

CHEMICAL REACTOR DESIGN

CHENG 323 Dr Shaker Haji

1

Student Outcomes

2

- *Student outcomes of concern in CHENG 323:*
 - SO 1: an ability to identify, formulate, and solve complex engineering problems by applying principles of engineering, science, and mathematics.
 - SO 2: an ability to apply engineering design to produce solutions that meet specified needs with consideration of public health, safety, and welfare, as well as global, cultural, social, environmental, and economic factors

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Lecture 1

Prepared by: Dr Shaker Haji - CHENG 323

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What are the Core Subjects of Chemical Engineering?


20 min

4

- 1) Chemical Engineering Thermodynamics
- 2) Transport Phenomena
 - a. Momentum Transfer/Fluid Mechanics.
 - b. Mass Transfer/Separation Processes.
 - c. Heat Transfer
- 3) Chemical Reaction Engineering

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What Do Chemical Kinetics and Chemical Reaction Engineering Involve?

5

Chemical kinetics is the study of chemical reaction rates and mechanisms.

The study of **chemical reaction engineering (CRE)** combines the study of *chemical kinetics* with the *design of the reactors* in which the reaction occur.

It is primary the knowledge of **chemical reaction engineering (CRE)** that distinguishes the chemical engineer from other engineers.

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What Does Chemical Engineering Thermodynamics Involve?

6

It involves:

- Calculations of heat and work requirements for physical and chemical processes.
- Determination of equilibrium compositions/conditions in cases of:
 - chemical reactions
 - transfer of chemical species between phases

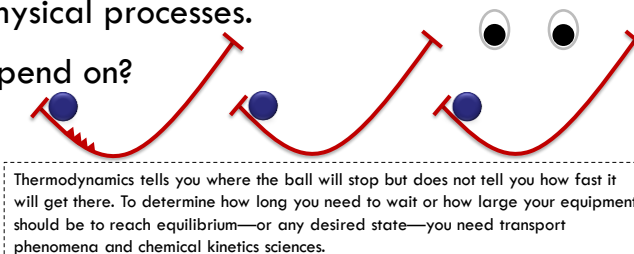
6

What Thermodynamics Cannot Predict?

1. Thermodynamic consideration do not establish the *rates* of chemical and physical processes.

What do rates depend on?

- driving force
- resistance



Although driving forces are thermodynamic variables, resistances are not.

2. Neither can thermodynamics, reveal the microscopic mechanisms of physical and chemical processes.

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Time Out: Generalized Equation for Flux

- Rates depend on Driving Force & Resistance
- The governing eq. for any flux (rate/area) can be generalized as: $J = M \cdot F$
 J = Flux, F = Driving Force Gradient, M = Coupling Coefficient, Conductivity, or $1/\text{Resistivity}$
- Examples:

Current Density (Ohm's Law): $I = V/R$ where $R = \rho L/A$

$$j'' = \frac{I}{A} = \frac{1}{\rho} \cdot \frac{V}{L} = \sigma \cdot \frac{V}{L} \quad \text{or} \quad j'' = \sigma \cdot \frac{dV}{dx} \quad (\text{C/s} \cdot \text{cm}^2 \text{ or } \text{A/cm}^2)$$

Molar Flux (Fick's Law of Diffusion): $N_A'' = -D_{AB} \cdot \frac{dC_A}{dx}$ (mol/s·m²)

Heat Flux (Conduction): $q_x'' = -k \cdot \frac{dT}{dx}$ (J/s·m² or W/m²)

Other (Flux = Conductance X Driving Force):

$$q'' = h \cdot \Delta T \quad q'' = U \cdot (T_a - T) \quad N_A'' = k_c \cdot \Delta C_A$$

8

What does each science enable you to know?

same material, same mass, insulated container.

$T_0=50^{\circ}\text{C}$

$T_0=100^{\circ}\text{C}$

$\longrightarrow$

$T_f=75^{\circ}\text{C}$

$T_f=75^{\circ}\text{C}$

after infinite time

Thermodynamics

$\longrightarrow$

$T_{\text{final}} = T_{\text{equilibrium}} = 75^{\circ}\text{C}$

Heat Transfer

$\longrightarrow$

It takes 3 minutes to reach this temperature

10

What does each science enable you to know?

Water-gas shift reaction carried out in a reactor at 827°C & 10 bar.

$\text{CO} + \text{H}_2\text{O} \leftrightarrow \text{CO}_2 + \text{H}_2$

1 mol

1 mol

1 mol

0 mol

33.3%

33.3%

33.3%

0 mol%

$\longrightarrow$

$\text{CO} + \text{H}_2\text{O} \leftrightarrow \text{CO}_2 + \text{H}_2$

0.67 mol

0.67 mol

1.33 mol

0.33 mol

22.3%

22.3%

44.3%

11 mol%

What is the mixture composition after infinite time?

Thermodynamics

$\longrightarrow$

Final/equilibrium composition is: $y_{\text{CO}}=y_{\text{H}_2\text{O}}=0.223$, $y_{\text{CO}_2}=0.443$, & $y_{\text{H}_2}=0.11$; equilibrium conversion of CO is 33%.

Chemical Reaction Engineering

$\longrightarrow$

To approach this equilibrium composition/conversion,

-How long should I wait? (Batch reactor)

-How big the reactor should be? (Continuous-flow reactor)

Next

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Chemical Reaction Engineering

13

Chemical reaction engineering is at the heart of virtually every chemical process.

Industries that draw heavily on Chemical Reaction Engineering (CRE) are called CPI (Chemical Process Industries).

Examples of CPI?

GPIC; SABIC (~20 companies): Ibn Sina, Yansab, Ibn Rushd;

Dow; DuPont; Shell; Chevron; Bapco

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Chemical Reaction Engineering

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Company	2012 Sales, US\$ billion
BASF	95.1
Sinopec	64.9
ExxonMobil	60.9
Dow Chemical	56.8
SABIC	50.4
Shell	45.8
LyondellBasell	45.3
DuPont	34.8
Mitsubishi	32.8
INEOS	29.9

The top 10 chemical companies in the world ranked by 2012 sales

Company	2012 Sales, US\$ millions
SABIC	50,407
Petro Rabigh	16,536
Tasnee	4,779
Saudi Kayan	2,529
Yanbu National Petrochemical Co.	2,480
Saudi Industrial Investment Group	1,482
Safco	1,328
Sipchem	1,046
Advanced Petrochemicals	659
Alujain	563

The top 10 chemical companies in Saudi Arabia ranked by 2012 sales

Ref: Gerlowski, L., & Al Othman, A. (2014, August). Saudi Arabia's Chemicals Industry Continues to Grow. *Chemical Engineering Progress (CEP, an AIChE publication)*, 64-68.

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Areas of Applications

15

In addition to the more traditional areas of the manufacturing of chemicals & pharmaceuticals, the *Chemical Reaction Engineering (CRE)* principles can also be applied in areas such as

- waste treatment
- microelectronics
- nanoparticles
- living systems

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Smog (Ch. 1, Ch. 7)

Wetlands (Ch. 4)

Nitroaniline Plant Explosion
Exothermic Reactions That Runaway

Plant Safety
(Ch. 8 & 9)

Oil Recovery
(Ch. 5)

Cobra Bites
(Ch. 6)

Pharmacokinetics of Cobra Bites
Multiple Reactions in a Batch (Batch) Reactor

Lubricant Design
(Ch. 7)

Effective Lubricant Design
Scavenging Free Radicals

Manufacture of Phthalic Anhydride (Ch. 3)

Mask, Etch, then Strip Mask

CVD, Mask, Etch, Strip Mask

CVD of Final Layer

16

16



35 min

How much to study?!

19

How much time is needed to study for this course?

You will need at least 6 hours per week for this course:

- Plan A:
 - 1 hr after each lecture ($1 \times 3 = 3$ hr) [Sun, Tue, & Thu]
 - 3 hr during the weekend to solve the suggested problems
- Plan B:
 - 1.5 hr before each lecture ($1.5 \times 2 = 3$ hr) [Mon & Wed]
 - 3 hr during the weekend to solve the suggested problems

Attend
Classes

Read Book/
YouTube Lec.

Examples

Problems

MCQs

Previous
Exams

- Start from Today!

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How much do I study for this course?

20



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Materials on the Web and CDROM

CDROM & Web: <http://www.umich.edu/~elements/5e/>

Elements of
Chemical Reaction Engineering
(2020)

Essentials of
Chemical Reaction Engineering
(2016)

Welcome to Chemical Reaction Engineering!

