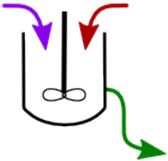
Introduction to Reactor Design

ChE 3K4



Kevin Dunn, 2013

(with credit to Dr. P. Mhaskar for many of the slides)

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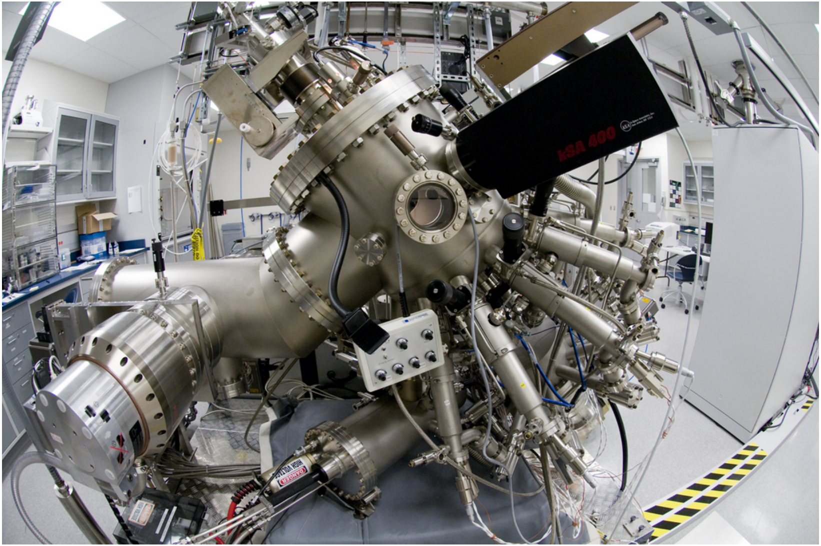
Overall revision number: 28 (January 2013)

Batch system

TABLE 3-3. STOICHIOMETRIC TABLE FOR A BATCH SYSTEM

Species	*Initially* (mol)	*Change* (mol)	*Remaining* (mol)
A	N_{A0}	$-(N_{A0}X)$	$N_A = N_{A0} - N_{A0}X$
B	N_{B0}	$-\frac{b}{a}(N_{A0}X)$	$N_B = N_{B0} - \frac{b}{a}N_{A0}X$
C	N_{C0}	$\frac{c}{a}(N_{A0}X)$	$N_C = N_{C0} + \frac{c}{a}N_{A0}X$
D	N_{D0}	$\frac{d}{a}(N_{A0}X)$	$N_D = N_{D0} + \frac{d}{a}N_{A0}X$
I (inerts)	N_{I0}	—	$N_I = N_{I0}$
Totals	N_{T0}		$N_T = N_{T0} + \left(\frac{d}{a} + \frac{c}{a} - \frac{b}{a} - 1\right)N_{A0}X$

Batch systems (derivation on board)



[Argone National Laboratory, batch deposition reactor]

Flow system: columns 1, 2, 3, 4

TABLE 3-4. STOICHIOMETRIC TABLE FOR A FLOW SYSTEM

Species	*Feed Rate to Reactor* (mol/time)	*Change within Reactor* (mol/time)	*Effluent Rate from Reactor* (mol/time)
A	F_{A0}	$-F_{A0}X$	$F_A = F_{A0}(1-X)$
B	$F_{B0} = \Theta_B F_{A0}$	$-\frac{b}{a}F_{A0}X$	$F_B = F_{A0}\left(\Theta_B - \frac{b}{a}X\right)$
C	$F_{C0} = \Theta_C F_{A0}$	$\frac{c}{a}F_{A0}X$	$F_C = F_{A0}\left(\Theta_C + \frac{c}{a}X\right)$
D	$F_{D0} = \Theta_D F_{A0}$	$\frac{d}{a}F_{A0}X$	$F_D = F_{A0}\left(\Theta_D + \frac{d}{a}X\right)$
I	$F_{I0} = \Theta_I F_{A0}$	—	$F_I = F_{A0}\Theta_I$
	F_{T0}		$F_T = F_{T0} + \left(\frac{d}{a} + \frac{c}{a} - \frac{b}{a} - 1\right)F_{A0}X$
			$F_T = F_{T0} + \delta F_{A0}X$

Flow system: column 5 (concentration)

$$C_A = \frac{F_A}{v} = \frac{F_{A0}(1-X)}{v} = \frac{F_{A0}(1-X)}{v_0(1+\varepsilon X)}\left(\frac{T_0}{T}\right)\frac{P}{P_0} = C_{A0}\left(\frac{1-X}{1+\varepsilon X}\right)\frac{T_0}{T}\left(\frac{P}{P_0}\right)$$

$$C_B = \frac{F_B}{v} = \frac{F_{A0}[\Theta_B-(b/a)X]}{v} = \frac{F_{A0}[\Theta_B-(b/a)X]}{v_0(1+\varepsilon X)}\left(\frac{T_0}{T}\right)\frac{P}{P_0} = C_{A0}\left(\frac{\Theta_B-(b/a)X}{1+\varepsilon X}\right)\frac{T_0}{T}\left(\frac{P}{P_0}\right)$$

$$C_C = \frac{F_C}{v} = \frac{F_{A0}[\Theta_C+(c/a)X]}{v} = \frac{F_{A0}[\Theta_C+(c/a)X]}{v_0(1+\varepsilon X)}\left(\frac{T_0}{T}\right)\frac{P}{P_0} = C_{A0}\left(\frac{\Theta_C+(c/a)X}{1+\varepsilon X}\right)\frac{T_0}{T}\left(\frac{P}{P_0}\right)$$

$$C_D = \frac{F_D}{v} = \frac{F_{A0}[\Theta_D+(d/a)X]}{v} = \frac{F_{A0}[\Theta_D+(d/a)X]}{v_0(1+\varepsilon X)}\left(\frac{T_0}{T}\right)\frac{P}{P_0} = C_{A0}\left(\frac{\Theta_D+(d/a)X}{1+\varepsilon X}\right)\frac{T_0}{T}\left(\frac{P}{P_0}\right)$$

$$C_I = \frac{F_I}{v} = \frac{F_{A0}\Theta_I}{v} = \frac{F_{A0}\Theta_I}{v_0(1+\varepsilon X)}\left(\frac{T_0}{T}\right)\frac{P}{P_0} = \frac{C_{A0}\Theta_I}{1+\varepsilon X}\left(\frac{T_0}{T}\right)\frac{P}{P_0}$$

Let's derive where this all comes from.

