CHE 402
Kinetics & Reactor Design

Fall 2008

Dr. Eid Al-Mutairi

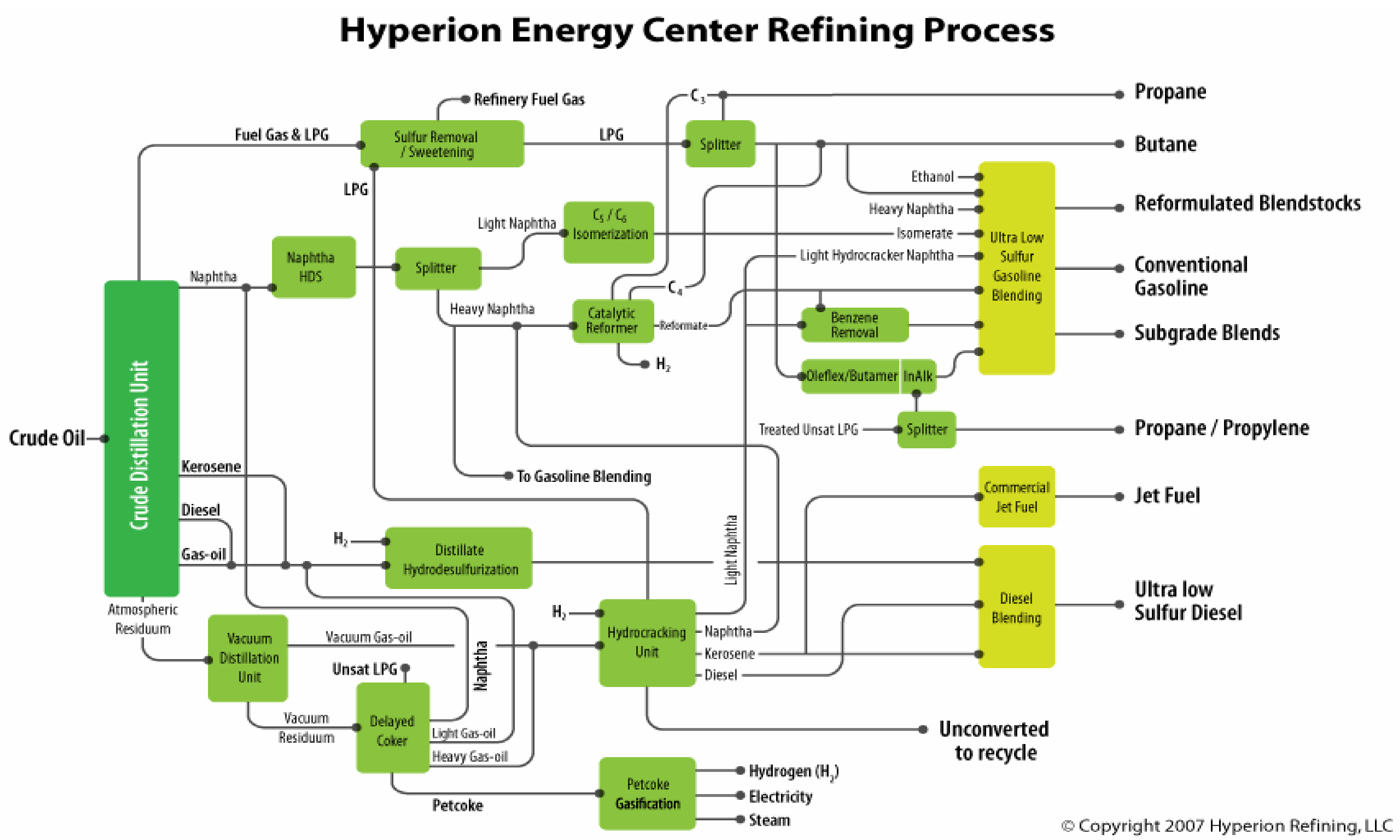
Instructor

- Dr. Eid Al-Mutairi
- Off: 16-266
- Email: mutairi@kfupm.edu.sa

Students

- Who you are?
- Why you become chemical engineer?
- What does “kinetics & rector design” mean to you?

Chemical Engineering Field



Reaction Kinetics & Reactor Design

Course Contents

- Addressing basic concepts of chemical reactions kinetics
- Conversion and Reactor Sizing
- Isothermal reactor design
- Collection and Analysis of Rate Data
- Multiple reactions
- Non-Isothermal Reactor Design
- Catalysis and Catalytic Reactors

Grading Policy

Homework	10%
Quizzes	10%
Major Exams	40%
Final Exam	40%

Chapter 1: Mole Balances

- Define the rate of chemical reaction.
- Apply the mole balance equations to a batch reactor, CSTR, PFR, and PBR.
- Describe two industrial reaction engineering systems.
- Describe photos of real reactors.
- Describe how to surf the CD-ROM attached with this text.

