Chemical Reaction Engineering I

Chapter 2
Conversion and Reactor Sizing

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Chapter Description

Aims

- Define and compute conversion for any reactive unit
- Rewrite the design equations as the functions of conversion

Expected Outcomes

- Size the reactors based on the rate given as a function of conversion

References & other information

- Elements of Chemical Reaction Engineering',
  by H. Scott Fogler

Subtopics

2.1 Conversion

2.2 Space Time and Velocity

2.3 Mean Residence Time of Flow Reactor

Conversion

Consider reaction

aA + bB $\rightarrow$ cC + dD

Using basis stoichiometric coefficients,

A is a limiting reactant

Thus, $$A+\frac{b}{a}B\rightarrow\frac{c}{a}C+\frac{d}{a}D$$

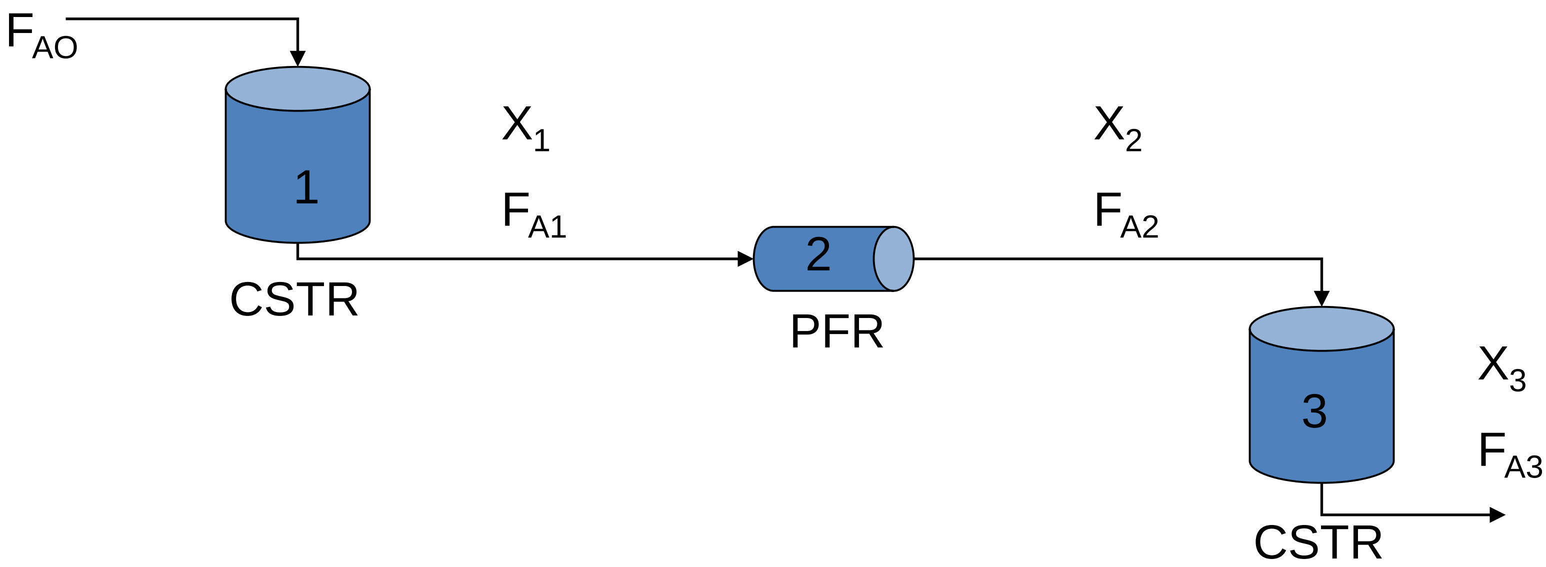
So,

Conversion of A is

Constant volume only

$$X_A=\frac{moles\ of\ A\ reacted}{moles\ of\ A\ fed}=\frac{N_{A0}-N_A}{N_{A0}}=\frac{F_{A0}-F_A}{F_{A0}}=\frac{C_{A0}-C_A}{C_{A0}}$$

