## Introduction to Reactor Design

## ChE 3K4



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## Chapter 2: Major ideas for this section

A Definition of conversion
B Reactor design for a specified conversion
C Graphical interpretation/solution of CSTR and PFR design equations

## Conversion

Consider

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

Consider species $A$ to be the basis (usually we pick the one which gets consumed to completion first, i.e. the limiting reagent).

Useful to express extent of reaction in terms of conversion of $A$ :

$$
X_{A}=\frac{\text { moles } A \text { reacted }}{\text { moles } A \text { fed }}
$$

To simplify notation, use $X$ (without subscript).

## Conversion

## Remarks

- In a batch reactor, $X$ is a function of time
- For irreversible reaction, $X \rightarrow 1$ as $t \rightarrow \infty$
- For reversible reaction, $X \rightarrow X_{e}$ (equilibrium conversion) as $t \rightarrow \infty$
- In flow reactors (CSTR and PFR) the $X$ is a function of volume, which reflects the amount of time reactants spend in the reactor


## Design equations in terms of conversion

In this section we consider rewriting the previously derived equations from Chapter 1 (called the design equations) in terms of conversion.
We had previously used concentration $C_{A}$ and molar flow $F_{A}$. Now we will use $X$, conversion.

We consider our 4 reactors (numbers refer to Fogler):
2.2 Batch
2.3.1 CSTR
2.3.2 PFR
2.3.3 PBR

## Batch systems

First express $N_{A}$ in terms of $X$
$\binom{$ moles $A}{$ reacted }$=\binom{$ moles $A}{$ fed }$\cdot\left(\frac{\text { moles } A \text { reacted }}{\text { moles } A \text { fed }}\right)$

$$
=N_{A 0} \cdot X
$$

$\binom{$ moles $A$ at }{ time $t}=\binom{$ initial }{ moles $A}-\binom{$ moles $A}{$ consumed }

$$
\begin{aligned}
& N_{A}=N_{A 0}-N_{A 0} \cdot X \\
& N_{A}=N_{A 0}(1-X)
\end{aligned}
$$

## Batch systems

- Recall the mole balance equation (assumptions?):

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

- Integral form:

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

Design feature for batch systems: time

## Flow systems: CSTRs, PFRs and PBRs

$$
\begin{aligned}
& F_{A 0} X=\left(\frac{\text { moles } A \text { fed }}{\text { time }}\right) \cdot\left(\frac{\text { moles } A \text { reacted }}{\text { moles } A \text { fed }}\right) \\
& F_{A 0} X=\frac{\text { moles } A \text { reacted }}{\text { time }}
\end{aligned}
$$

$\binom{$ molar rate of }{$A$ leaving }$=\binom{$ molar rate }{ of $A$ fed }$-\binom{$ molar rate of }{$A$ consumed }

$$
\begin{aligned}
& F_{A}=F_{A 0}-F_{A 0} X \\
& F_{A}=F_{A 0}(1-X)
\end{aligned}
$$

Draw a picture here $\rightarrow$

## CSTR

- Recall the mole balance equation (what were the assumptions?):

$$
\begin{aligned}
& V=\frac{F_{A 0}-F_{A}}{-r_{A}} \\
& V=\frac{F_{A 0}-F_{A 0}(1-X)}{-r_{A}} \\
& V=\frac{F_{A 0} X}{-r_{A}}
\end{aligned}
$$

- $r_{A}$ : taken inside the reactor $=$ exit conditions

Design feature for CSTR systems: volume

## PFR

Recall the mole balance equation (what were the assumptions?):

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

But $F_{A}=F_{A 0}(1-X)$

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

Integral form:

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

Design feature for PFR systems: volume

## PBR

Follows a similar derivation:

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

Integral form:

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

Design feature for PBR systems: catalyst weight

Summary so far Apply to a 1st order system Remark: we generally obtain $-r_{A}$ vs $X$ from rate equation, e.g. $-r_{A}=k C_{A}$. Consider a flow reactor:

$$
\begin{aligned}
& F_{A}=F_{A 0}(1-X) \\
& C_{A}=\frac{F_{A}}{q}=\frac{F_{A 0}(1-X)}{q}
\end{aligned}
$$