ENHANCED BY Google

Select Chapter

Complete Introduction

Chapter 1

Chapter 2

Chapter 3

Chapter 4

Chapter 5

Chapter 6

Chapter 7

Chapter 8

Chapter 9

Appendices

Chapter 10

Chapter 11

Chapter 12

Chapter 13

Chapter 14

Chapter 15

Chapter 16

Chapter 17

Chapter 18

Let's Get Started

Lecture Notes

Software

Undergraduate (ChE 344)

Homepage

Graduate (ChE 528)

Homepage

Asynchronous Learning

Additional Textbook

Websites

Additional Resources

SafeChemE Website

Interactive Computer Games

Web Modules

Thoughts on Problem Solving

FAQs

Fun YouTube Videos

Updates and Typos

23

BY CHAPTER

HIDE

Objectives

Living Example Problems

Extra Help

Summary Notes

LearnChemE

Screencasts

FAQs

Interactive Computer Modules

Additional Material

Self Test

Clicker Questions

Professional Reference Shelf

BY CONCEPT

HIDE

Interactive Modules

Web Modules

Interactive Computer Games

Living Example Problems

U OF M

HIDE

Asynchronous Learning

ChE 344

ChE 528

Chapter 1: Mole Balances

Objective

Hello completing Chapter 1 of the text and associated website material, the reader will be able to:

Define the rate of chemical reaction.

Apply the mole balance equations to a BR, CSTR, PFR, and PBR.

Describe photos of real reactors.

Useful Links

Living Example Problems

Polymath, Python, Matlab and Wolfram code to help visualize and deeper understand certain concepts

Extra Help

LearnChemE

Screencasts, Summary Notes, FAQs, and Interactive Computer Modules that provide for deeper understanding of important concepts

Additional Materials

New Technical Material, Detailed Derivations and Web Modules with Novel Applications, along with expanded explanations and examples that didn't make it in

Professional Reference Shelf

Material important to the practicing engineer that is not necessarily covered in all CRE courses.

Computer Simulation Problem Statements

Digital problems using Wolfram and Python as well as Matlab and Polymath

Youtube Videos

Humorous videos covering topics varying from example problems to light hearted breaks from studying

Evaluation

Self Tests

Interactive problems with solutions to provide extra practice of concepts

Clicker Questions

Interactive multiple choice questions to help access your understanding of the material

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24

CHENG 323

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BY CHAPTER

HIDE

- Objectives
- Living Example Problems
- Extra Help
 - Summary Notes
 - LearnChemE
 - Screencasts
 - FAQs
 - Interactive Computer Modules
- Additional Material
- Self Test
- i>Clicker Questions
- Professional Reference Shelf

BY CONCEPT

HIDE

- Interactive Modules
 - Web Modules
 - Interactive Computer Games
- Living Example Problems

U OF M

HIDE

- Asynchronous Learning
- ChE 344
- ChE 528

Chapter 1: Mole Balances

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Hello completing **Chapter 1** of the text and :

- Define the rate of chemical reaction
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BY CHAPTER

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Chapter 1: Mole Balances

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Interactive multiple choice questions to help access your understanding of the material

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The screenshot shows a course navigation interface. On the left is a sidebar with three main sections, each with a 'HIDE' button and a right-pointing arrow:

- BY CHAPTER** (circled in red):
 - Objectives
 - Living Example Problems
 - Extra Help
 - Summary Notes
 - LearnChemE
 - Screencasts
 - FAQs
 - Interactive Computer Modules
 - Additional Material
 - Self Test
 - Clicker Questions
 - Professional Reference Shelf
- BY CONCEPT** (circled in red):
 - Interactive Modules (indicated by a blue arrow pointing to it)
 - Web Modules
 - Interactive Computer Games
 - Living Example Problems
- U OF M** (circled in red):
 - Asynchronous Learning
 - ChE 344
 - ChE 528

The main content area on the right features a dark blue background with white and yellow text, framed to look like a screen. It reads:

Focus on Creative Problem Solving:
Strategies for Developing Creative Engineers

Kinetic Challenge I

Jonas Daunoravicius
Stephan Su
Prof. H. Scott Fogler

University of Michigan
Department of Chemical Engineering

Optimized for 800x600 resolution Continue

Below this screen, the text **INTERACTIVE COMPUTER MODULES** is displayed. Underneath it are links: [Kinetics Challenge 1 -- Quiz Show](#), [Introduction to Kinetics, Status: Final Release](#), [Details](#), and **Objectives for [Chapter One](#)**.

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The slide has a blue header bar at the top. On the left side of this bar is an orange square containing the number '28'. To the right of the square, the text 'Lecture 2' is written in white. The main body of the slide is white with horizontal lines. At the bottom, centered, is the text 'Prepared by: Dr Shaker Haji - CHENG 323'.

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Course Policies



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Course Policies

The course guidelines include, but are not limited to, the following:

1. The students are expected to:
 - arrive on time for all classes (lectures/tutorials). Latecomers are expected to enter the classroom quietly.
 - have their mobile phone on "Silent" and refrain from using it. I don't want to see your mobile phone!
 - be attentive in class and engage in classroom activities. Side conversations are not allowed.
 - learn both the conceptual and computational aspects of the covered materials.
 - print and bring the lecture notes and the appendices to all sessions (a must). They are available on Blackboard or MS Teams as PDF files.
 - compile all the fundamental equations in one place (e.g., A4 papers) to be used in the classroom (not allowed in quizzes or exams)

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Course Policies

2. A list of fundamental equations and textbook appendices will be given in the exams. You will not need to derive the necessary equations unless you are asked to or if they are not provided.
3. Attendance is taken at the beginning of the class.
4. Coursework (project report or other work) submitted after the stated deadline will be subjected to grade deductions.
5. There will be both announced and unannounced quizzes. If you miss a quiz, you will receive a grade of zero for that quiz (no make-up quizzes).
6. Recording classroom activities or taking pictures in the classroom is not allowed.
7. There is zero tolerance for cheating and plagiarism.

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1 Mole Balances

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In this Chapter

33

Introduction
Definitions
General Mole Balance Equation
Batch, CSTR, PFR, PBR

33

Chemical Reaction Engineering (CRE)



10 min

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Chemical Reaction Engineering (CRE) is the field that studies:

1. the rates and mechanisms of chemical reactions (chemical kinetics), and
2. the design of the reactors in which they take place.

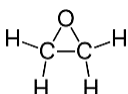
34

Chemical Identity

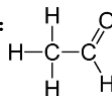
35

- The identity of a chemical species is determined by the *kind, number, & configuration* of that species' atoms.
- Changing one of the above leads to completely different chemical species; examples:
 - ▢ changing kind of atoms: O_2 vs. CO
 - ▢ changing number of atoms: O_2 vs. O_3
 - ▢ changing configuration of atoms (structure): C_2H_4O

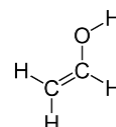
Ethylene Oxide:



Acetaldehyde:



Ethenol:



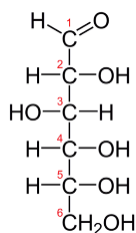
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Chemical Identity

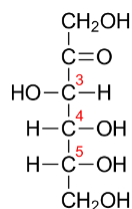
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Test yourself:

- Sucrose (table sugar) is digested in the body via the enzyme sucrase to **glucose** (blood sugar) and **fructose** (fruit sugar).
- What makes these two compounds different chemical species although they have the same chemical formula ($C_6H_{12}O_6$)?
- Is it the *kind, number, or configuration* of the atoms?



glucose



fructose

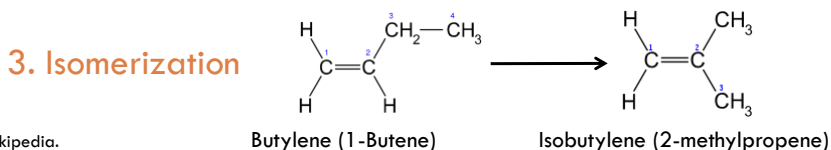
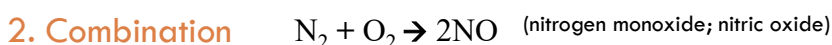
Ref: Wikipedia.com

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Chemical Identity

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- A chemical species is said to have reacted when it has lost its chemical identity.
- There are three basic ways a species may lose its chemical identity:



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Reaction Rate



20 min

38

- During a chemical reaction, some species are consumed while others are generated.
- In this classical approach to chemical change, it is assumed that the total mass is neither created nor destroyed.
- Chemical rxn: $\text{H}_2 + \frac{1}{2} \text{O}_2 \rightarrow \text{H}_2\text{O}$
- Is there a non-classical approach to chemical change?
Another type of rxns?

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Reaction Rate

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- The **reaction rate** is the rate at which a species loses its chemical identity per unit volume.
- i.e. the rxn rate is the number of moles of species i reacted per unit volume per unit time.
- The rate of a reaction (mol/L·s) can be expressed as either
the rate of Disappearance (Consumption): $-r_i$
or as
the rate of Formation (Generation): r_i

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Reaction Rate

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Consider the isomerization **A → B**

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

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

What is r_B ?

