopy

Textbook website:

http://www.umich.edu/~elements/5e/

The website will be needed for the Living Example Problems

Chemical reaction engineering (CRE)

CRE is the field that studies the rates and mechanisms of chemical reactions and the design of the reactors in which they take place. You may also hear people call this class "kinetics" which is the study of the rates of chemical reactions. However, chemical kinetics does not necessarily include the design of reactors.

Designing chemical reactors is an area that is <u>unique to chemical engineers</u>.

It will combine aspects of
- Fluid mechanics
- Heat and mass transport
- Thermodynamics

By reading and understanding the book you will take a major step into becoming a chemical engineer.

Course objective:

Ability to design chemical reactors for the conversion of undesired species to desired species. The goal is for you to be able to learn the fundamentals needed to solve important problems for society involving chemical reactions.

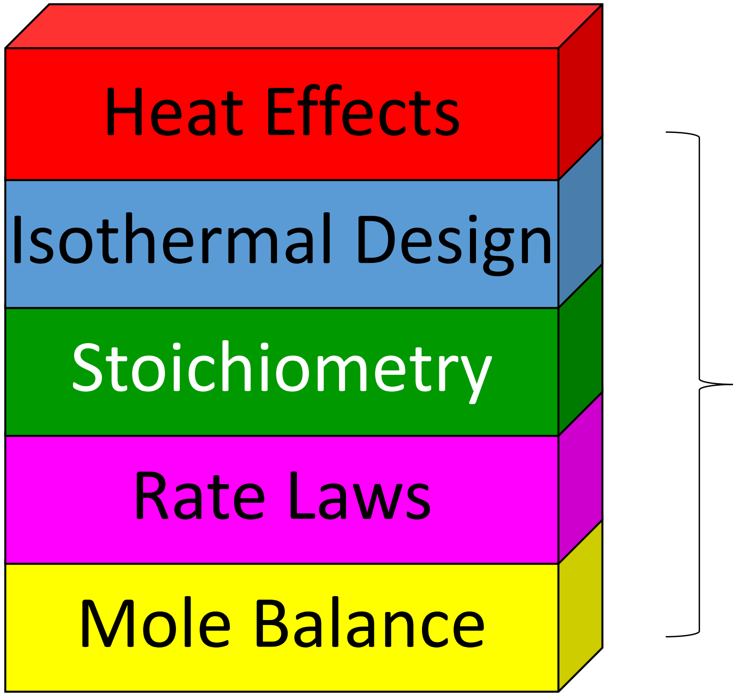
Course outcomes:

- Size reactors including isothermal/adiabatic/non-adiabatic
- Multiple reactions and determine selectivity/yield
- Reaction order including reaction mechanisms
- Reactor safety (continuing with safety modules you have seen in other classes)