Chemical Reactions

- Examples
- Types
- Our life and chemical reactions

Chemical Identity

- A chemical species is said to have reacted when it has lost its chemical identity. The identity of a chemical species is determined by the *kind* , *number* ,and *configuration* of that species' atoms .

Three ways a chemical species can lose its chemical identity

decomposition	combination	isomerization
$CH_3CH_3 \rightarrow H_2 + H_2C = CH_2$	$N_2 + O_2 \rightarrow 2NO$	$C_2H_5CH = CH_2 \rightarrow CH_2 = C(CH_3)_2$

Reaction Rate

- Measures how fast a number of moles of one chemical species are consumed to form another chemical.

$$CCl_3CHO + 2C_6H_5Cl \longrightarrow (C_6H_4Cl)_2CHCCl_3 + H_2O$$

$$A + 2B \longrightarrow C + D$$

Reaction Rate

- The reaction rate is the rate at which a species looses its chemical identity per unit volume. The rate of a reaction can be expressed as the rate of disappearance of a reactant or as the rate of appearance of a product. Consider species A:

$$A \longrightarrow B$$

r_A = the rate of formation of species A per unit volume

$-r_A$ = the rate of a disappearance of species A per unit volume

r_B = the rate of formation of species B per unit volume

The rate of reaction, $-r_A$, is the number of moles of A reacting (disappearing) per unit time per unit volume

Reaction Rate: Example I

$$A \longrightarrow B$$

- If B is being created Sat 0.2 moles per decimeter cubed per second, i.e,
  r_B = 0.2 mole/dm^3/s
- Then A is disappearing at the same rate:
  $-r_A$ = 0.2 mole/dm^3/s
- For a catalytic reaction, we refer to $-r_A'$, which is the rate of disappearance of species A on a per mass of catalyst basis.

Reaction Rate

- Consider species j:
- r_j is the rate of formation of species j per unit volume [e.g. mol/dm3*s]
- r_j is a function of concentration, temperature, pressure, and the type of catalyst (if any)
- r_j is independent of the type of reaction system (batch, plug flow, etc.)
- r_j is an algebraic equation, <u>not</u> a differential equation
- We use an algebraic equation to relate the rate of reaction, -rA, to the concentration of reacting species and to the temperature at which the reaction occurs [e.g. $-r_A = k(T)C_A^2$].

Reaction Rate: Example II

$$CCl_3CHO + 2C_6H_5Cl \longrightarrow (C_6H_4Cl)_2CHCCl_3 + H_2O$$

$$A + 2B \longrightarrow C + D$$

e.g. $-r_A = 4\ mole/dm^3/s$

$r_A = -4\ mole/dm^3/s$

$-r_B = 8\ mole/dm^3/s$

$r_B = -8\ mole/dm^3/s$

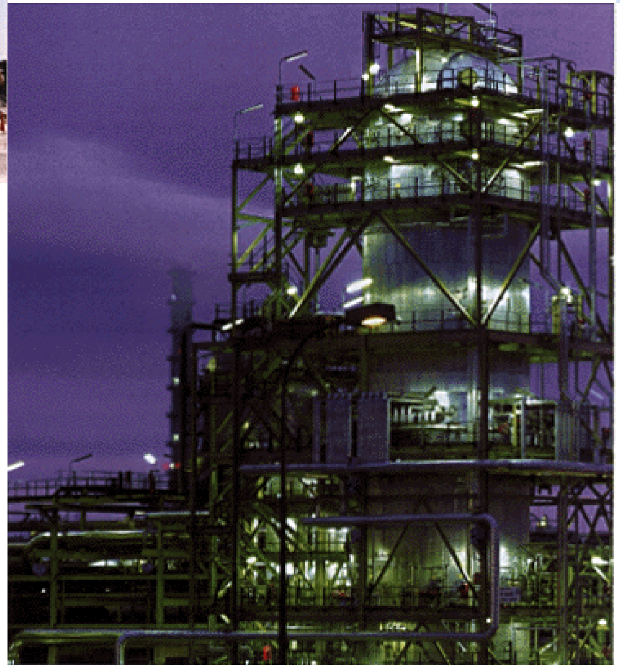
$r_C = 4\ mole/dm^3/s$

Reactors

- Plug Flow Reactor (PFR) or Tubular Reactor
- Continuous Stirred Tank Reactor (CSTR)
- Batch Reactor