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

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Reaction Rate

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□ Example: $A \rightarrow B$ (isomerization)

If species B is being formed at a rate of 0.2 moles per decimeter cubed per second, i.e., $r_B = 0.2 \text{ mole/dm}^3/\text{s}$, then A is disappearing at the same rate.

▣ A is disappearing at a rate which is written as:

$$-r_A = 0.2 \text{ mole/dm}^3/\text{s}$$

▣ The rate of formation (generation) of A is

$$r_A = -0.2 \text{ mole/dm}^3/\text{s}$$

▣ Do you recall Kirchhoff's current law?!

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Reaction Rate

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- The **reaction rate** is the rate at which a species loses its chemical identity per unit volume ($\text{mol/dm}^3/\text{s}$).
- 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 ($\text{mol/g}_{\text{cat}}/\text{s}$).
- The heterogeneous reaction rate can also be expressed on a per catalyst surface area, where it is referred to as $-r_A''$ ($\text{mol/m}^2/\text{s}$).

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Mathematical Definition of Reaction Rate

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- The *mathematical definition* of a chemical reaction rate has been a source of confusion in the literature.
- It is common to see the rate of rxn defined as: $r_A = \frac{dC_A}{dt}$
- This definition is wrong! dC_A/dt is not the rate of reaction.
- The above eq. is simply the mole balance for a constant volume batch reactor
- This eq. does not apply to any continuous flow reactor operated at steady state (e.g. CSTR where $C_A \neq f(t)$)

[Read @ home](#)

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Mathematical Definition of Reaction Rate

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- So what is the rate of rxn and what is its equation?
- The rate of rxn (r_i) is the number of moles of species i generated per unit volume per unit time.
- The equation of the rxn rate (i.e., rate law) is an algebraic equation that is solely a function of the properties of the reacting materials and reaction conditions at a point in the sys.
- The rate equation is independent of the type of reactor (e.g., batch or continuous flow) in which the reaction is carried out.
- However, because the properties and rxn conditions of the reacting materials may vary with position in a chemical reactor, it can vary from point to point in the system.

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Mathematical Definition of Reaction Rate

45

- The reaction rate equation (rate law) is an algebraic equation, not a differential equation.
- For example, for $A \rightarrow B$, the reaction rate could be:

$$-r_A = kC_A \quad -r_A = kC_A^2 \quad -r_A = \frac{k_1 C_A}{1 + k_2 C_A}$$

45

Reaction Rate

46

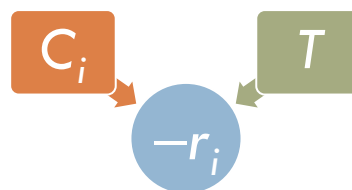
- The reaction rate, and therefore, the reaction rate equation (rate law) is function of the:
 - ▣ properties of the reacting materials (H_2 vs. N_2)
 - ▣ reaction conditions (T , C_{i0} , P , etc.)
- The reaction rate equation is independent of the type of reactor (batch or continuous-flow, etc.)

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Reaction Rate

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- The reaction rate is function of the properties of the reacting materials and reaction conditions
- For a given set of reacting materials and rxn environment (solvent, phase...etc), **the rxn rate is mainly function of the:**
 - reactants' concentrations
 - temperature
- For catalyzed reactions, the rxn rate is also function of the catalyst activity.

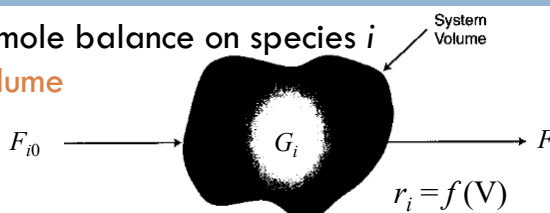


47

1.2 The General Mole Balance Equation

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We want to perform a mole balance on species i around the **system volume** shown here:



Recall that for conserved quantities the balance is:

$$\text{Accumulation} = \text{Input} - \text{Output}$$

While for non-conserved quantities it is:

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

$$\text{Or: } \text{In} - \text{Out} + \text{Generation} = \text{Accumulation} \quad [\text{mol/s}]$$

(to the
sys)

(from
the sys)

(within
the sys)

(within
the sys)

48

1.2 The General Mole Balance Equation



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- Examine the **system volume** shown below:

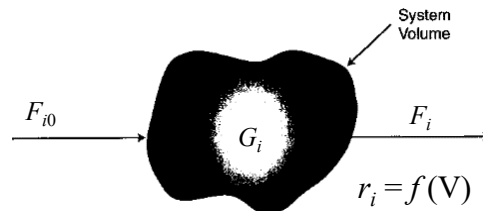
- What are F_{i0} , F_i , & G_i ?

- Units of $G_i = \text{mole } i/\text{s}$

$$r_i = \text{mole } i/\text{L}\cdot\text{s}$$

- Why $r_i = f(V)$?

- Calculate G_i from r_i .



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1.2 The General Mole Balance Equation

50

- Examine the **system volume** shown below:

- What are F_{i0} , F_i , & G_i ?

- Units of $G_i = \text{mole } i/\text{s}$

$$r_i = \text{mole } i/\text{L}\cdot\text{s}$$

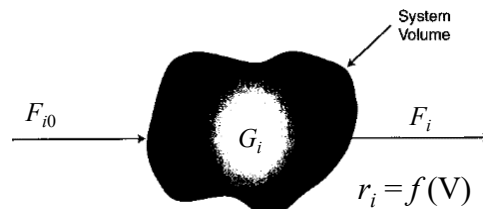
- Why $r_i = f(V)$?

- Calculate G_i from r_i .

- Calculate G_i if all the sys. variables (e.g. C_i , T , P , cat activity) are spatially uniform throughout the sys. volume.

- If $r_i \neq f(V)$, then $G_i = r_i V$.

- However, this is not the case here, i.e. $r_i = f(V)$.

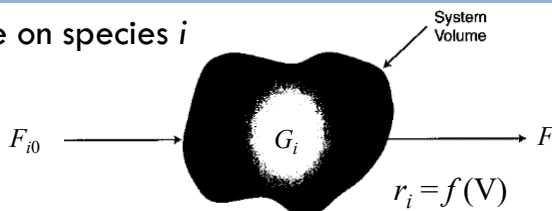


50

1.2 The General Mole Balance Equation

51

Perform a mole balance on species i
in the **system volume**
shown here:



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

51

General Mole Balance

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$$F_{i0} - F_i + \int_0^V r_i \cdot dV = \frac{dN_i}{dt}$$

- From this **general mole balance equation**, we can develop the design equations for the various types of industrial reactors: batch, semibatch, & continuous-flow.
- Upon evaluation of these equations, we can determine the **time** (batch) or **reactor volume** (continuous-flow) necessary to convert a specified amount of reactants to products.

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Lecture 3

General Mole Balance Equation:

1. Batch Reactor

2. Continuous Stirred Tank Reactor (CSTR)

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1.3 Batch Reactors

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- A batch reactor has neither inflow nor outflow of reactants or products while a reaction is being carried out.
- The reaction takes place during that time.
- A typical batch reactor consists of a tank with an agitator and integral heating/cooling system.

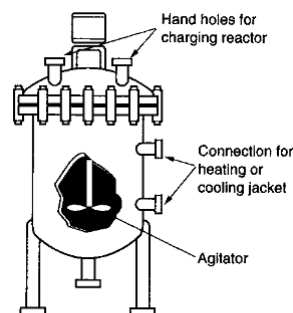


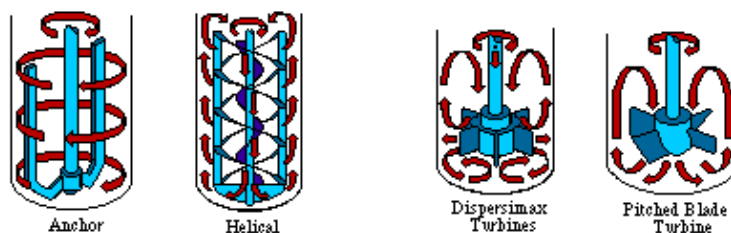
Figure 1-5(a) Simple batch homogeneous reactor. [Excerpted by special permission from *Chem. Eng.*, 63(10), 211 (Oct. 1956). Copyright 1956 by McGraw-Hill, Inc., New York, NY 10020.]

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1.3 Batch Reactors

55

- In the batch reactor, it is assumed that the reaction mixture is perfectly mixed.
- What does that imply?
- Therefore, there is no variation in the rate of reaction throughout the reactor volume.



Mixing patterns in a batch reactor or CSRT [Encyclopedia of Equipment]

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1.3 Batch Reactors

56

- What are the batch reactor uses, advantages, and disadvantages?