Ability to upgrade reactants into more desirable species

Overview of next several weeks

Chemical Reaction Engineering Algorithm



Heat Effects

Ch.5 Lecture 6-7 Isothermal Design

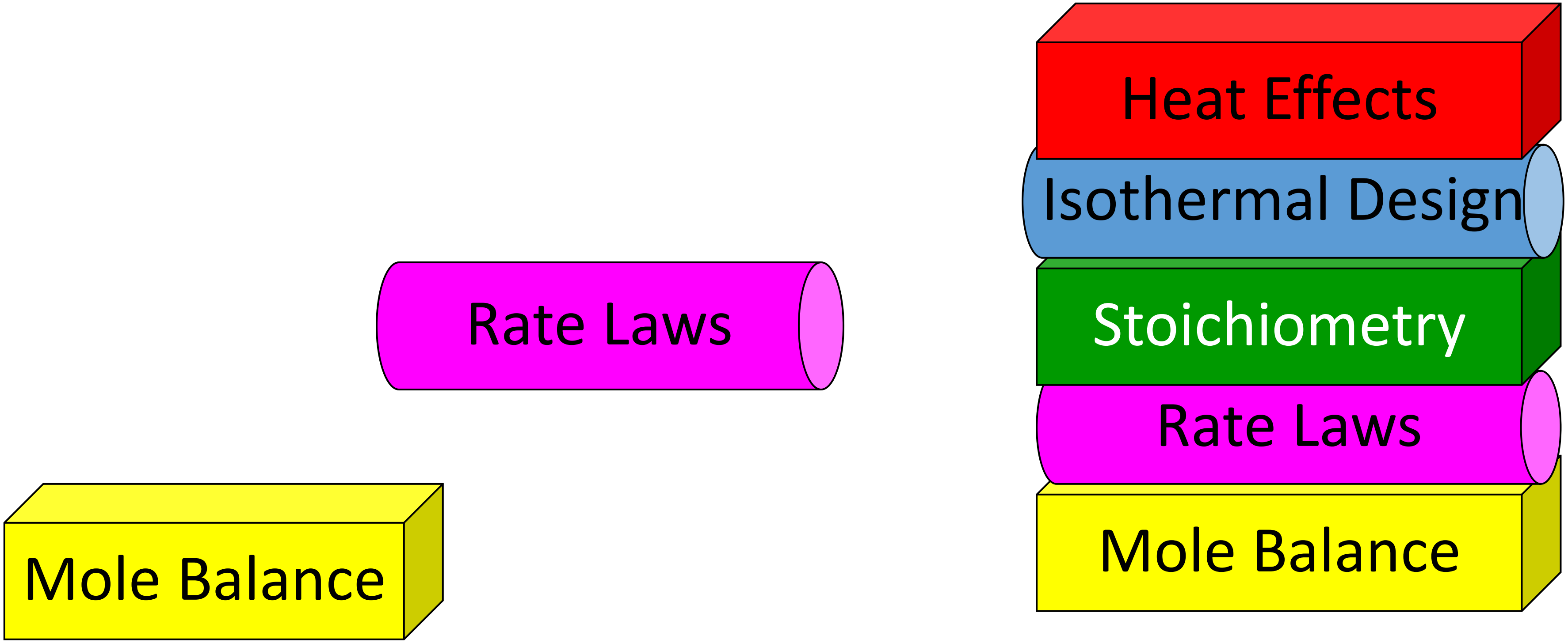
Ch.4 Lecture 4-5 Stoichiometry

Ch.3 Lecture 3 Rate Laws

Ch.1 Lecture 1 Mole Balance

Midterm 1

Be careful not to cut corners on any of the CRE building blocks while learning this material…



Rate Laws

Mole Balance

Heat Effects

Isothermal Design

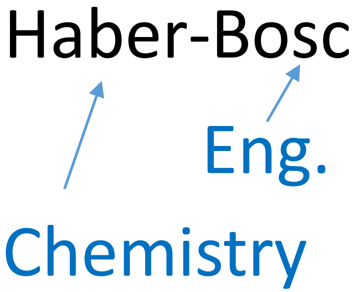
Stoichiometry

Rate Laws

Mole Balance

Otherwise, your Algorithm becomes unstable!

Real world applications of chemical reaction engineering



Haber-Bosch process

Eng.

Chemistry

$$N_2 + 3H_2 \rightarrow 2NH_3$$

(Used for fertilizer)

175 million tonnes of ammonia per year (~24 kg per person). Fertilizer from this process is responsible for half of the world's food but requires only 1% of world's energy.

Other applications:

- Environmental (Catalytic converter, removing CO)
- Energy conversion (Cracking reactions for fuels)
- Chemicals (Plastics)
- Pharmaceuticals (homogeneous catalysis)

More applications of chemical reaction engineering and kinetics

Sustainable fuels

Wastewater treatment

Drug delivery

(Ch 14 textbook website)

(AIChE) “Evolution of Drug Delivery”

Chemical identity

What type of atoms? N? C? O? H?

How many atoms? N_2? NH_3? CO_2? CO?

Configuration of atoms?

For a reaction to occur, bonds must be broken and/or formed. A chemical species has reacted if it has lost its chemical identity

Writing down a reaction

aA + bB ⇄ cC + dD

a, b, c, d are how many moles are made or consumed by the reaction. The “stoichiometric coefficient, ν_i” is positive this value for products, and negative for reactants (consumed).

$$\nu_A = -a \qquad \nu_C = c$$

$$\nu_B = -b \qquad \nu_D = d$$

Types of reactions

Reactant

Product

1. Decomposition $$A \rightarrow 2B$$
2. Combination $$2A \rightarrow B$$
3. Isomerization $$A \rightarrow B$$

Reaction rate law: An equation that tells you how fast a reaction proceeds (e.g., per unit volume)

r_j is rate of reaction of species j

Negative = disappearing

Positive = forming

$r_j = \nu_i r$ where r is the rate of reaction

Units of r_j are: $\frac{mol\ j}{L \cdot s}$

Example reaction: $A \to B$

$$r = r_B = -r_A = k(C_A)^1$$

$$r_B = -r_A = k(C_A)^1$$

r_j is a function of concentration, temperature, pressure and type of catalyst (if any)

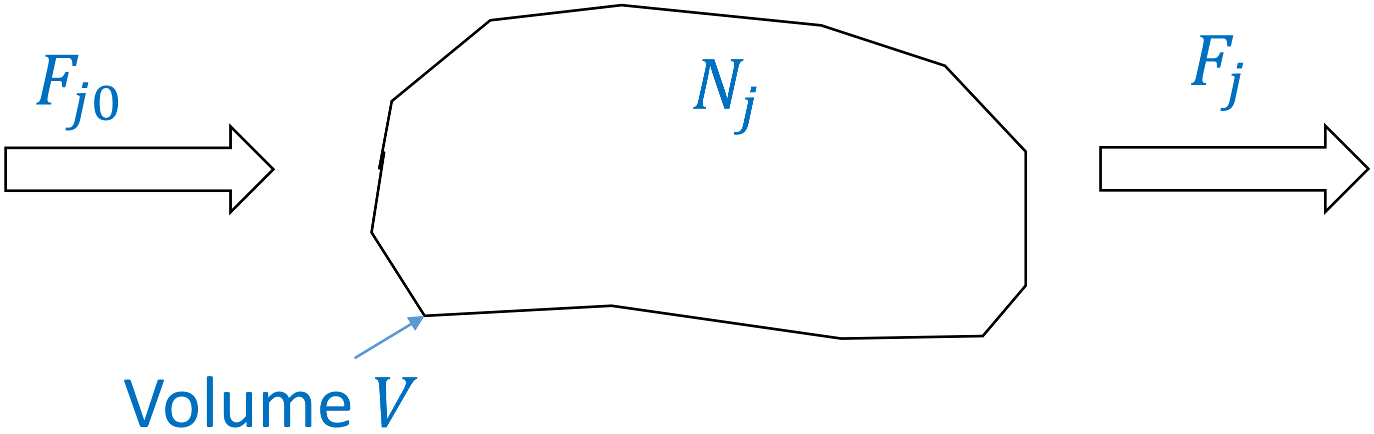
r_j is independent of type of reactor system