Industrial Reactor

Reactor System Used at Amoco

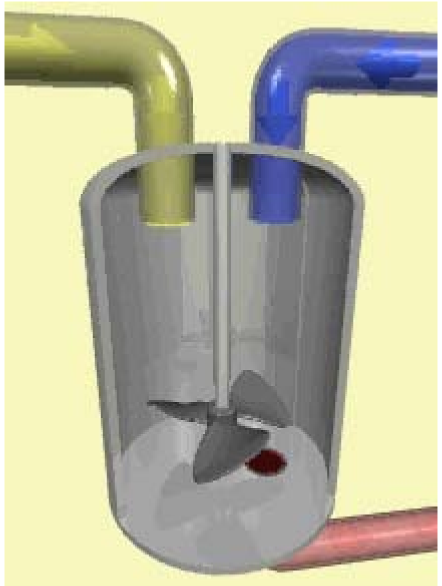


Sasol Advanced Synthol (SAS) Reactor

Fixed Bed Reactor

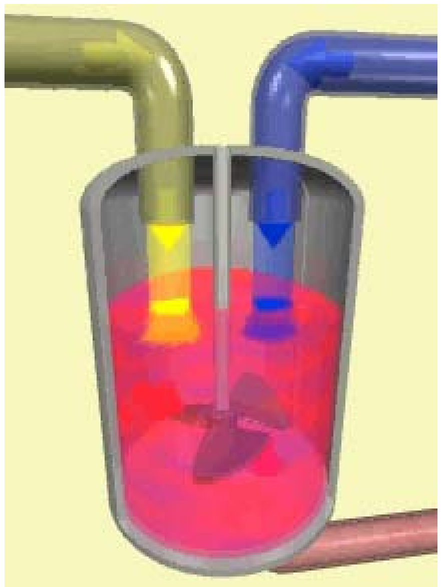
Batch Reactors

- Batch reactors are the simplest reactors used in chemical processes.
- Reactants are first placed inside the reactor and then allowed to react over time.
- Applications: typically used for liquid phase reactions.
  - When only a small amount of product is desired (process in testing phase OR product is expensive)



CSTR

- CSTRs are very well mixed ►contents have uniform properties (temperature, density, etc)
- Reactants are continuously introduced into the reactor, while products are continuously removed.



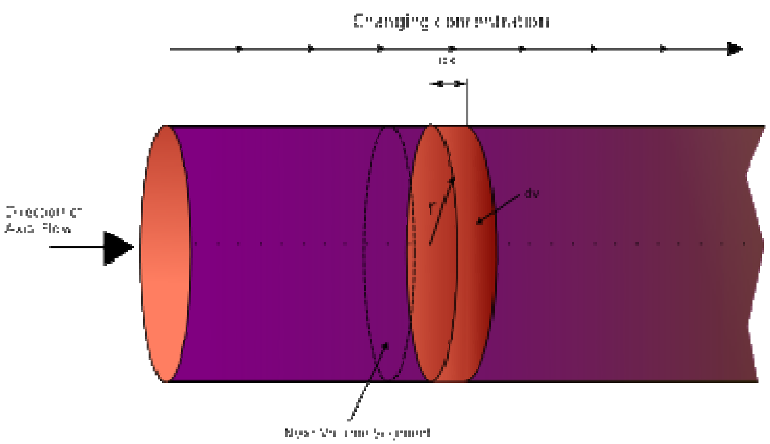
PFR (Tubular)

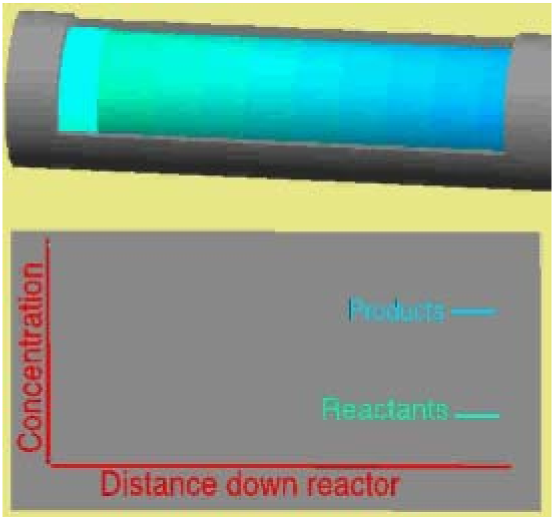
Plug flow or tubular reactors consist of a hollow pipe or tube through which reactants and products to flow through.