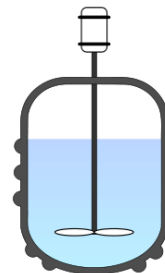


56

1.3 Batch Reactors

57

- A batch reactor is used for:
 - ▣ Study reactions in labs (kinetic data)
 - ▣ Testing new processes that have not been fully developed
 - ▣ Small-scale operation (low demand or expensive products)
 - ▣ Processes that are difficult to convert to continuous operations



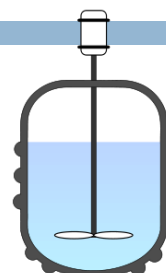
Batch reactor symbol [wiki]

57

1.3 Batch Reactors

58

- Advantages of batch reactors
 - ▣ High conversions through leaving the reaction mixture in the reactor for long periods of time.
- Disadvantages of batch reactor:
 - ▣ High labor costs per batch
 - ▣ The variability of products from batch to batch
 - ▣ Difficulty of large scale production

Batch reactor symbol
[wiki]

58

1.3 Batch Reactors



59

Starting from the general mole balance equation, derive the **batch reactor mole balance**.

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

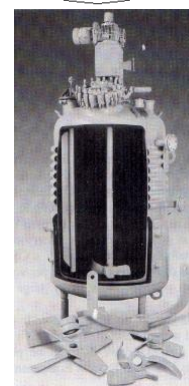
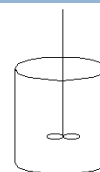
$$F_{A0} = F_A = 0$$

Well mixed

$$\int r_A dV = r_A V$$

Design Equation of Batch Reactor.

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



59

1.3 Batch Reactors

60

Starting from the batch reactor mole balance, find the time, t_1 , necessary to reduce the initial number of moles of A from N_{A0} to a final desired number N_{A1} .

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

Differential Form of Batch Reactor Design Equation

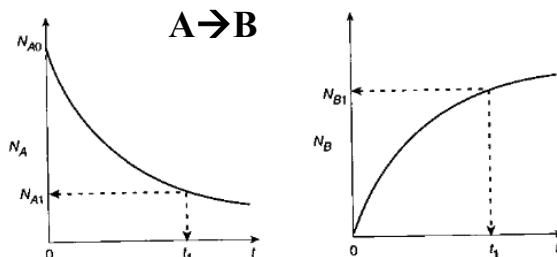


Figure 1-6 Mole-time trajectories.

$$t_1 = \int_{N_{A1}}^{N_{A0}} \frac{dN_A}{-r_A V}$$

Integral Form of Batch Reactor Design Equation

60

How Long Does the RXN Take?



61

CDP1-A:

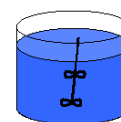
(solve in < 15 min)

A 200-L constant-volume batch reactor is pressurized to 20 atm with a mixture of 75% A and 25% inert. The gas-phase reaction ($A \rightarrow B + C$) is carried out isothermally at 227°C.

- Assuming that the ideal gas law is valid, how many moles of A are in the reactor initially? What is the initial concentration of A?

$$(R = 0.08206 \text{ L}\cdot\text{atm}/\text{mol}\cdot\text{K})$$

$$N_{A0} = 73.1 \text{ mol}, C_{A0} = 0.365 \text{ M}$$



61

How Long Does the RXN Take?

62

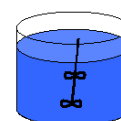
CDP1-A:

(solve in < 15 min)

A 200-L constant-volume batch reactor is pressurized to 20 atm with a mixture of 75% A and 25% inert. The gas-phase reaction ($A \rightarrow B + C$) is carried out isothermally at 227°C.

- If the reaction is first order, $-r_A = kC_A$ with $k = 0.1 \text{ min}^{-1}$, calculate the time necessary to consume 99% of A. [Solve the ODE in terms of N_A]

$$t = 46 \text{ min}$$



62

How Long Does the RXN Take?

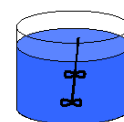
63

CDP1-A:

(solve in < 15 min)

A 200-L constant-volume batch reactor is pressurized to 20 atm with a mixture of 75% A and 25% inert. The gas-phase reaction ($A \rightarrow B + C$) is carried out isothermally at 227°C.

- Determine the pressure at the calculated time



63

How Long Does the RXN Take?

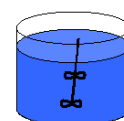
64

CDP1-A:

(solve in < 15 min)

A 200-L constant-volume batch reactor is pressurized to 20 atm with a mixture of 75% A and 25% inert. The gas-phase reaction ($A \rightarrow B + C$) is carried out isothermally at 227°C.

- Determine the pressure at the calculated time



$P = 34.85 \text{ atm}$

64

How Long Does the RXN Take?

65

CDP1-A (modified):

A 200-L constant-volume batch reactor is pressurized to 20 atm with a mixture of 75% A and 25% inert. The gas-phase reaction is carried out isothermally at 227°C.

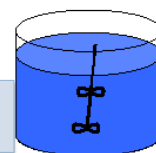
- Assuming that the ideal gas law is valid, how many moles of A are in the reactor initially? What is the initial concentration of A?

$$(R = 0.08206 \text{ L}\cdot\text{atm}/\text{mol}\cdot\text{K})$$

- If $-r_A = kC_A^2$ with $k = 0.7 \text{ L}/\text{mol}\cdot\text{min}$, calculate the time necessary to consume 99% of A.

- Determine the pressure at the calculated time.

$$N_{A0} = 73.1 \text{ mol}, C_{A0} = 0.365 \text{ M}, P = 34.85 \text{ atm}, t = 386.9 \text{ min}$$



65

Done by Marwa Alwadi 20195477

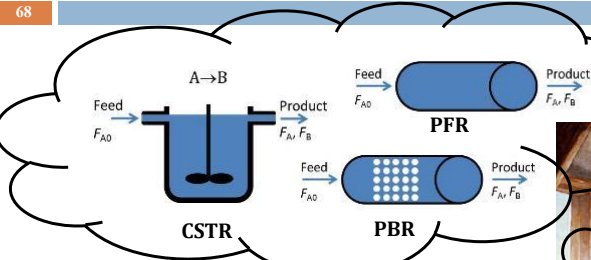


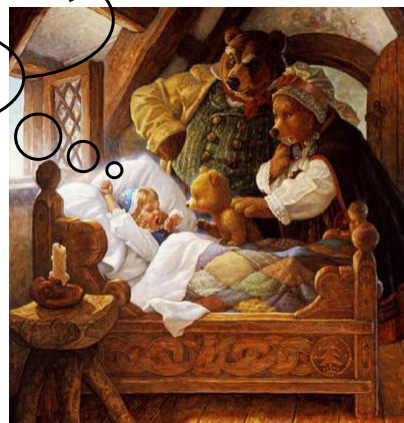
66

66

 30 min

1.4 Continuous-Flow Reactors





The story of:

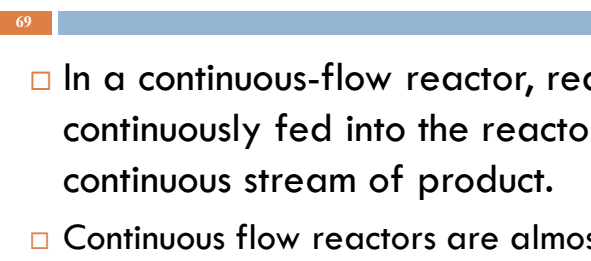
Goldilocks and the Three Continuous-Flow Reactors

www.rounds.com

68

 30 min

1.4 Continuous-Flow Reactors



- In a continuous-flow reactor, reactants are continuously fed into the reactor and emerge as continuous stream of product.
- Continuous flow reactors are almost always operated at steady state.
- We will consider three types:
 - ▣ Continuous Stirred Tank Reactor (CSTR)
 - ▣ Plug Flow Reactor (PFR)
 - ▣ Packed Bed Reactor (PBR)

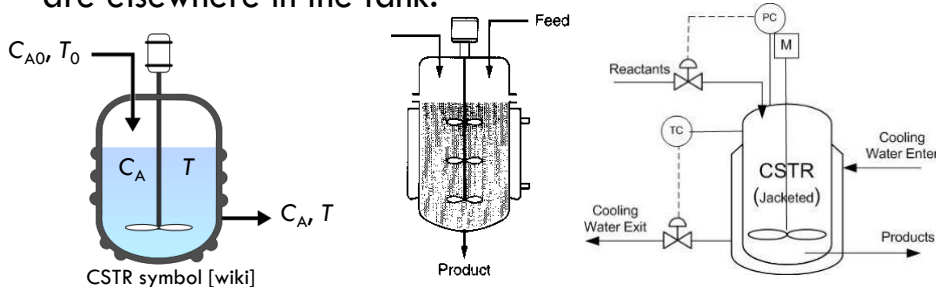
} Tubular Reactors

69

1.4.1 Continuous-Stirred Tank Reactor

70

- CSTR is used primarily for liquid phase reactions and is normally operated at steady state.
- It is assumed to be perfectly mixed. So?
- Therefore, T & C_i are the same at the exit point as they are elsewhere in the tank.