C_A is the concentration of species A (mol/L)

k is the "rate constant", and is always positive

General mole balance equation

In – out + (generation – consumption) = accumulation



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

N_j is the # of moles of species j in volume V at a given time

F_{j0} is the # of moles of species j flowing IN per unit time

F_j is the # of moles of species j flowing OUT per unit time

G_j is net generation of species j in volume V per unit time

Generation/consumption term: We can generate or consume a species by reacting it!

If the volume V is spatially uniform:

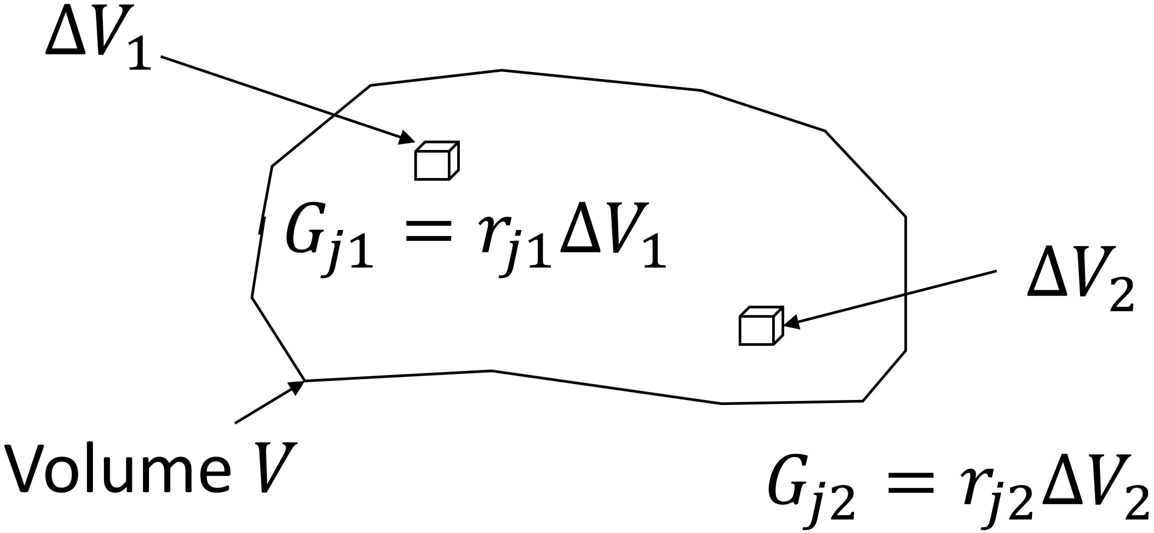
$$G_j = r_j V$$

So we can control the total amount generated/consumed by changing the volume V. This is essentially reactor design, if V is the volume of our reactor!

For heterogeneous reactions, we write the rate with respect to mass or area of catalyst, rather than volume.

$$r_j' [=] \frac{mol\ j}{g_{catalyst} \cdot s} \qquad r_j'' [=] \frac{mol\ j}{area_{catalyst} \cdot s}$$

If the volume V is *not* spatially uniform (meaning r_j is different depending on location due to T, conc. differences):



