## 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


## Review Lecture 1

## Reactor Mole Balances Summary

The GMBE applied to the four major reactor types (and the general reaction $A \rightarrow B$ )
$\begin{array}{ll}\text { Reactor } & \text { Differential } \\ \text { Batch } & \frac{d N_{A}}{d t}=r_{A} V\end{array}$
Algebraic Integral

$$
t=\int_{N_{A 0}}^{N_{A}} \frac{d N_{A}}{r_{A} V} \underbrace{N_{A}}_{\mathrm{t}}
$$

CSTR

$$
V=\frac{F_{A 0}-F_{A}}{-r_{A}}
$$

$$
V=\int_{F_{A 0}}^{F_{A}} \frac{d F_{A}}{d r_{A}}
$$

$$
\frac{d F_{A}}{d V}=r_{A}
$$



PFR

$$
\frac{d F_{A}}{d W}=r_{A}^{\prime}
$$

$$
W=\int_{F_{A 0}}^{F_{A}} \frac{d F_{A}}{r_{A}^{\prime}} \underbrace{\mathrm{F}_{\mathrm{A}}}_{\mathrm{W}}
$$

## Review Lecture 1

## CSTR - Example Problem

Given the following information, Find V
$v_{0}=10 \mathrm{dm}^{3} / \mathrm{min}$
$C_{A 0}$
$F_{A 0}=v_{0} C_{A 0}$

$$
\begin{aligned}
& v=v_{0}=10 \mathrm{dm}^{3} / \mathrm{min} \\
& C_{A}=0.1 C_{A 0} \\
& F_{A}=v C_{A}
\end{aligned}
$$

Liquid phase

$$
\begin{aligned}
& v=v_{0} \\
& F_{A}=v_{0} C_{A}
\end{aligned}
$$

## Review Lecture 1

## CSTR - Example Problem

(1) Mole Balance:

$$
V=\frac{F_{A 0}-F_{A}}{-r_{A}}=\frac{v_{0} C_{A 0}-v_{0} C_{A}}{-r_{A}}=\frac{v_{0}\left[C_{A 0}-C_{A}\right]}{-r_{A}}
$$

(2) Rate Law:
$-r_{A}=k C_{A}$
(3) Stoichiometry:
$C_{A}=\frac{F_{A}}{v}=\frac{F_{A}}{v_{0}}$

## Review Lecture 1

## CSTR - Example Problem

(4) Combine:
$V=\frac{v_{0}\left[C_{A 0}-C_{A}\right]}{k C_{A}}$
(5) Evaluate:
$C_{A}=0.1 C_{A 0}$
$V=\frac{\frac{10 \mathrm{dm}^{3}}{\min }\left[C_{A 0}-0.1 C_{A 0}\right]}{\left(0.23 \min ^{-1}\right)\left(0.1 C_{A 0}\right)}=\frac{10[1-0.1]}{(0.23)(0.1)} \mathrm{dm}^{3}$
$V=\frac{900}{2.3}=391 \mathrm{dm}^{3}$

## Define conversion, $X$

Consider the generic reaction:

$$
\mathrm{aA}+\mathrm{bB} \longrightarrow \mathrm{cC}+\mathrm{dD}
$$

Chose limiting reactant $A$ as basis of calculation:

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

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

## Batch

$$
\begin{aligned}
& {\left[\begin{array}{l}
\text { Moles } A \\
\text { remaining }
\end{array}\right]=\left[\begin{array}{l}
\text { Moles } A \\
\text { initially }
\end{array}\right]-\left[\begin{array}{l}
\text { Moles } A \\
\text { reacted }
\end{array}\right]} \\
& \quad N_{A}=N_{A 0}-N_{A 0} X \\
& d N_{A}=0-N_{A 0} d X \\
& \frac{d N_{A}}{d t}=-N_{A 0} \frac{d X}{d t}=r_{A} V
\end{aligned}
$$

## Batch

$$
\frac{d N_{A}}{d t}=-\frac{r_{A} V}{N_{A 0}} \quad \begin{array}{lll}
t=0 & X=0 \\
t=t & X=X
\end{array}
$$

Integrating,
$t=N_{A 0} \int_{0}^{X} \frac{d X}{-r_{A} V}$
The necessary $t$ to achieve conversion $X$.