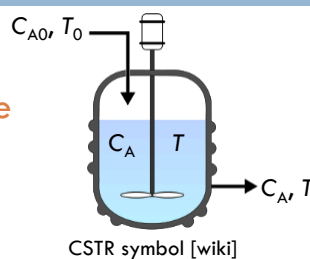


70

1.4.1 Continuous-Stirred Tank Reactor

71

Starting from the general mole balance equation, derive the **CSTR mole balance equation** for A.



71

1.4.1 Continuous-Stirred Tank Reactor

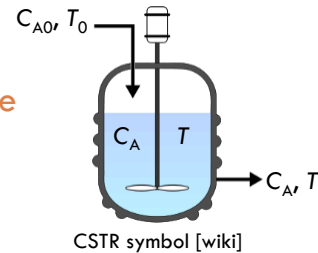
72

Starting from the general mole balance equation, derive the **CSTR mole balance equation** for A.

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

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

CSTR Design Equation.



The CSTR design equation gives the reactor volume V necessary to reduce the entering flow rate of species A, from F_{A0} to the exit flow rate F_A , when species A is disappearing at a rate of $-r_A$.

72

1.4.1 Continuous-Stirred Tank Reactor

73

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

CSTR mole balance equation.

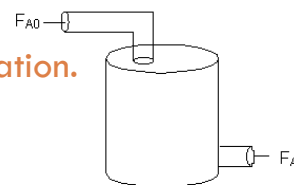
Solve for F_A :

$$F_A = F_{A0} + V \cdot r_A$$

Compare to the mole balance in CHENG 111

$$(\dot{n}_i)_{out} = (\dot{n}_i)_{in} + v_i \cdot \dot{\xi}$$

What cannot be done with the CHENG 111 equation & why?



73

1.4.1 Continuous-Stirred Tank Reactor

74

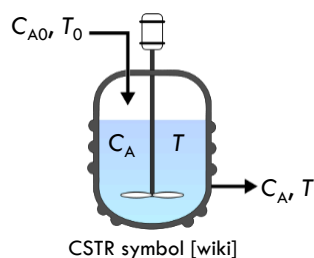
- For liquids, how the molar flow rate of A (F_A) is quantified?
- F_A can be calculated from the concentration C_A & the volumetric flow rate v (lowercase Upsilon) as:

$$F_A = C_A \cdot v$$

- Hence the design equation can be rewritten as:

$$V = \frac{v_0 C_{A0} - v C_A}{-r_A}$$

- How can C_A & v be measured?



74

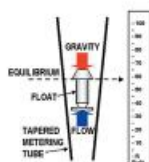
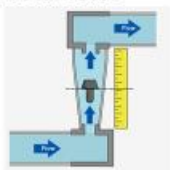
3.2b Flow Rate Measurement

Slide
form
CHENG
111

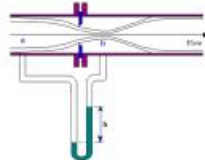
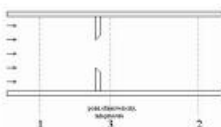
A **flowmeter** is a device mounted in a process line that provides a continuous reading of the flow rate in the line.

Two commonly used **flowmeters** are:

1. rotameter



2. orifice meter



75

76

Lecture 4

Prepared by: Dr Shaker Haji - CHENG 323

76

78

Lecture 4

General Mole Balance Equation:

- 3. Plug Flow Reactor (PFR)
- 4. Packed Bed Reactor (PBR)

} Tubular Reactors

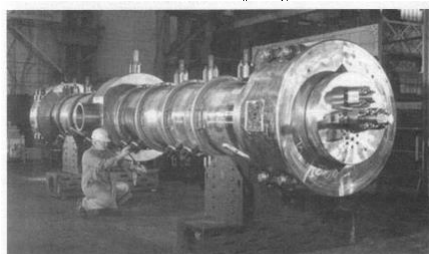
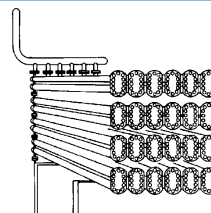
Prepared by: Dr Shaker Haji - CHENG 323

78

1.4.2 Plug Flow Tubular Reactor

79

- Tubular Reactor consists of cylindrical pipes and is normally operated at steady state.
- It is used most often for gas-phase reactions.



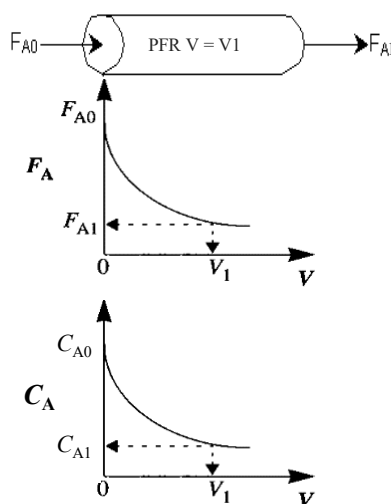
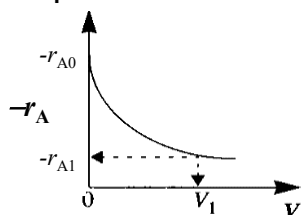
Polyethylene reactor; this 16-in inner-diameter reactor is designed to operate at 35,000 psi and 600°F; in operation, this reactor is in a vertical configuration. Courtesy of Autoclave Engineers, Division of Snap-tite, Inc.

79

1.4.2 Plug Flow Tubular Reactor

80

- In the tubular reactor, the reactants are continually consumed as they flow down the length of the reactor.
- Hence, the reaction rate varies axially (except for zero-order rxn)

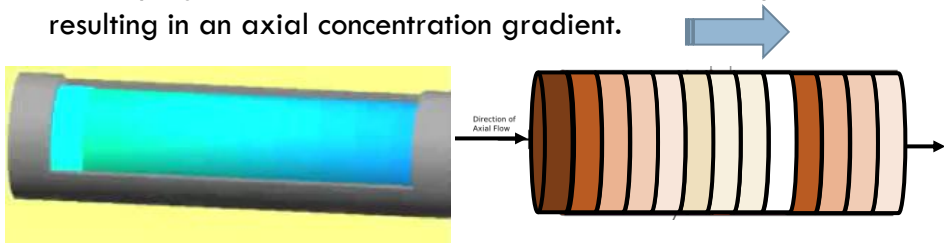


80

1.4.2 Plug Flow Tubular Reactor

81

- The fluid-flow through the tubular reactor may be modeled as a flow of a series of infinitely thin coherent "plugs", each with a uniform composition.
- The plugs are viewed to be traveling in the axial direction of the reactor, with each plug having a different composition from the ones before and after it.
- As the plug flows down the reactor the reaction takes place, resulting in an axial concentration gradient.

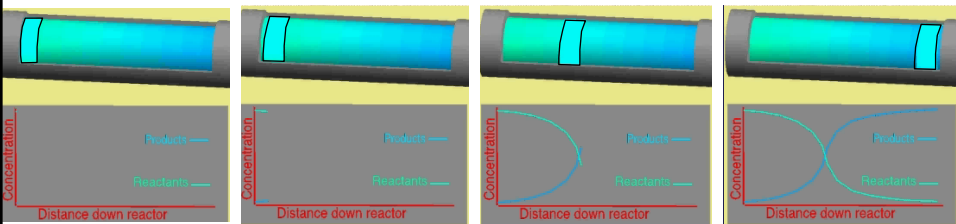


81

1.4.2 Plug Flow Tubular Reactor

82

- As the plug flows down the reactor the reaction takes place, resulting in an axial concentration gradient.



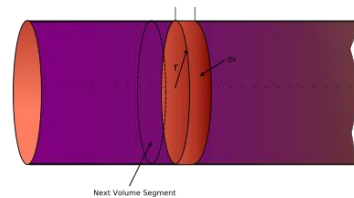
Operation of a PFR & the reactants & products concentration profile [Encyclopedia of Equipment]

82

1.4.2 Plug Flow Tubular Reactor

83

- The key assumption is that as a plug flows through a PFR, the fluid is perfectly mixed in the radial direction but not in the axial direction (forwards or backwards).
- What can each plug be modeled as? i.e. what type of reactor (Batch/CSTR)?