$$G_j = G_{j1} + G_{j2} + \cdots$$

$$G_j = \sum_{i=1}^{N} r_{ji}\Delta V_i$$

$$G_j = \iiint r_j(x,y,z)\,dV = \int_0^V r_j\,dV$$

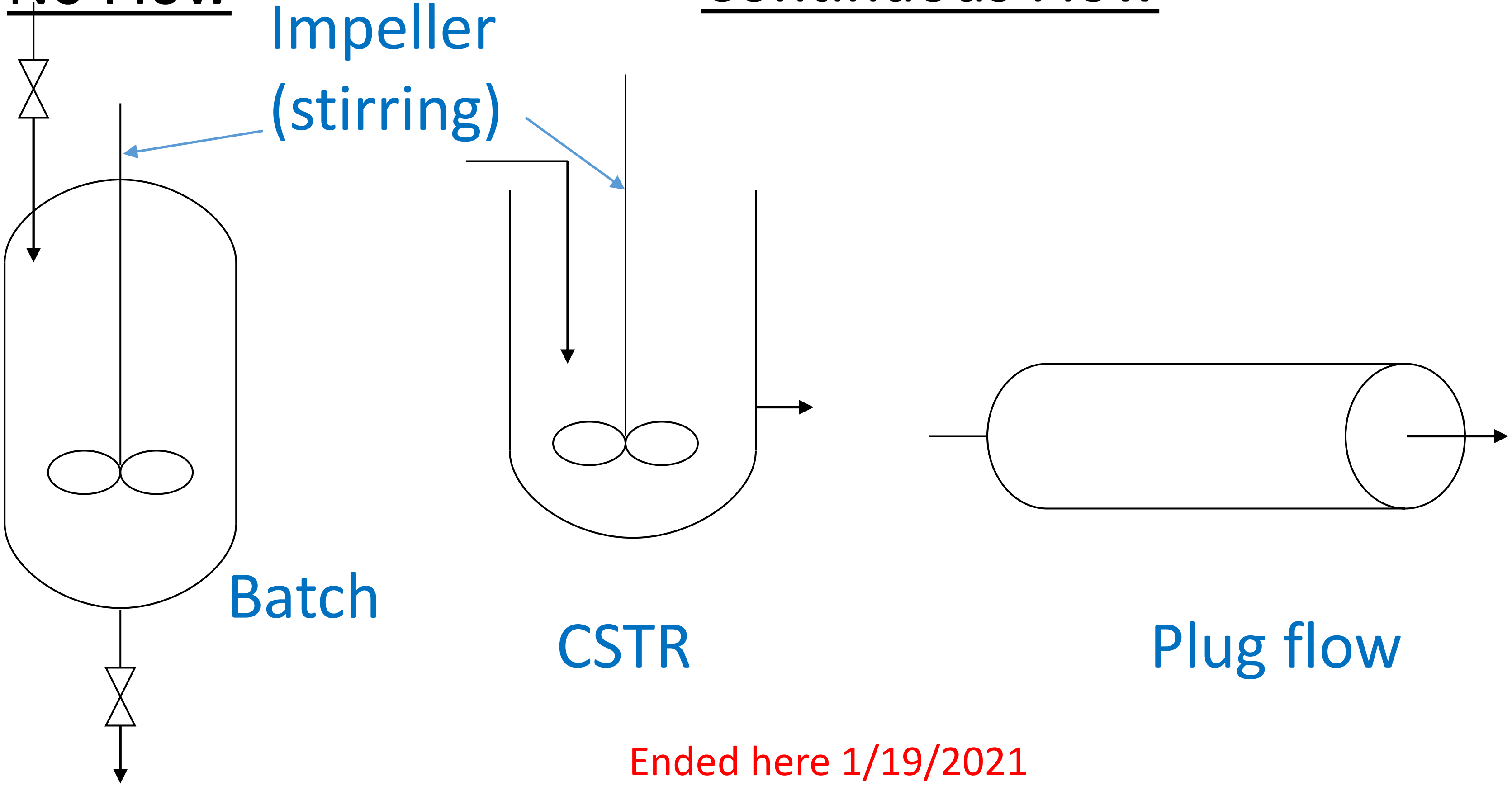
General Mole Balance Equation or reactor design equation

$$F_{j0} - F_j + \int_0^V r_j dV = \frac{dN_j}{dt}$$

Common types of reactors:

No Flow

Continuous Flow



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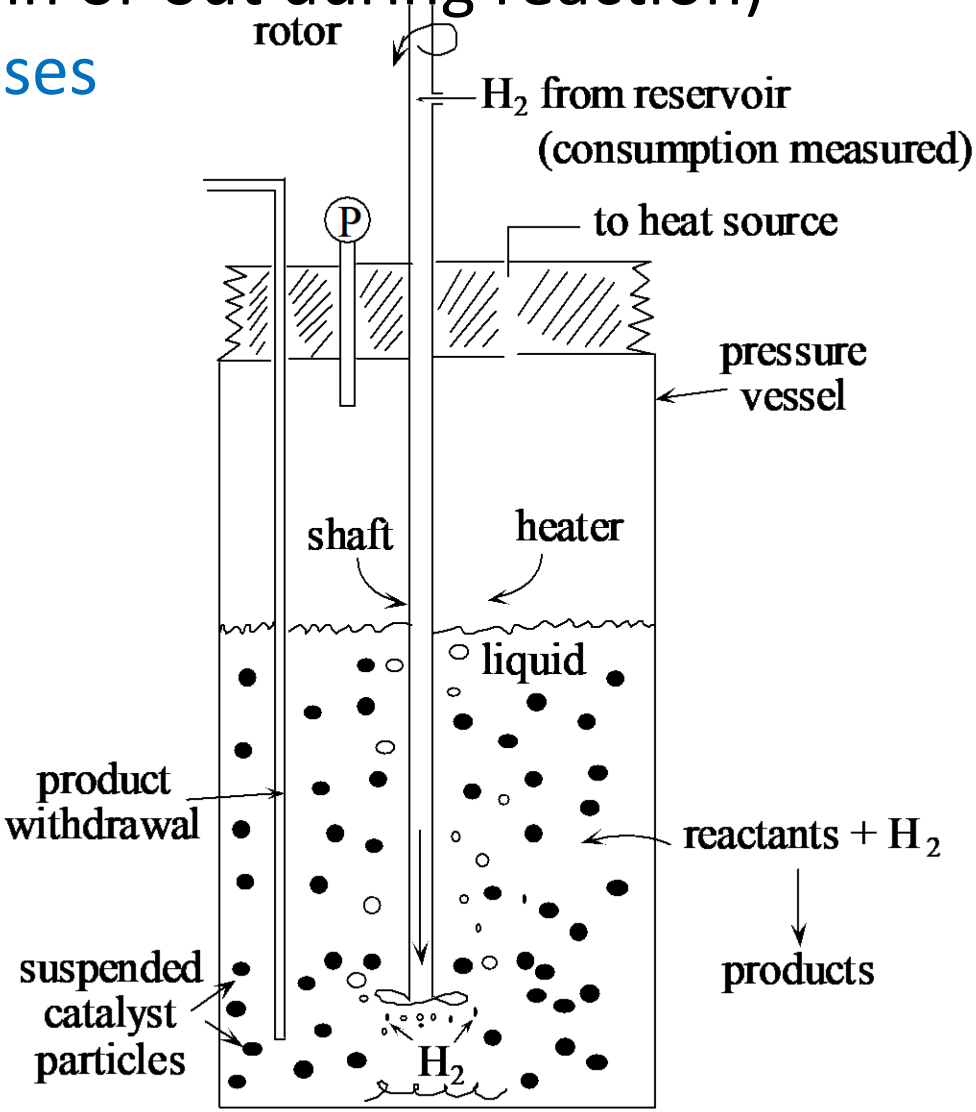
Batch reactors (no flow in or out during reaction)

