CHME 312, Reaction Engineering
Spring Semester 2011

◎ **Textbook**

- H. Scott Fogler, *Elements of Chemical Reaction Engineering*, 4th Ed., Prectice Hall International, 2006

◎ **Instructor**

- Kyoshik Park, Chemical Engineering Programme (park@metu.edu.tr, S-131)

Introduction to Chemical Reaction Engineering I

o **What is Chemical Reaction Engineering (CRE) ?**

- Studying the chemical kinetics

• Chemical rxn rates and rxn mechanisms

$$A \rightarrow B$$

If B is being created at a rate of 0.2 moles per liter per second, ie, the rate of formation of B is,

r_B **= 0.2 mole/l/s**

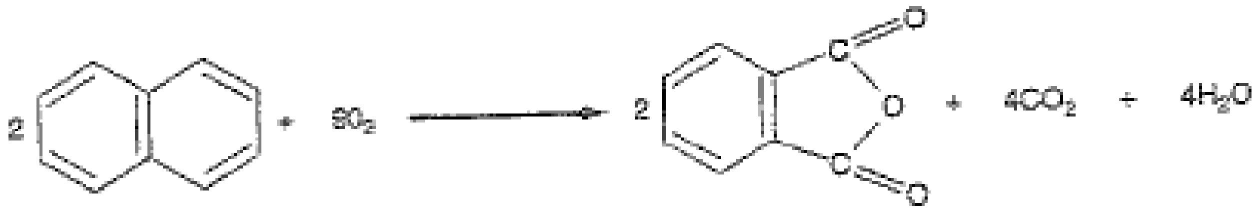
Then A is disappearing at the same rate:

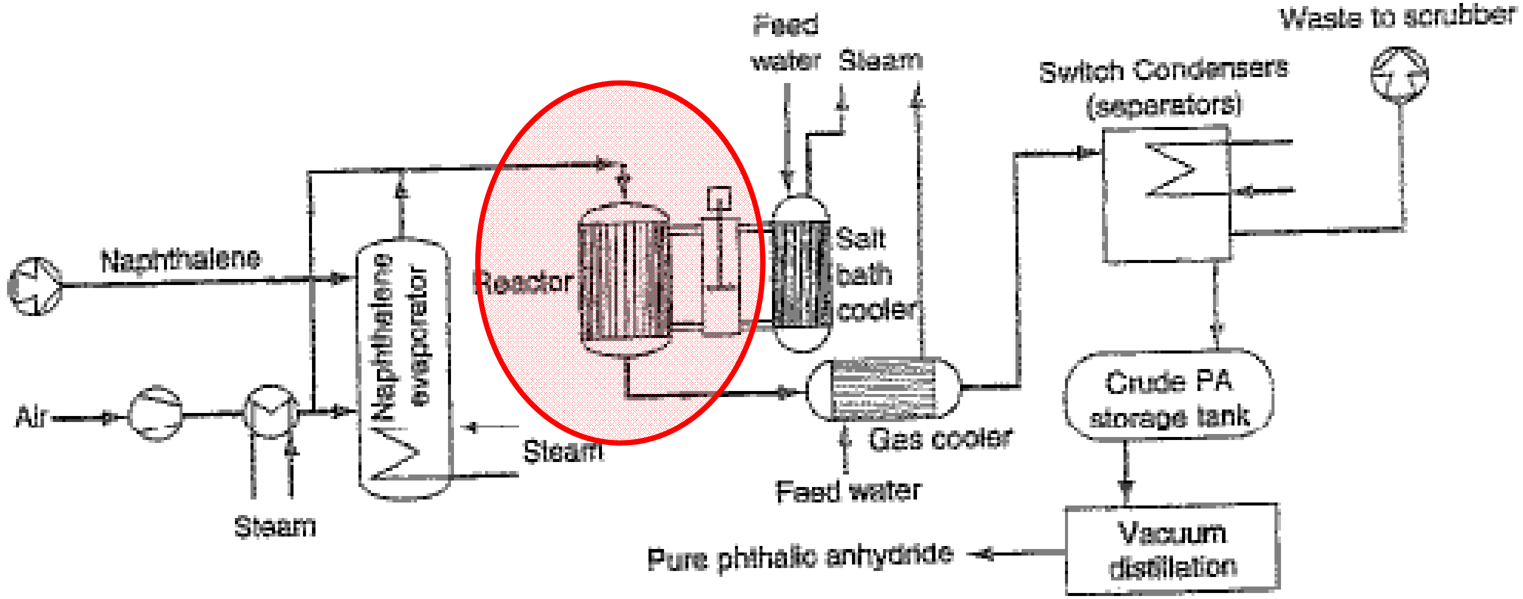
$-r_A$ **= 0.2 mole/l/s**

the rate of formation of A is

r_A **= -0.2 mole/l/s**

- Studying the reactors in which the reactions occurs





Manufacturing of Phthalic Anhydride

Introduction to Chemical Reaction Engineering II

- **CRE is at the heart of producing almost industrial chemicals**
  - **It is primarily a knowledge of chemical kinetics and reactor design that distinguishes the chemical engineer from other engineers**
- **Economic success of a plant**
  - **The selection of right reaction system**
    - **the safest and most efficient manner**
      - ☜ **large amount of undesirable product may cause subsequent purification and separation cost**

Structure of CRE

Goal	Multiple Rxns
Mass transfer	Mass transfer operations
Therm.	Nonisothermal operations, Multiple st. st.
Physical characteristic	Modeling real reactor, RTD, Dispersion, Segregation
Rxn analysis	Analysis of rate data, Lab reactors, Least-square analysis
Reactor analysis	Design of chemical reactors, PF, CSTR, Batch, Semibatch, Packed bed