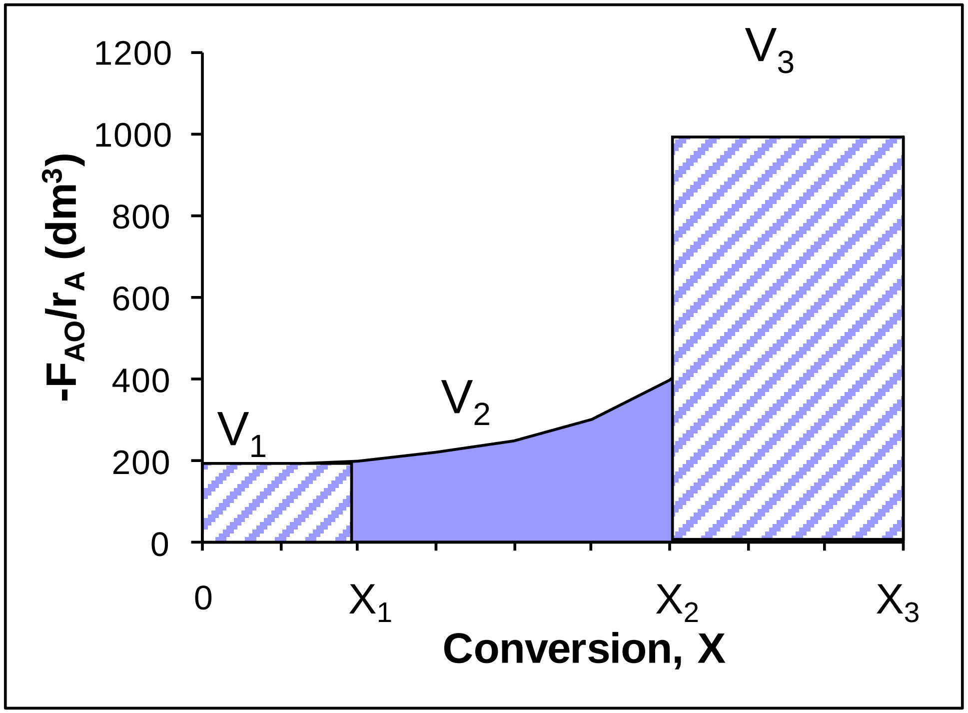
Conversion for Reactor in Series



$$X_n = \frac{Moles\ of\ A\ reacted\ up\ to\ reactor\ n}{Moles\ of\ A\ feed\ to\ first\ reactor}$$

$\therefore$ Valid with no side stream*

Reactor in Series



$$V_1 = \frac{F_{A0} X_1}{-r_{A1}}$$

$$V_2 = \int_{X_1}^{X_2} \frac{F_{A0}}{-r_A} dX$$

$$V_2 = \frac{F_{AO}\left(X_2 - X_1\right)}{-r_{A2}}$$

$$V_3 = \frac{F_{AO}\left(X_3 - X_2\right)}{-r_{A3}}$$

Space Time and Space Velocity

- The conversion of reactants in a chemical reactor relates to the *time* that the chemical species spend in the reactor.

- Two types of time-parameters are commonly used in chemical reaction engineering are:
  - space time
  - residence time

- Space time is often used as a scaling parameter in reactor design

Space Time and Space Velocity

<u>*Space Time (τ)*</u> *:* $$\tau = \frac{V}{v_o}$$

Time required to process 1 reactor volume of fluid at inlet conditions

<u>*Space Velocity*</u>: $$SV = \frac{v_o}{V}$$

- *LHSV- Liquid Hourly Space Velocity*
  (liquid feed rate at 60 or75 °F)
- *GHSV - Gas Hourly Space Velocity*
  (gas feed rate at STP)

<u>*Actual Residence Time*</u>*:* The time actually spent by fluid inside the reactor.

Mean Residence Time of Flow Reactor

We should be clearly aware of the distinction between these two measures of time, $\bar{t}$ and τ. They are defined as follows:

$$\tau = \begin{pmatrix} \text{time needed to} \\ \text{treat one reactor} \\ \text{volume of feed} \end{pmatrix} = \frac{V}{v_0} = \frac{C_{A0}V}{F_{A0}}, \quad [\text{hr}] \qquad \textbf{(6) or (8)}$$

$$\bar{t} = \begin{pmatrix} \text{mean residence time} \\ \text{of flowing material} \\ \text{in the reactor} \end{pmatrix} = C_{A0}\int_0^{X_A} \frac{dX_A}{(-r_A)(1+\varepsilon_A X_A)}, \quad [\text{hr}] \qquad \textbf{(24)}$$

For constant density systems (all liquids and constant density gases)

$$\tau = \bar{t} = \frac{V}{v}$$

Summary

	Differential Equation	Algebraic Equation	Integral Equation
Batch	$N_{A0}\frac{dX}{dt} = -r_A V$		$t = N_{A0}\int_0^X \frac{dX}{-r_A V}$
CSTR		$V = \frac{F_{A0}(X_{out} - X_{in})}{-(r_A)_{out}}$	
PFR	$F_{A0}\frac{dX}{dV} = -r_A$		$V = F_{A0}\int_{X_{in}}^{X_{out}} \frac{dX}{-r_A}$
PBR	$F_{A0}\frac{dX}{dW} = -r'_A$		$W = F_{A0}\int_{X_{in}}^{X_{out}} \frac{dX}{-r'_A}$

Authors Information

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