- Used for new processes
- Quality control



Batch-slurry reactor for hydrogenation of specialty chemicals.

Batch reactor design equation

- Not steady state
- Rate doesn't depend on position (makes these also sometimes called well-mixed reactors)
- No flows in or out

$$\cancelto{0}{F_{j0}} - \cancelto{0}{F_j} + \int_0^V r_j dV = \frac{dN_j}{dt}$$

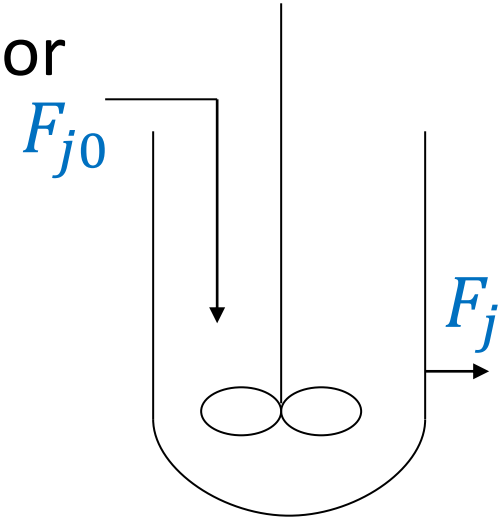
$$\boxed{r_j V = \frac{dN_j}{dt}}$$

$$dt = \frac{dN_j}{r_j V} \qquad \int_0^{t_1} dt = \int_{N_{j0}}^{N_{j1}} \frac{1}{r_j V} dN_j$$

Ended here 1/6/2022

Constant/continuous stirred tank reactor (CSTR)

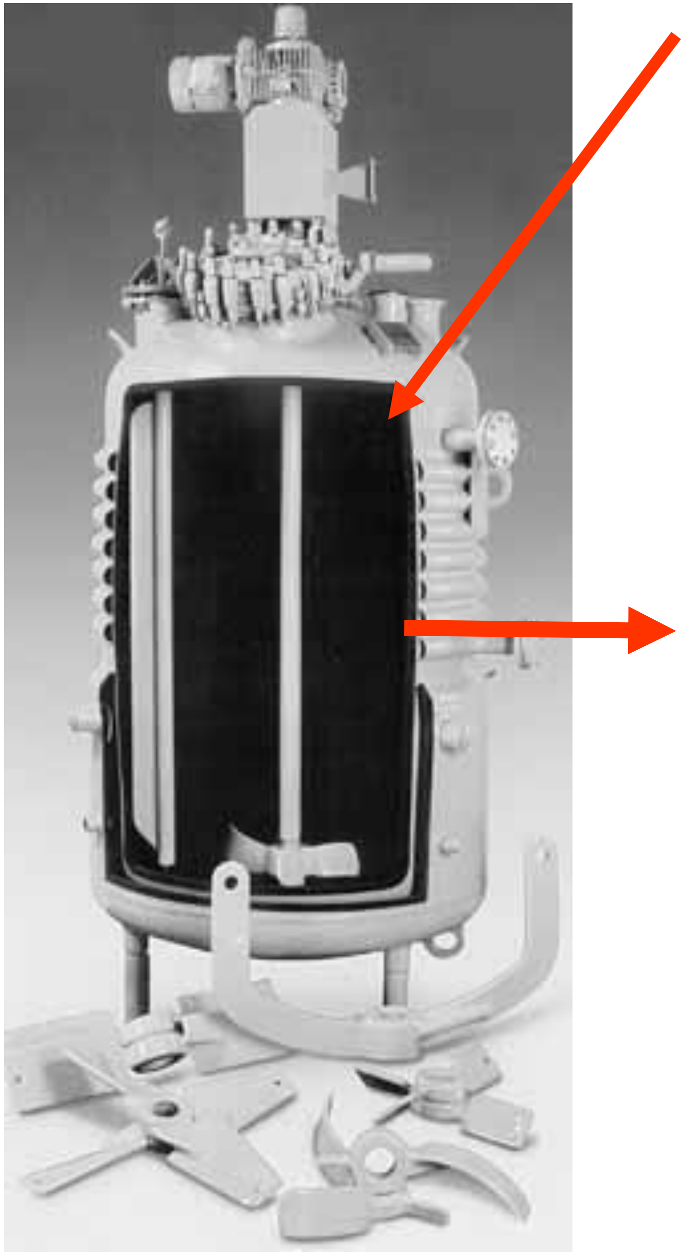
Inlet stream conc. are different than in reactor