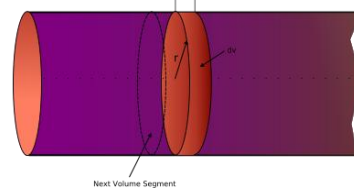
Schematic diagram of a Plug Flow Reactor (PFR) [wiki]

83

1.4.2 Plug Flow Tubular Reactor

84

- The key assumption is that as a plug flows through a PFR, the fluid is perfectly mixed in the radial direction but not in the axial direction (forwards or backwards).
- What can each plug be modeled as? i.e. what type of reactor (Batch/CSTR)?
- Each plug of differential volume is considered as a separate entity, effectively an infinitesimally small batch reactor, limiting to zero volume.
- Plugs of reactants are continuously fed into the reactor.
- Here, we are looking at the FLOW as small PLUGS.



Schematic diagram of a Plug Flow Reactor (PFR) [wiki]

84

1.4.2 Plug Flow Tubular Reactor



85

- Now we will look at the REACTOR as small SEGMENTS.
- What can each segment be modeled as? i.e. what type of reactor (Batch/CSTR)?
- PFR can also be viewed and modeled as large number of CSTRs in series.
- Every segment, which is infinitesimally small, can be viewed as a CSTR.

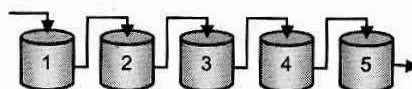


Figure 2-5 Modeling a PFR with CSTRs in series.

85

1.4.2 Plug Flow Tubular Reactor

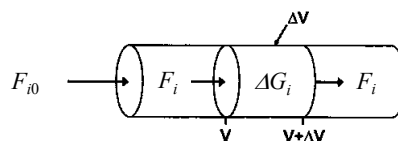


87

$$F_{i0} - F_i + \int_0^V r_i \cdot dV = \frac{dN_i}{dt} \rightarrow \text{GMBE}$$

- The PFR **design equation** can be derived from the GMBE in two ways:

1. Apply GMBE on ΔV



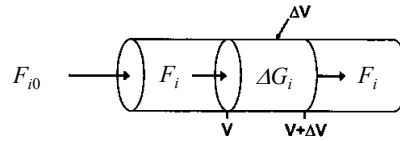
2. Apply GMBE on the whole V , then differentiate wrt to V



87

1. Apply GMBE on ΔV

The ΔV is chosen sufficiently small such that there are no spatial variation in reaction rate within this volume.



88

88

$$F_{i0} - F_i + \int_0^V r_i \cdot dV = \frac{dN_i}{dt} \rightarrow \text{GMBE}$$

2. Apply GMBE on the whole V , then differentiate wrt to V



89

89

1.4.2 Plug Flow Tubular Reactor

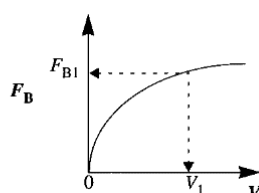
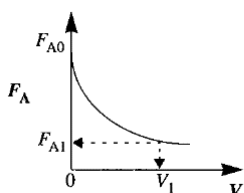
90

Differential Form of
PFR Design Eq.

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



Find the volume, V , necessary to reduce the entering molar flow rate from F_{A0} to the exit molar flow rate of F_A .



$$V = \int_{F_{A0}}^{F_A} \frac{dF_A}{r_A}$$

Integral form of
PFR Design Eq.

90

1.4.2 Packed-Bed Reactor



92

PBR:



The fluid-solid heterogeneous rxns take place on the surface of the catalyst.

Consequently, the rxn rate is based on mass of solid catalyst, W , rather than on reactor volume, V .

The rate of rxn of a substance A is, therefore, defined as:

$$-r'_A = \text{mol A reacted/s} \cdot \text{g catalyst}$$

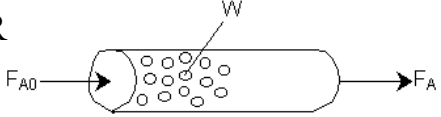
The mass of solid catalyst is used because the amount of the catalyst is what is important to the rate of product formation.

92

1.4.2 Packed-Bed Reactor

94

PBR


$$F_{A0} - F_A + \int r'_A dW = \frac{dN_A}{dt}$$

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

$$F_{A0} - F_A + \int r'_A dW = 0$$

Differentiate with respect to W and rearrange

$$\frac{dF_A}{dW} = r'_A$$

94

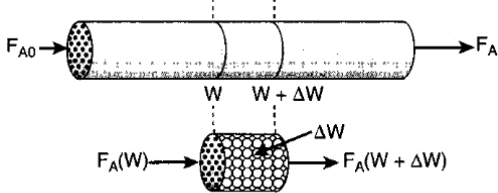


Figure 1-14 Packed-bed reactor schematic.

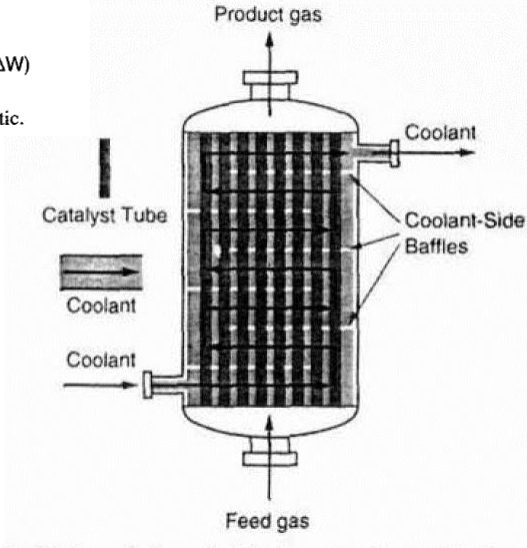


Figure 1-13 Longitudinal catalytic packed-bed reactor.

95



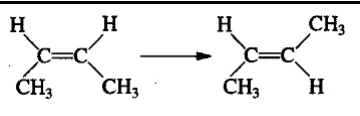
96

تفاني . مثابرة . تصميم . دأب . عزم

Dedication, Perseverance. Persistence. Willpower

96

How Large is the Reactor?



cis-2-butene *trans*-2-butene

30 min

97

Example 1-1: (solve in < 10 min)

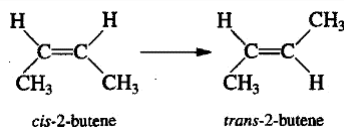
Consider the liquid phase *cis* – *trans* isomerization of 2-butene shown above which can be written symbolically as **A**→**B**.

The first order ($-r_A = kC_A$) rxn is carried out, isothermally, in a tubular reactor in which the volumetric flow rate, ν , is constant.

- Starting from the design equation, derive an algebraic eq. that relates V to C_{A0} , C_A , ν , & k .

97

How Large is the Reactor?



98

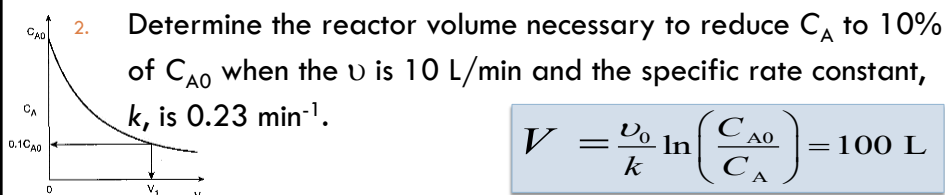
Example 1-1:

(solve in < 10 min)

Consider the liquid phase *cis* – *trans* isomerization of 2-butene shown above which can be written symbolically as $A \rightarrow B$.

The first order ($-r_A = kC_A$) rxn is carried out, isothermally, in a tubular reactor in which the volumetric flow rate, v , is constant.

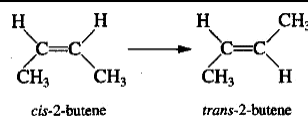
- Starting from the design equation, derive an algebraic eq. that relates V to C_{A0} , C_A , v , & k .



$$V = \frac{v_0}{k} \ln \left(\frac{C_{A0}}{C_A} \right) = 100 \text{ L}$$

98

How Large is the Reactor?



99

Problem 1-6:

$$[C_A = 0.1 C_{A0}, v = 10 \text{ L/min}, k = 0.23 \text{ min}^{-1}, -r_A = kC_A]$$

For the same conditions & requirements of

Example 1-1 (PFR), calculate the volume of a CSTR.

$$V \approx 400 \text{ L}$$

99

How Large is the Reactor?

cis-2-butene *trans*-2-butene

100

Problem 1-6: $[C_A=0.1\ C_{A0},\ v = 10\ \text{L/min},$
 $k=0.23\ \text{min}^{-1},\ -r_A = kC_A]$

For the same conditions & requirements of Example 1-1 (PFR), calculate the volume of a CSTR.

Which volume is larger, the PFR or the CSTR? Explain why.

