Lecture 2

Chemical Reaction Engineering (CRE) is the field that studies the rates and mechanisms of chemical reactions and the design of the reactors in which they take place.

Lecture 2 – Tuesday 1/15/2013

- Review of Lecture 1
- Definition of Conversion, X
- Develop the Design Equations in terms of X
- Size CSTRs and PFRs given $-r_A = f(X)$
- Conversion for Reactors in Series
- Review the Fall of the Tower of CRE

Reactor Mole Balances Summary

The GMBE applied to the four major reactor types (and the general reaction $A \rightarrow B$)



Review Lecture 1

CSTR – Example Problem

Given the following information, Find V



Liquid phase

 $\upsilon = \upsilon_0$ $F_A = \upsilon_0 C_A$

CSTR – Example Problem

(1) Mole Balance: $V = \frac{F_{A0} - F_A}{-r_A} = \frac{\upsilon_0 C_{A0} - \upsilon_0 C_A}{-r_A} = \frac{\upsilon_0 [C_{A0} - C_A]}{-r_A}$

(2) Rate Law: $-r_A = kC_A$

(3) Stoichiometry: $C_{A} = \frac{F_{A}}{\upsilon} = \frac{F_{A}}{\upsilon_{0}}$

Review Lecture 1

CSTR – Example Problem

(4) Combine:

$$V = \frac{\upsilon_0 \left[C_{A0} - C_A \right]}{kC_A}$$

$$\frac{(5) \text{ Evaluate:}}{C_A = 0.1C_{A0}}$$

$$V = \frac{\frac{10dm^3}{\min} [C_{A0} - 0.1C_{A0}]}{(0.23 \min^{-1})(0.1C_{A0})} = \frac{10[1 - 0.1]}{(0.23)(0.1)} dm^3$$

$$V = \frac{900}{2.3} = 391 \, dm^3$$

Define conversion, X

Consider the generic reaction:

 $a A + b B \longrightarrow c C + d D$

Chose limiting reactant A as basis of calculation:

$$A + \frac{b}{a}B \longrightarrow \frac{c}{a}C + \frac{d}{a}D$$

Define conversion, X $X = \frac{\text{moles A reacted}}{\text{moles A fed}}$

Batch

$$\begin{bmatrix} Moles \ A \\ remaining \end{bmatrix} = \begin{bmatrix} Moles \ A \\ initially \end{bmatrix} - \begin{bmatrix} Moles \ A \\ reacted \end{bmatrix}$$
$$N_A = N_{A0} - N_{A0}X$$
$$dN_A = 0 - N_{A0}dX$$
$$\frac{dN_A}{dt} = -N_{A0}\frac{dX}{dt} = r_AV$$

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Batch

$$\frac{dN_A}{dt} = -\frac{r_A V}{N_{A0}}$$

$$t = 0 \quad X = 0$$
$$t = t \quad X = X$$

Integrating,

$$t = N_{A0} \int_{0}^{X} \frac{dX}{-r_{A}V}$$

The necessary *t* to achieve conversion X.

CSTR

Consider the generic reaction:

 $a A + b B \longrightarrow c C + d D$

Chose limiting reactant A as basis of calculation: $A + \frac{b}{a}B \longrightarrow \frac{c}{a}C + \frac{d}{a}D$

Define conversion, X $X = \frac{\text{moles A reacted}}{\text{moles A fed}}$

CSTR

Steady State

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

Well Mixed

$$V = \frac{F_{A0} - F_{A}}{-r_{A}}$$
$$\int r_{A} dV = r_{A} V$$

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CSTR

$$\begin{bmatrix} Moles \ A \\ leaving \end{bmatrix} = \begin{bmatrix} Moles \ A \\ entering \end{bmatrix} - \begin{bmatrix} Moles \ A \\ reacted \end{bmatrix}$$

$$F_{A} = F_{A0} - F_{A0}X$$

$$F_{A0} - F_{A} + \int r_{A}dV = 0$$

$$V = \frac{F_{A0} - (F_{A0} - F_{A0}X)}{-r_{A}}$$

$$V = \frac{F_{A0}X}{-r_{A}}$$

CSTR volume necessary to achieve conversion X.

PFR

$$\frac{dF_A}{dV} = r_A$$
$$F_A = F_{AO} - F_{AO}X$$

$$\mathbf{I}_A - \mathbf{I}_{A0} \quad \mathbf{I}_{A0}^{\mathbf{I}}$$

Steady State d

$$dF_A = 0 - F_{A0}X$$

$$\frac{dX}{dV} = \frac{-r_A}{F_{A0}}$$

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PFR

$$V = 0 \quad X = 0$$
$$V = V \quad X = X$$

Integrating,

$$V = \int_{0}^{X} \frac{F_{A0}}{-r_{A}} dX$$

PFR volume necessary to achieve conversion X.

Reactor Mole Balances Summary

in terms of conversion, X



Levenspiel Plots

Reactor Sizing

Given $-r_A$ as a function of conversion, $-r_A = f(X)$, one can size any type of reactor. We do this by constructing a Levenspiel plot. Here we plot either $(F_{A0}/-r_A)$ or $(1/-r_A)$ as a function of X. For $(F_{A0}/-r_A)$ vs. X, the volume of a CSTR and the volume of a PFR can be represented as the shaded areas in the Levenspiel Plots shown as:

$$\frac{F_{A0}}{-r_A} = g(X)$$



X





Levenspiel Plots



Numerical Evaluations of Integrals

 The integral to calculate the PFR volume can be evaluated using method as Simpson's One-Third Rule: (See Appendix A.4)



$$V = \int_{0}^{X} \frac{F_{A0}}{-r_{A}} dX = \frac{\Delta x}{3} F_{A0} \left[\frac{1}{-r_{A}(0)} + \frac{4}{-r_{A}(X/2)} + \frac{1}{-r_{A}(X)} \right]$$

Other numerical methods are:

- Trapezoidal Rule (uses two data points)
- Simpson's Three-Eight's Rule (uses four data points)
- Five-Point Quadrature Formula

Given: r_A as a function of conversion, one can also design any sequence of reactors in series by defining X:

 $X_{i} = \frac{\text{total moles of A reacted up to point i}}{\text{moles of A fed to first reactor}}$

Only valid if there are no side streams.

Molar Flow rate of species A at point i:

$$F_{Ai} = F_{A0} - F_{A0}X_i$$



Reactor 1:

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Reactor 2:

$$V_{2} = \int_{X_{1}}^{X_{2}} \frac{F_{A0}}{-r_{A}} dX$$



Reactor 3:

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Space time τ is the time necessary to process 1 reactor volume of fluid at entrance conditions.



KEEPING UP

• The tower of CRE, is it stable?



These topics build upon one another.



CRE Algorithm



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



Otherwise, your Algorithm becomes unstable.

End of Lecture 2