If $q=q_{0}$ (under what conditions would this hold?):

$$
\begin{aligned}
& C_{A}=\frac{F_{A 0}}{q_{0}}(1-X) \\
& C_{A}=C_{A 0}(1-X)
\end{aligned}
$$

and

$$
-r_{A}=k C_{A}=k C_{A 0}(1-X)
$$

## Example: data collected

Table 2-2. Processed Data

| $X$ | 0.0 | 0.1 | 0.2 | 0.4 | 0.6 | 0.7 | 0.8 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $-r_{A}\left(\frac{\mathrm{~mol}}{\mathrm{~m}^{3} \cdot \mathrm{~s}}\right)$ | 0.45 | 0.37 | 0.30 | 0.195 | 0.113 | 0.079 | 0.05 |
| $\left(1 /-r_{\Lambda}\right)\left(\frac{\mathrm{m}^{3} \cdot \mathrm{~s}}{\mathrm{~mol}}\right)$ | 2.22 | 2.70 | 3.33 | 5.13 | 8.85 | 12.7 | 20 |
| $\left(F_{\mathrm{AO} 0} /-r_{\mathrm{A}}\right)\left(\mathrm{m}^{3}\right)$ | 0.89 | 1.08 | 1.33 | 2.05 | 3.54 | 5.06 | 8.0 |

- $F_{A 0}=0.4 \mathrm{~mol} . \mathrm{s}^{-1}$
- Isothermal and constant pressure; gas-phase
- We have no idea what the reaction order is


## Example: plotted



## Example: plotted (with best-fit line added)



## CSTR solution



## PFR solution



## Simpson's rules

- Got 3 equally-spaced points; with spacing $=h$ ?

$$
\int_{x_{0}}^{x_{2}} f(x) d x \approx \frac{h}{3}\left[f\left(x_{0}\right)+4 f\left(x_{1}\right)+f\left(x_{2}\right)\right]
$$

- Got 4 equally-spaced points; with spacing $=h$ ?

$$
\int_{x_{0}}^{x_{3}} f(x) d x \approx \frac{3 h}{8}\left[f\left(x_{0}\right)+3 f\left(x_{1}\right)+3 f\left(x_{2}\right)+f\left(x_{3}\right)\right]
$$

- See Appendix A for other formulas (more general)


## CSTR vs PFR



## Profiles along the reactor: $r_{A}$



How was this found?

## Profiles along the reactor: $X$



How was this
found?

## Reactors in series: multiple CSTRs

South Africa, the Ergo tailings plant


## Flotation cells: Bolivia

See flotation cells in series on flickr.com

## Reactors in series: multiple CSTRs



## CSTR solution



## Rule for conversions in series

## $X_{n}=\frac{\text { total moles of A reacted leaving reactor } n}{\text { moles A fed to first reactor }}$

e.g. for 2 reactors in series

$$
\begin{aligned}
V_{2} & =\frac{F_{A 1}-F_{A 2}}{-r_{A 2}} \\
& =\frac{F_{A 0}\left(1-X_{1}\right)-F_{A 0}\left(1-X_{2}\right)}{-r_{A 2}} \\
& =\frac{F_{A 0}\left(X_{2}-X_{1}\right)}{-r_{A 2}}
\end{aligned}
$$



## Reactors in series: multiple CSTRs

- Consider N CSTRs in series

We observe that system approximates performance of a PFR of volume

$$
V_{\text {PFR }} \approx V_{1}+V_{2}+\cdots+V_{N}
$$

Approximation improves as $N$ increases.

## Homework exercise

- Example on page 56 (F2011)
- Example on page 62 (F2006)


## 3 reactors in series



## 3 reactors in series



## Some further definitions

- Space time, or residence time:

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

time necessary to process one reactor volume of fluid based on entrance conditions