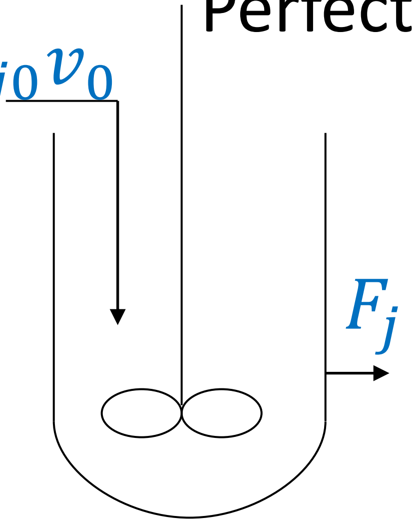
All conc. at outlet and in reactor are the same

CSTR

Batch + Flow at Steady State = CSTR



Constant/continuous stirred tank reactor (CSTR)



Inlet stream conditions $F_{j0} = C_{j0}v_0$ are different than in reactor

Perfect mixer

F_j

All conditions at outlet and in reactor are the same

- Flow in and out (v is volumetric flow rate
- Well-mixed
- Steady state

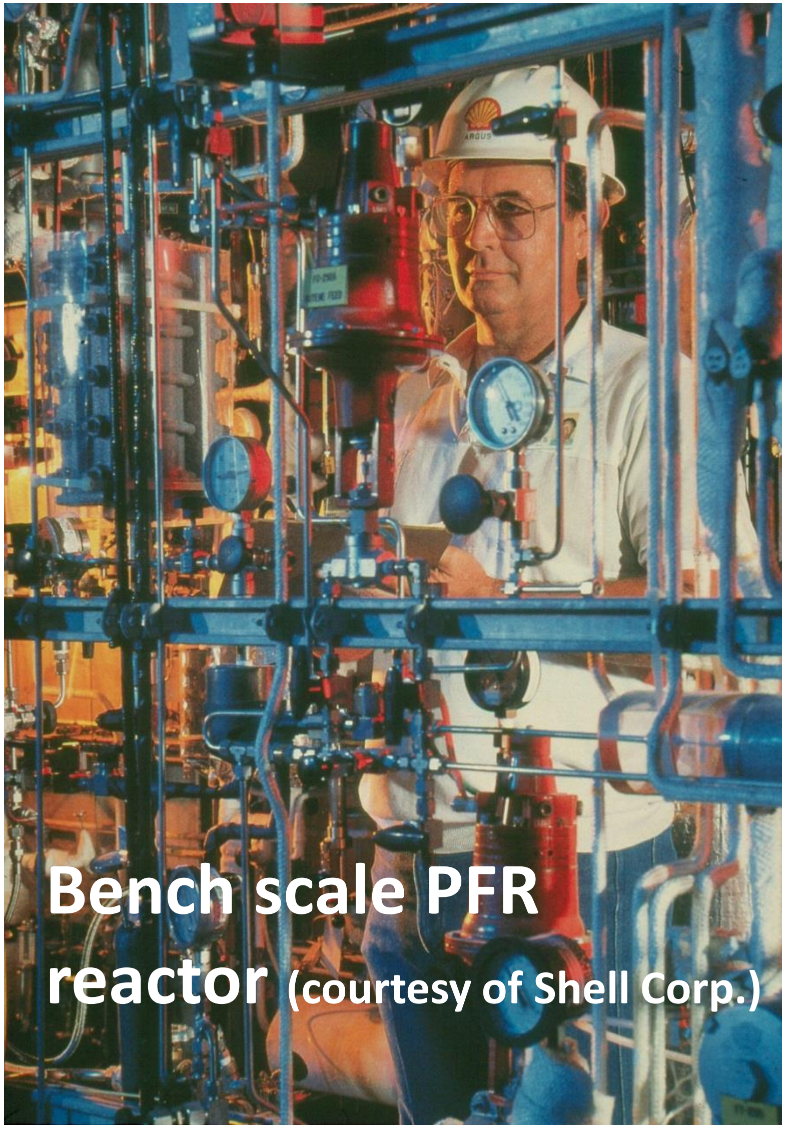
$$F_{j0} - F_j + \int_0^V r_j dV = \cancelto{0}{\frac{dN_j}{dt}}$$