Mole Balances

Stoichiometry

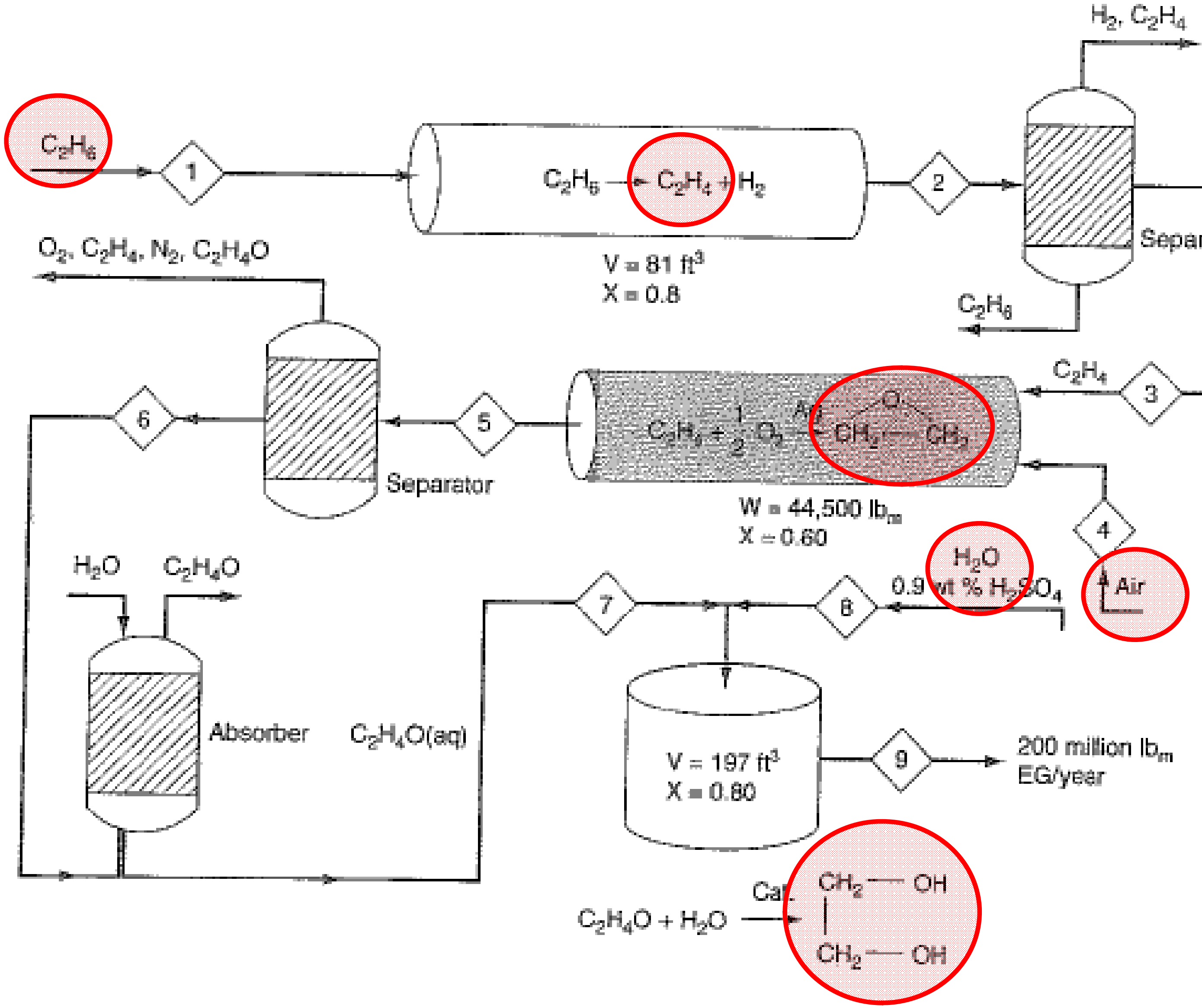
Diffusion

Energy Balances

Contacting

Rate Laws

Examples of CRE I



Examples of CRE I

- **Manufacturing of ethylene glycol**
  - **Economy**

Profit = **EG cost** - **Ethane cost**

$$\frac{\$0.38}{lb_m} \times 2 \times 10^8 \frac{lb_m}{year} \qquad \frac{\$0.04}{lb_m} \times 4 \times 10^8 \frac{lb_m}{year}$$

- **SA cost** - **Operating cost**

$$\frac{\$0.43}{lb_m} \times 2.26 \times 10^6 \frac{lb_m}{year} \qquad \$8,000,000$$

= \$76,000,000 - \$16,000,000 - \$54,000 - \$8,000,000
= \$52 million

Examples of CRE II

- **Modeling the Accumulation and Depletion of Smog in Los Angeles**
  - **- CRE is in everything... including the air!“**
    - **Can be used to model not only industrial processes but also everyday situations**

Examples of CRE II

LOS ANGELES FACT SHEET

- **Founded on September 4, 1781, under the name “El Pueblo de Los Angeles” and was incorporated to the USA on April 4, 1850.**
- **As of 2002 the population of Los Angeles County was 9,806,577.**
- **28% of the population in Los Angeles is under age 18.**
- **The county of Los Angeles covers approximately 4,061 square miles (10,518 square kilometers).**
- **The median household income for the city of Los Angeles in 1999 was $42,189.**
- **The mean travel time to work was 29.4 min as of 2000.**
- **Over 81% of all Los Angeles workers drive to work every day.**
- **Los Angeles has over 15,600 acres of parkland.**
- **Los Angeles is home to Griffith Park, the largest municipal park in the United States.**

Examples of CRE II

SMOG FACTS

Pollutants tend to accumulate in the lowest layer of the atmosphere, the troposphere, especially over the cities. This is due to the phenomenon of thermal inversion. When this occurs a layer of warm air above traps the pollutants. In addition, the topography of a city can worsen this effect, being the case of L.A. since it is surrounded by mountains.