In order to answer the above question, compare the following:

	V	C_A	$-r_A$
PFR		range:	range:
CSTR			

100

How Large is the Reactor?

cis-2-butene *trans*-2-butene

102

Problem 1-6:

For the same conditions & requirements of Example 1-1 (PFR), calculate the volume of a CSTR.

Which volume is larger, the PFR or the CSTR? Explain why.

In order to answer the above question, compare the following:

	V	C_A	$-r_A$
PFR	~100	range: $C_{A0} - 0.1\ C_{A0}$	range: $kC_{A0} - 0.1\ kC_{A0}$
CSTR	~400	$0.1\ C_{A0}$	$0.1\ kC_{A0}$

102

How Large is the Reactor?

C/C=C/C
cis-2-butene

$\longrightarrow$

C/C=C\C
trans-2-butene

103

C_{A0}

$0.1 C_{A0}$

$0.1 C_{A0}$

$[C_A = 0.1 C_{A0}, v = 10 \text{ L/min},$
 $k = 0.23 \text{ min}^{-1}, -r_A = k C_A]$

C_{A0}

$0.1 C_{A0}$

	V	C_A	$-r_A$
PFR	~ 100	range: $C_{A0} - 0.1 C_{A0}$	range: $k C_{A0} - 0.1 k C_{A0}$
CSTR	~ 400	$0.1 C_{A0}$	$0.1 k C_{A0}$

103



104

105

Lecture 5 – Week 2

- Industrial Reactors & Reactions

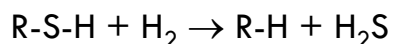
Prepared by: Dr Shaker Haji - CHENG 323

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Examples of Industrial Reactions

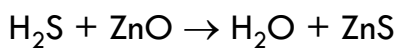
106

- Hydrodesulfurization Reactor (small vessel), NiMo catalyst:



- Two H_2S
Absorbers/Reactors,

Zinc Oxide Bed:



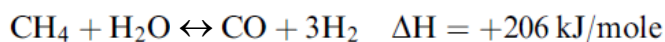
106

Examples of Industrial Reactions

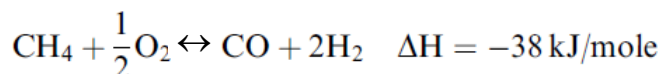
107

In industry, synthesis gas (H_2/CO) is produced from natural gas (CH_4) through:

1. Steam Reforming:



2. Partial Oxidation:



3. Autothermal Reforming:

both together in the same reactor

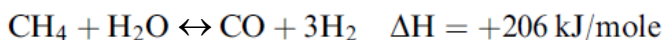
107

Industrial Reactors:

Hydrogen Production:

Natural Gas Reforming –

Steam Reforming



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Examples of Industrial Reactions

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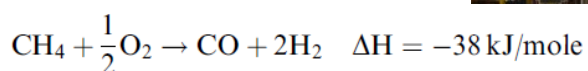
Industrial Reactors:

Hydrogen Production:

Natural Gas Reforming -

Catalytic Partial Oxidation

(secondary reformer)

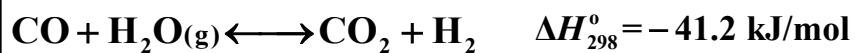


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Examples of Industrial Reactions

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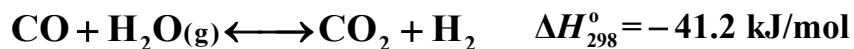
High Temperature & Low Temperature Water Gas Shift Reactors



110

Industrial Reactors

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High Temperature Shift Reactor

Catalyst: Fe Oxide-based

 $T = 330\text{--}470^{\circ}\text{C}$ $V_{HT} = 40\%$ of V_{total} $X = 75\%$ (in the reactor) $X_1 = 75\%$

Low Temperature Shift Reactor

Catalyst: Cu Oxide-based

 $T = 200\text{--}250^{\circ}\text{C}$ $V_{LT} = 40\text{--}50\% > V_{HT}$ $X = 90\%$ (in the reactor) $X_2 = 98\%$ (compared to HT feed)

The above values are typical values for WGS reactors

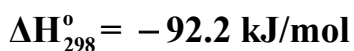
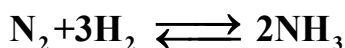
111

Examples of Industrial Reactions



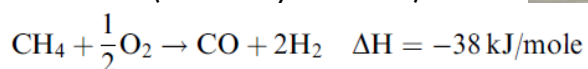
112

Ammonia Converter



Catalytic Partial Oxidation

(secondary reformer)



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Industrial Reactors

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Industrial Reactors:
Hydrotreating Reactors

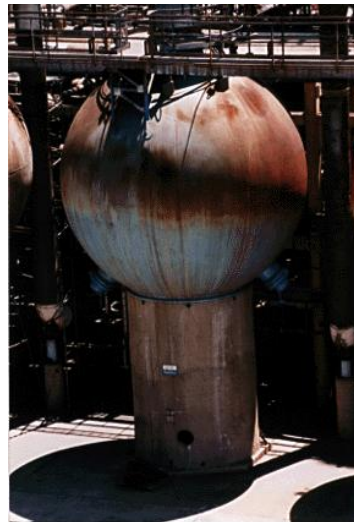


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Industrial Reactors

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Industrial Reactors:
Spherical Reactors



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Industrial Reactors

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Industrial Reactors:
Batch Reactor



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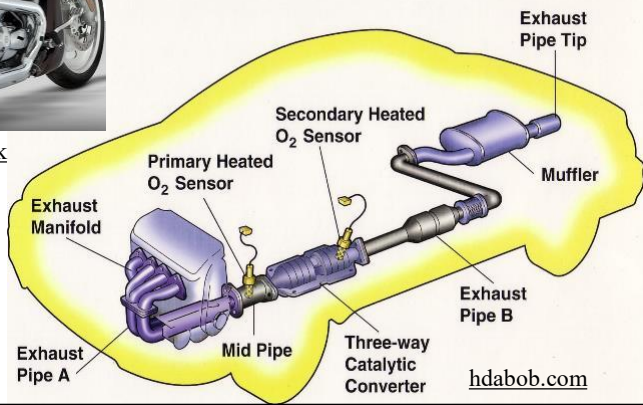
Industrial Reactors

116

Industrial Reactors:
Automotive Catalytic Converter:



www.harleycustom.co.uk



hdabob.com

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Industrial Reactors

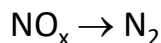
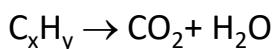
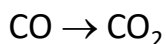
117

Industrial Reactors:

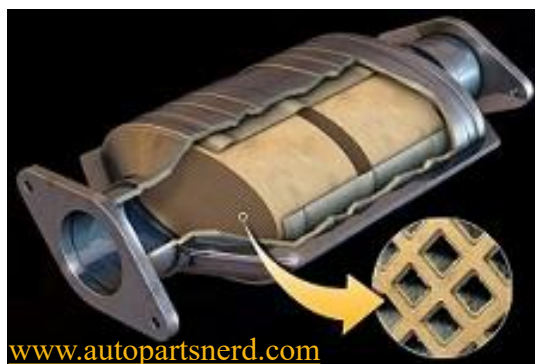
Automotive Catalytic Converter:

toxic byproducts $\xrightarrow[\text{exhaust}]{\text{Cat}}$ less toxic

Converts:



www.europeancarweb.com



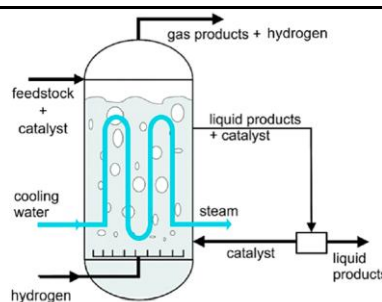
www.autopartsnerd.com

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Industrial Reactors

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Slurry Phase Distillate Reactor



Schematic diagram of a typical slurry-phase hydrocracker.

Energy Fuels 2019, 33, 9, 7917–7949

Slurry reactors:

They are three-phase reactors, meaning they can be used to react solids, liquids, and gases simultaneously.

They usually consist of a catalyst (solid) suspended in a liquid, through which a gas is bubbled.

Example: Sasol Low Temperature Fischer Tropsch™

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Industrial Reactors

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Industrial Reactors:

Fixed Bed Reactors



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Industrial Reactors



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Straight Through Transport Reactor (STTR) in use for a *Fisher-Tropsch* synthesis reaction



The Fischer–Tropsch process:
is a collection of chemical reactions
that converts a mixture of CO & H₂
into liquid hydrocarbons (fuel).

<http://www.oryxgtl.com.qa>

ORYX GTL Plant,
Qatar →



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1.5.1 Liquid-Phase Reactions

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Semibatch reactors and CSTRs are used primarily for liquid-phase rxns. (what is semibatch reactor?)