$$F_{j0} - F_j + r_j V = 0$$

$$V_{CSTR} = \frac{F_{j0} - F_j}{-r_j}$$

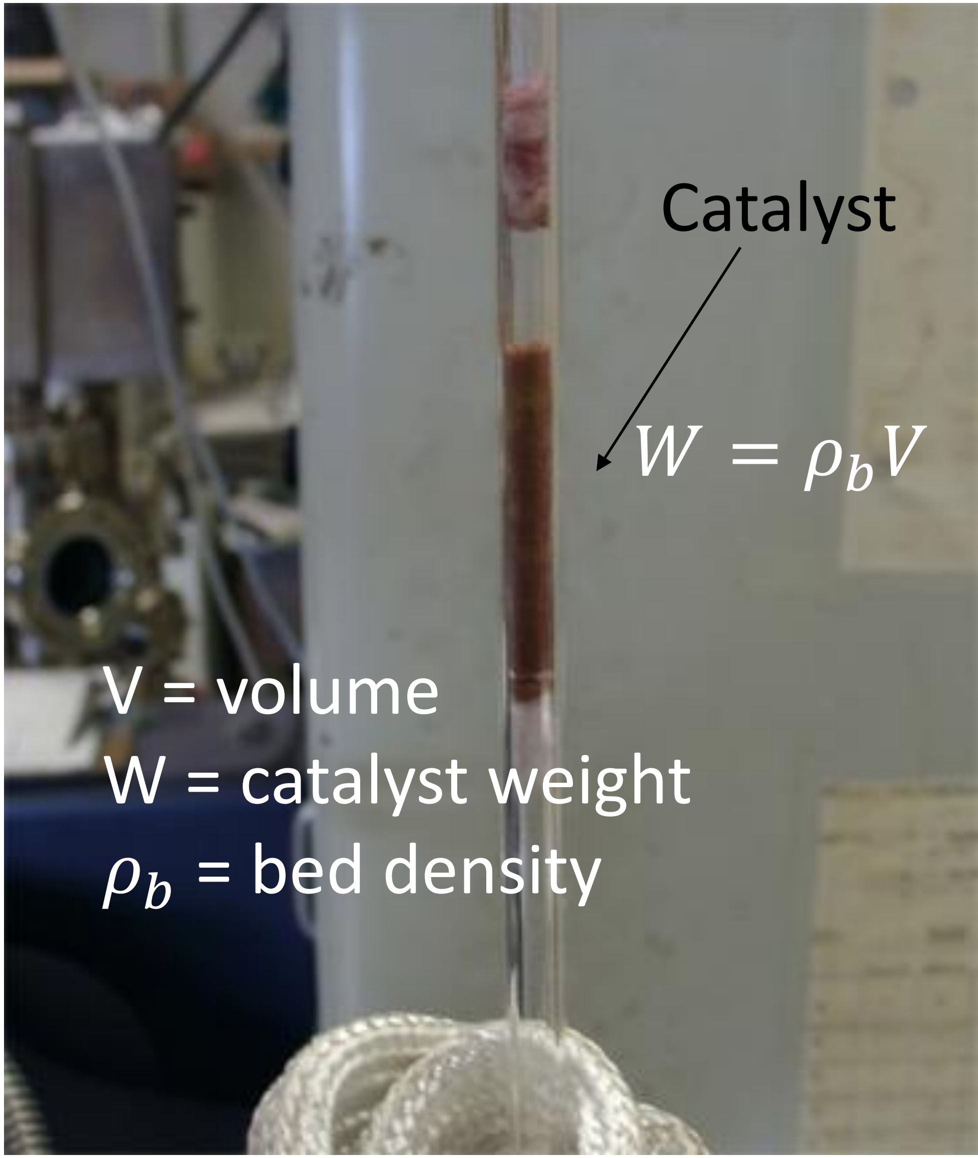
$$F_j = C_j v$$

Plug Flow Reactor (PFR)



Bench scale PFR reactor (courtesy of Shell Corp.)

Packed Bed Reactor (PBR)



Catalyst

$$W = \rho_b V$$

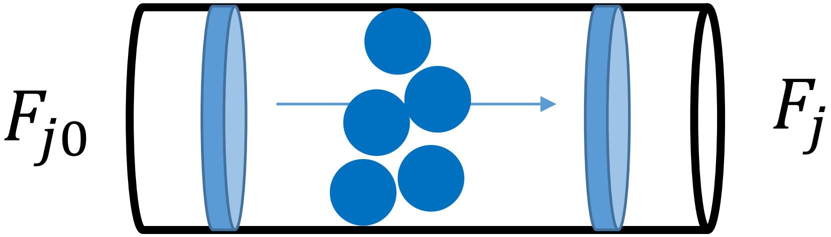
V = volume

W = catalyst weight

ρ_b = bed density

Plug flow reactor or packed bed reactor

- No radial variation
- No parabolic profile
- Each ΔV of fluid is treated as an ideal CSTR (steady state)

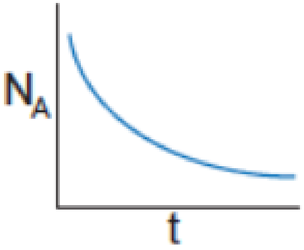
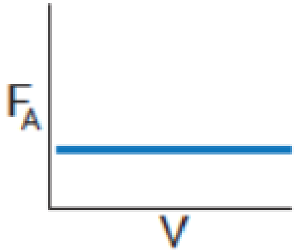
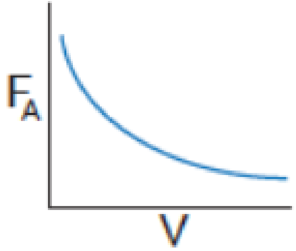


$$F_{j0} - F_j + \int_0^V r_j dV = \cancelto{0}{\frac{dN_j}{dt}}$$

$$F_{j,V} - F_{j,V+\Delta V} + r_j \Delta V = 0$$

$$r_j = \frac{dF_j}{dV}$$

Chapter 1 Summary: Reactor Mole Balances/Design Eqs

Reactor	Assumptions	Mole Balance	Reactant Profile
Batch	Spatially uniform, no inlet/outlet streams	$r_j V = \frac{dN_j}{dt}$	
CSTR	Spatially uniform, steady state	$V = \frac{F_j - F_{j0}}{r_j}$	
PFR	No radial variation, steady state	$r_j = \frac{dF_j}{dV}$	
PBR		$r_j' = \frac{dF_j}{dW}$	W is catalyst weight

Think about and discuss with your neighbors:

If we think of a hippo's stomach as a reactor, which would be the most appropriate reactor to use as a model?