REACTIONS INVOLVED

$$NO_2 + h\nu \rightarrow NO + O$$

$$O + O_2 \rightarrow O_3$$

$$O_3 + NO \rightarrow NO_2 + O_2$$

$$NO_2 + VOC \rightarrow \text{products such as PAN (peroxyacrilnitrate)}$$

$$O_3 + VOCs \rightarrow \text{aldehydes and free radicals}$$

Examples of CRE II

FACTORS THAT INFLUENCE SMOG FORMATION

- **Winds may blow smog away, which is the case in the problem you are about to explore.**
- **Temperature inversions can increase the production of smog, due to the reduction of atmospheric mixing. Therefore, the pollutants concentrate in the troposphere.**
- **Topography is another factor, since hills and mountains surrounding a community may reduce the flow of air, and as a consequence develop temperature inversions.**

☞ **Perform an unsteady-state mole balance on CO as it is depleted from the basin area**

Examples of CRE II

Problem - Questions

a) How many pound moles of gas are in the system we have chosen for the Los Angeles basin if the temperature is 75°F and the pressure is 1 atm?

b) What is the rate, $F_{CO,A}$, at which all autos emit carbon monoxide into the basin (lb mol CO/h)?

c) What is the volumetric flow rate (ft^3/h) of a 15 mph wind through the corridor 20 miles wide and 2000 feet high?

d) At what rate, $F_{CO,S}$, does the Santa Ana wind bring carbon monoxide into the basin (lb mol CO/h)?

e) Assuming that the volumetric flow rates entering and leaving the basin are identical $v = v_o$ show that the unsteady mole balance on CO within the basin becomes

$$F_{CO,A} + F_{CO,S} - v_O C_{CO} = V(dC_{CO}/dt)$$

f) Verify that the solution to the previous equation is

$$t = \frac{V}{v_o} \ln\left(\frac{\left[F_{CO,A} + F_{CO,S}\right] - v_o C_{CO,0}}{\left[F_{CO,A} + F_{CO,S}\right] - v_o C_{CO,f}}\right)$$

Examples of CRE II

Problem – Questions

g) If the initial concentration of carbon monoxide in the Los Angeles basin before the Santa Ana wind starts to blow is 8 ppm (2.04×10^{-8} lb mol/ft^3), calculate the time required for the carbon monoxide to reach a level of 2 ppm.

h) There is heavier traffic in the L.A. basin in the mornings and in the evenings as workers go to and from work in downtown L.A. Consequently, the flow of CO into the L.A. basin might be better represented by the sine function over a 24-hour period.

$$F_{CO,A} = a + b \sin(\pi * t/6)$$

The time, t = 0, starts at midnight. Where a = 35,000 lb mol/h and b = 30,000 lb mol/h. The general material balance equation now becomes

$$a + b \sin(\pi * t/6) + F_{CO,S} - v_O C_{CO} = V(dC_{CO}/dt)$$

Examples of CRE II

Problem – Solutions (Ex)

a) How many pound moles of gas are in the system we have chosen for the Los Angeles basin if the temperature is 75°F and the pressure is 1 atm?