A semibatch reactor has essentially the same disadvantages as the batch reactor. (mention 3 of these)

However, it has the **advantages** of:

- *T* control by regulation of the feed rate
- the capability of minimizing unwanted side rxns through the maintenance of a low conc. of one of the reactants:

$$A + B \rightarrow D \quad \text{desired rxn}$$
$$A + D \rightarrow U \quad \text{undesired rxn}$$

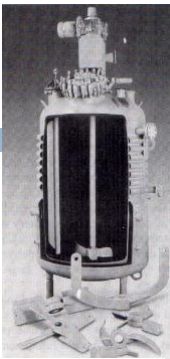
The semibatch reactor is also used for two-phase rxns in which a gas usually is bubbled continuously through the liquid.

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1.5.1 Liquid-Phase Reactions

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A CSTR is used when intense agitation is required.



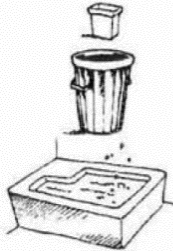


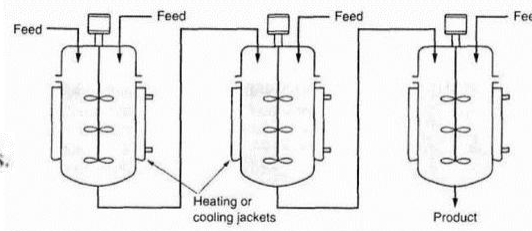
TABLE 1-1. REPRESENTATIVE PFAUDLER CSTR/BATCH REACTOR SIZES AND 2004 PRICES

Volume	Price	Volume	Price
5 Gallons (wastebasket)	\$29,000	1000 Gallons (2 Jacuzzis)	\$85,000
50 Gallons (garbage can)	\$38,000	4000 Gallons (8 Jacuzzis)	\$150,000
500 Gallons (Jacuzzi)	\$70,000	8000 Gallons (gasoline tanker)	\$280,000

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The CSTR can either be used by itself or as part of a series or battery of CSTRs.

Figure 1-16 Battery of stirred tanks.



Advantage: Easy to maintain good T control with a CSTR; why?
Because it is well mixed.

Disadvantage: The concentration of reactant per volume of reactor in CSTR is the smallest of the flow reactors. So?

So, very large reactors are necessary to obtain high conversion.
If you are not able to afford to purchase a new reactor, it may be possible to find a used reactor that may fit your needs.

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1.5.2 Gas-Phase Reactions

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- Gas-phase reactions are often carried out in tubular reactors.
- The tubular reactor is relatively easy to maintain (no moving parts).
- It usually produces the highest conversion per reactor volume of any of the flow reactors.
- The disadvantage of the tubular reactor is that it is difficult to control T within the reactor & hot spots can occur when the rxn is exothermic.
- Most homogeneous liquid-phase flow reactors are CSTRs, whereas most homogeneous gas-phase flow reactors are tubular.

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1.5.2 Gas-Phase Reactions

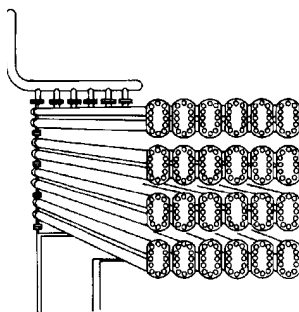


125

- The tubular reactor is commonly found either in the form of one long tube or as one of a number of shorter reactors arranged in a tube bank.



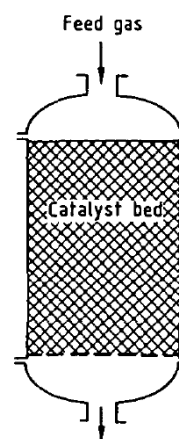
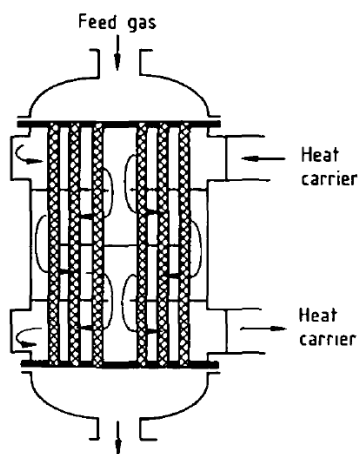
<http://www.stamixco-usa.com/>



www.hydrocarbonprocessing.com

125

- The cost of PFRs and PBRs (without catalyst) are similar to the costs of heat exchangers.
- A packed-bed (also called a fixed-bed) reactor is essentially a tubular reactor that is packed with solid catalyst particles.



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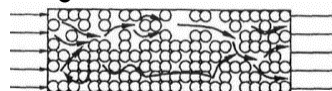
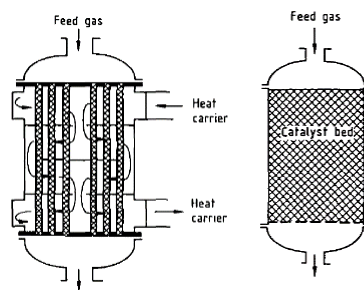
Fixed Bed Reactor, by GERHART EIGENBERGER

126

- This heterogeneous reaction system is most often used to catalyze gas reactions.

- **Disadvantages:**

- This reactor has the same difficulties with T control as the other tubular reactors.
- The catalyst is usually troublesome to replace.
- Channeling of the gas flow occurs, resulting in ineffective use of part of the reactor bed.

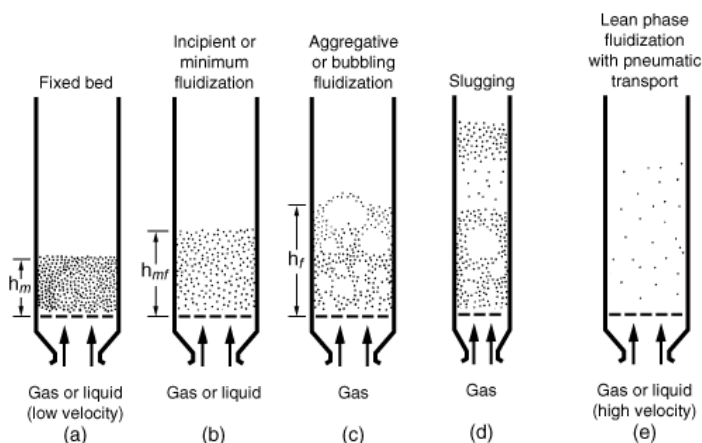


- **Advantage** of the packed-bed reactor:

- For most reactions PBR gives the highest conversion per weight of catalyst of any catalytic reactor.

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- Another type of catalytic reactor in common use is the Fluidized-bed reactor.

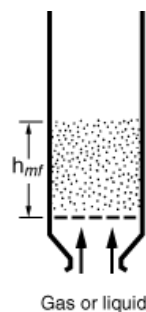


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D. Kunii and O. Levenspiel, Fluidization Engineering

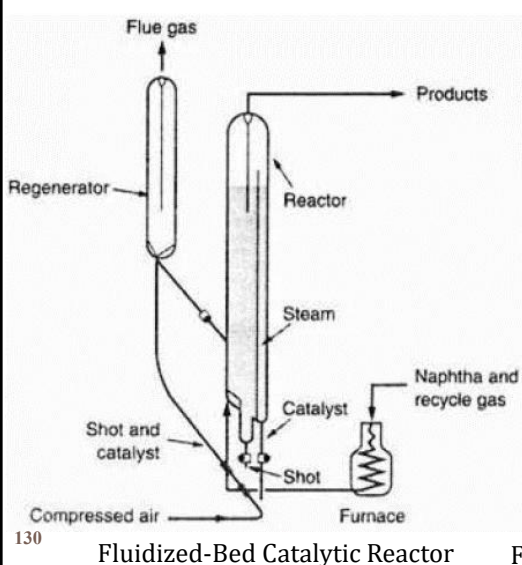
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- The fluidized-bed reactor is analogous to the CSTR in that its contents, though heterogeneous, are well mixed.
- Which results in an even T distribution throughout the bed, thus avoiding hot spots.
- The fluidized-bed reactor can only be approximately modeled as a CSTR; for higher precision it requires a model of its own.
- This type of reactor can handle large amounts of feed & solids and has good T control; thus it is used in a large number of applications.
- **Advantages:** the ease of catalyst replacement or regeneration.



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- The advantages of the ease of catalyst replacement or regeneration are sometimes offset by the high cost of the reactor and catalyst regeneration equipment.



Bapco's

Fluidized Catalytic Cracking Unit, FCCU

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- In this chapter, and on the CD-ROM, we've introduced each of the major types of industrial reactors: batch, semibatch, stirred tank, tubular, fixed bed (packed bed), and fluidized bed.
- Many variations and modifications of these commercial reactors are in current use.

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Note 1

Note 2

Complete
Suggested
Problems #1

Quiz
#1
3 days from
today, as
announced

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