## CSTR

Consider the generic reaction:

$$
\mathrm{aA}+\mathrm{bB} \longrightarrow \mathrm{cC}+\mathrm{dD}
$$

Chose limiting reactant A as basis of calculation:

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

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

## CSTR

Steady State

$$
\frac{d N_{A}}{d t}=0
$$

Well Mixed

$$
\begin{gathered}
V=\frac{F_{A 0}-F_{A}}{-r_{A}} \\
\int r_{A} d V=r_{A} V
\end{gathered}
$$

## CSTR

$$
\begin{gathered}
{\left[\begin{array}{l}
\text { Moles } A \\
\text { leaving }
\end{array}\right]=\left[\begin{array}{l}
\text { Moles } A \\
\text { entering }
\end{array}\right]-\left[\begin{array}{l}
\text { Moles } A \\
\text { reacted }
\end{array}\right]} \\
F_{A}=F_{A 0}-F_{A 0} X \\
F_{A 0}-F_{A}+\int r_{A} d V=0 \\
V=\frac{F_{A 0}-\left(F_{A 0}-F_{A 0} X\right)}{-r_{A}} \\
V=\frac{F_{A 0} X}{-r_{A}}
\end{gathered}
$$

CSTR volume necessary to achieve conversion X.

## PFR

$$
\begin{gathered}
\frac{d F_{A}}{d V}=r_{A} \\
F_{A}=F_{A 0}-F_{A 0} X
\end{gathered}
$$

Steady State $\quad d F_{A}=0-F_{A 0} X$

$$
\frac{d X}{d V}=\frac{-r_{A}}{F_{A 0}}
$$

## PFR

$$
\begin{array}{ll}
V=0 & X=0 \\
V=V & X=X
\end{array}
$$

Integrating,

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

PFR volume necessary to achieve conversion $X$.

## Reactor Mole Balances Summary in terms of conversion, X

Reactor
Differential

$$
N_{A 0} \frac{d X}{d t}=-r_{A} V
$$

Batch

CSTR

PFR $\quad F_{A 0} \frac{d X}{d V}=-r_{A}$

$$
F_{A 0} \frac{d X}{d W}=-r_{A}^{\prime}
$$

PBR

Algebraic Integral
Integral

$$
V=\frac{F_{A 0} X}{-r_{A}}
$$

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


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

$$
W=\int_{0}^{X} \frac{F_{A 0} d X}{-r_{A}^{\prime}} \quad \frac{\mathrm{X}}{\mathrm{~W}}
$$

## 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 $\left(F_{A 0} /-r_{A}\right)$ or $\left(1 /-r_{A}\right)$ as a function of $X$. For $\left(F_{A 0} /-r_{A}\right)$ 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:

$$
\frac{F_{A 0}}{-r_{A}}=g(X)
$$

## Levenspiel Plots



## CSTR



## PFR



## 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)

| ${ }^{1}$ |  | $V=\int_{0}^{X} \frac{F_{A 0}}{-r_{A}} d X=\frac{\Delta x}{3} F_{A 0}\left[\frac{1}{-r_{A}(0)}+\frac{4}{-r_{A}(X / 2)}+\frac{1}{-r_{A}(X)}\right]$ |
| :---: | :---: | :---: |
| $\underline{1}$ |  |  |
|  |  | Other numerical methods are: |
| $\frac{1}{-r_{A}\left(X_{1}\right)}$ |  | - Trapezoidal Rule (uses two data points) |
| 1 |  | - Simpson's Three-Eight's |
| $-r_{A}(0)$ | $X_{1} X_{2}$ | Rule (uses four data points) |
|  |  | - Five-Point Quadrature Formula |

## Reactors in Series

Given: $r_{A}$ as a function of conversion, one can also design any sequence of reactors in series by defining X:

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

Only valid if there are no side streams.

Molar Flow rate of species A at point i :

$$
F_{A i}=F_{A 0}-F_{A 0} X_{i}
$$

## Reactors in Series



## Reactors in Series

Reactor 1:
$F_{A 1}=F_{A 0}-F_{A 0} X_{1}$

$$
V_{1}=\frac{F_{A 0}-F_{A 1}}{-r_{A 1}}=\frac{F_{A 0}-\left(F_{A 0}-F_{A 0} X_{1}\right)}{-r_{A 1}}=\frac{F_{A 0} X_{1}}{-r_{A 1}}
$$



## Reactors in Series

Reactor 2:
$V_{2}=\int_{X_{1}}^{X_{2}} \frac{F_{A 0}}{-r_{A}} d X$


## Reactors in Series

Reactor 3:

$$
\begin{aligned}
& F_{A 2}-F_{A 3}+r_{A 3} V_{3}=0 \\
& \left(F_{A 0}-F_{A 0} X_{2}\right)-\left(F_{A 0}-F_{A 0} X_{3}\right)+r_{A 3} V_{3}=0 \\
& V_{3}=\frac{F_{A 0}\left(X_{3}-X_{2}\right)}{-r_{A 3}}
\end{aligned}
$$



## Reactors in Series



## Reactors in Series

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

$$
\tau=\frac{V}{U_{0}}
$$



## KEEPING UP

The tower of CRE, is it stable?

## Reaction Engineering



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