A) CSTR

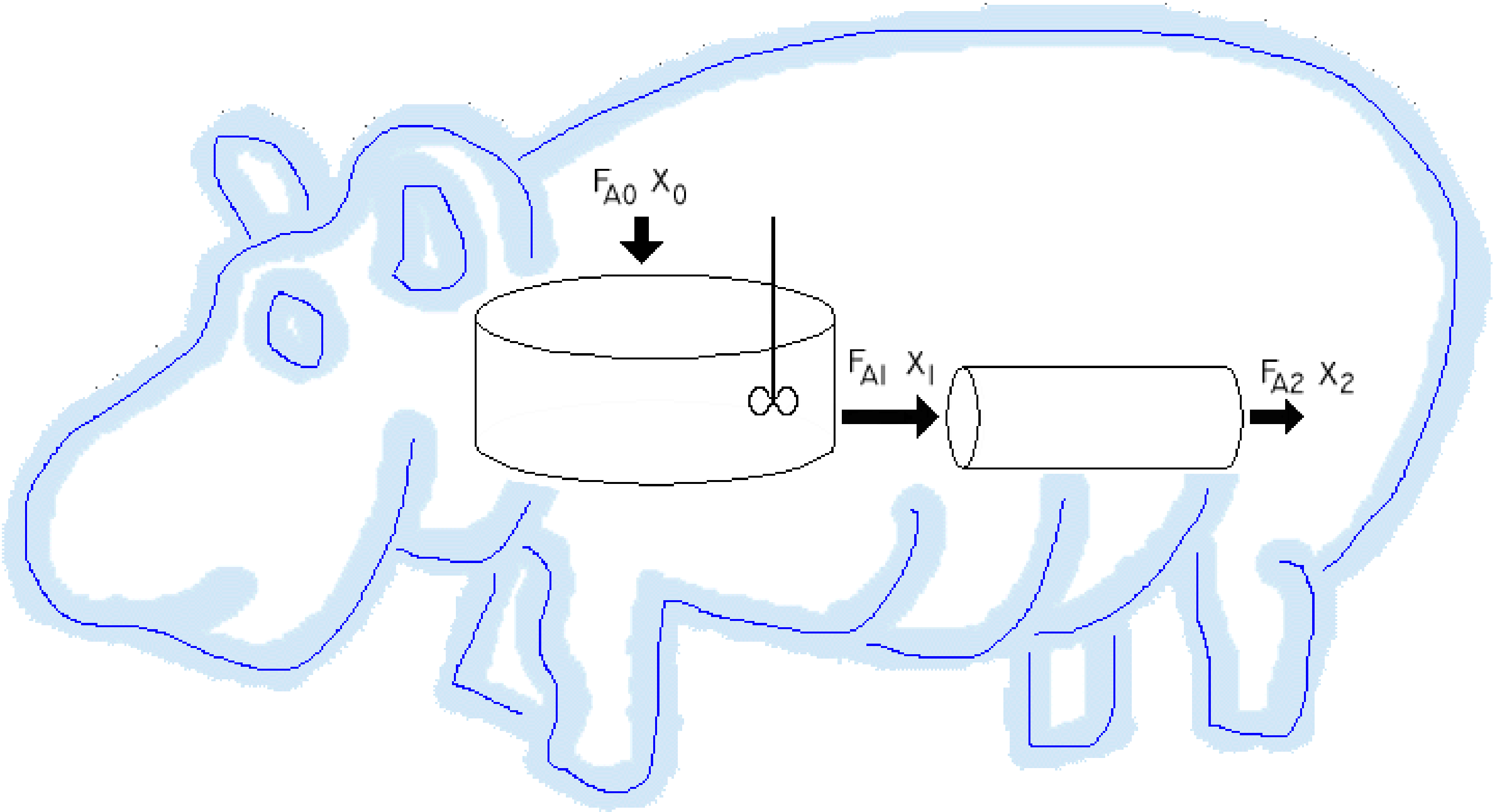
B) Batch

C) PFR

D) PBR

Assume that the hippo has to eat non-stop, and that although its stomach does not have an impeller, it is well mixed.

Flow in and out continuously, well mixed, must be a CSTR!



http://umich.edu/~essen/html/web_mod/hippo/equation4.htm

CSTR first, then flows out of stomach to gastrointestinal tract (more like a plug flow reactor).

We will learn about reactors in “series” soon!

Working on a problem together.

Let's model the reaction in the hippo's stomach (CSTR) with the following reaction and rate law

$$Food \rightarrow Products$$

$$A \rightarrow B$$

$$r_B = -r_A = kC_A$$

Based on the CSTR mole balance equation, is the molar flow rate out ($F_A = F_{A,out}$) higher or lower than in ($F_{A0} = F_{A,in}$)? What about for F_B vs. F_{B0}?

$$F_{A0} - F_A + r_A V = 0$$

$$F_{A0} - F_A - kC_A V = 0$$

$$F_{A0} - F_A = kC_A V; F_{A0} > F_A$$

$$F_{B0} - F_B + r_B V = 0$$

$$F_{B0} - F_B + kC_A V = 0$$

$$F_{B0} - F_B = -kC_A V; F_{B0} < F_B$$