<u>DATA</u>

$T = 75^{o}F$

$P = 1\ atm$

$V = (2*10^{10}\ ft^2)(2000\ ft)$

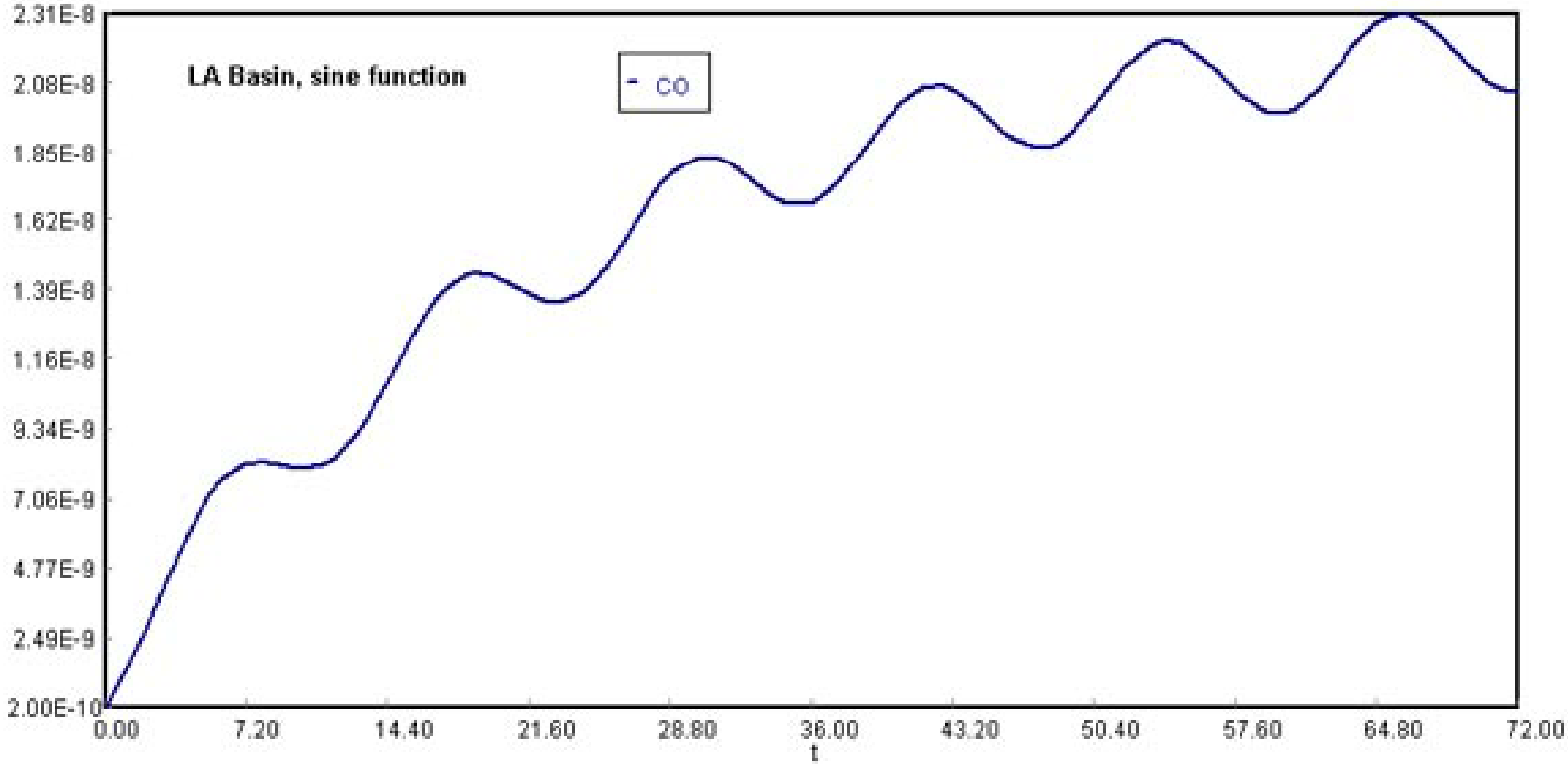
$= 4*10^{13}\ ft^3$

$R = 0.7302$

$PV = nRT$

$n = PV/RT = 1.024x10^{11}$ *lbmol*

Examples of CRE II



- **The time, t = 0, starts at midnight.**
  - **a = 35,000 lb mol/h and b = 30,000 lb mol/h.**
- **The general material balance equation now becomes**

$$a + b\sin(\pi * t/6) + F_{CO,S} - v_O C_{CO} = V(dC_{CO}/dt)$$

Examples of CRE III

$$A + M \rightarrow P + M$$

or more precisely

$$A \xrightarrow{\text{microbes}} P + \text{more\_microbes}$$

The rate law for the rate of disappearance of feed in the stomach is of the following form

$$-r_{AM1} = \frac{kC_A C_B}{K_M + C_A}, \left(\frac{kg}{m^3 * day}\right)$$