Applications: wide variety of operations (gas or liquid phases)

Gasoline production

Oil cracking

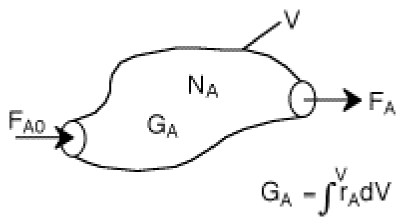




General Mole Balance Equation

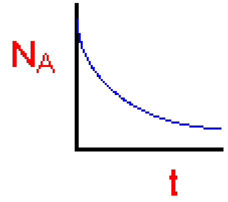
- IN - OUT + GENERATION = ACCUMULATION

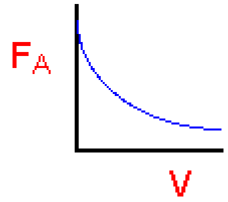
$$F_{A0} - F_A + \int_0^V r_A \, dV = \frac{dN_A}{dt}$$

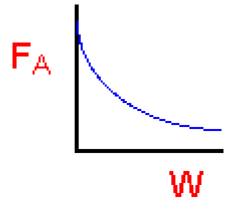


Mole Balance on Different Reactor Types

Reactor	Differential	Algebraic	Integral
Batch	$\frac{dN_A}{dt} = r_A V$		$t = \int_{N_{A0}}^{N_A} \frac{dN_A}{r_A V}$
CSTR		$V = \frac{F_{A0} - F_A}{-r_A}$	
PFR	$\frac{dF_A}{dV} = r_A$		$V = \int_{F_{A0}}^{F_A} \frac{dF_A}{r_A}$
PBR	$\frac{dF_A}{dW} = r'_A$		$W = \int_{F_{A0}}^{F_A} \frac{dF_A}{r'_A}$





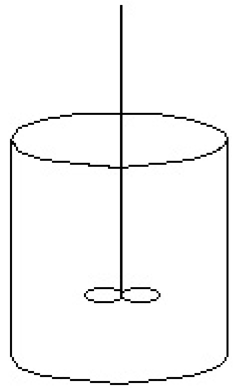


Batch Mole Balance

- General Mole Balance on System Volume V

$$\text{In} - \text{Out} + \text{Generation} = \text{Accumulation}$$

$$F_{A0} - F_A + \int r_A dV = \frac{dN_A}{dt}$$



-No inflow or outflow $F_{A0} = F_A = 0$

Assumptions

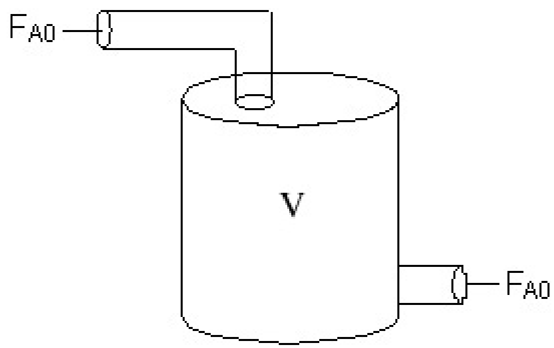
Well mixed $\int r_A dV = r_A V$ $\quad \left|\frac{dN_A}{dt} = r_A V\right.$

CSTR Mole Balance

- General Mole Balance on System Volume V

In − Out + Generation = Accumulation

$$F_{A0} - F_A + \int r_A dV = \frac{dN_A}{dt}$$



Assumptions

Steady State $\frac{dN_A}{dt} = 0$

Well mixed $\int r_A dV = r_A V$

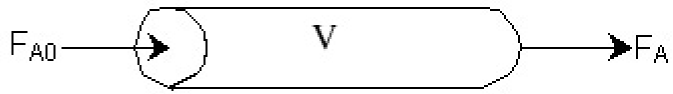
$$F_{A0} - F_A + r_A V = 0$$

$$V = \frac{F_{A0} - F_A}{-r_A}$$

PFR Mole Balance

- In − Out + Generation = Accumulation

$$F_{A0} - F_A + \int r_A dV = \frac{dN_A}{dt}$$



Steady State

$$\frac{dN_A}{dt} = 0$$

$$F_{A0} - F_A + \int r_A dV = 0$$

Differentiate with respect to V

$$0 - \frac{dF_A}{dV} = -r_A$$

$$\boxed{\frac{dF_A}{dV} = r_A}$$