Summary from last class

- $F_A = F_{A0}\left(1 - \frac{a}{a}X\right)$
- $F_B = F_{A0}\left(\Theta_B - \frac{b}{a}X\right)$
- $F_C = F_{A0}\left(\Theta_C + \frac{c}{a}X\right)$
- $F_D = F_{A0}\left(\Theta_D + \frac{d}{a}X\right)$

In general, we write:

$$F_j = F_{A0}\left(\Theta_j + \nu_j X\right)$$

- ν_j = stoichiometric ratio, accounting for sign
- $\nu_B = -\frac{b}{a}$
- $\nu_D = +\frac{d}{a}$

In the printed notes, page 115 (F2011)

- Create a "total concentration" (fictitious concentration)
- $C_T = \dfrac{P}{ZRT}$
- but, $C_T = \dfrac{F_T}{v}$ or, as I prefer: $C_T = \dfrac{F_T}{q}$

In the printed notes, page 116 (F2011)

- $C_T = \dfrac{F_T}{v} = \dfrac{P}{ZRT}$ ← applies anywhere along the reactor
- $C_{T0} = \dfrac{F_{T0}}{v_0} = \dfrac{P_0}{Z_0 R T_0}$ ← applies only at the feed point

Assuming $Z_0 = Z$

Most important equation for this page

$$v = v_0 \left(\frac{F_T}{F_{T0}}\right)\left(\frac{P_0}{P}\right)\left(\frac{T}{T_0}\right)$$

- How do we interpret this?
- Sign of $\left(\dfrac{P_0}{P}\right)$ and when is $\left(\dfrac{F_T}{F_{T0}}\right) = 1$?

In the printed notes, page 116/117

Recall the total flows (see columns 2 and 4)

- Entry flow $= F_{T0}$ mols per second
- Flow at any other point $= F_T$ mols per second

$$F_T = F_{T0} + F_{A0}\delta X$$

$$\frac{F_T}{F_{T0}} = 1 + \left(\frac{F_{A0}}{F_{T0}}\right)\delta X = 1 + \epsilon X$$

$$\epsilon = y_{A0}\delta$$

Back to our important equation ...

$$v = v_0\left(\frac{F_T}{F_{T0}}\right)\left(\frac{P_0}{P}\right)\left(\frac{T}{T_0}\right) = v_0\left(1+\epsilon X\right)\left(\frac{P_0}{P}\right)\left(\frac{T}{T_0}\right)$$

Middle of page 117 and top of page 118

- $C_j = \dfrac{F_j}{v}$ ← applies anywhere along the reactor
- Numerator: Sub in our definition for $F_j = F_{A0}\left(\Theta_j + \nu_j X\right)$
- Denominator: Sub in our important equation for volumetric flow, v

$$C_j = \frac{F_j}{v} = \frac{F_{A0}\left(\Theta_j + \nu_j X\right)}{v_0\left(1+\epsilon X\right)\left(\dfrac{P_0}{P}\right)\left(\dfrac{T}{T_0}\right)}$$

Top of page 118

The general concentration expression, for any species, at any point in the reactor:

$$C_j = \frac{C_{A0}\left(\Theta_j + \nu_j X\right)}{(1 + \epsilon X)} \left(\frac{P}{P_0}\right) \left(\frac{T_0}{T}\right)$$

What you should recall from chemistry

- y_A = mol fraction of A
- p_A = partial pressure of A
- P = total pressure
- $p_A = (y_A)(P)$ ← applies anywhere along the reactor
- $p_{A0} = (y_{A0})(P_0)$ ← applies only at the feed point
- but, $p_A = C_A RT$
- so, $(y_A)(P) = C_A RT$
- or $C_A = \dfrac{y_A P}{RT}$ ← applies anywhere along the reactor
- and $C_{A0} = \dfrac{y_{A0} P_0}{RT_0}$ ← applies only at the feed point

Flow system: columns 1, 2, 3, 4

TABLE 3-4. STOICHIOMETRIC TABLE FOR A FLOW SYSTEM

Species	*Feed Rate to Reactor* (mol/time)	*Change within Reactor* (mol/time)	*Effluent Rate from Reactor* (mol/time)
A	F_{A0}	$-F_{A0}X$	$F_A = F_{A0}(1-X)$
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C	$F_{C0} = \Theta_C F_{A0}$	$\frac{c}{a} F_{A0}X$	$F_C = F_{A0}\left(\Theta_C + \frac{c}{a} X\right)$
D	$F_{D0} = \Theta_D F_{A0}$	$\frac{d}{a} F_{A0}X$	$F_D = F_{A0}\left(\Theta_D + \frac{d}{a} X\right)$
I	$F_{I0} = \Theta_I F_{A0}$	—	$F_I = F_{A0}\Theta_I$
	F_{T0}		$F_T = F_{T0} + \left(\frac{d}{a} + \frac{c}{a} - \frac{b}{a} - 1\right) F_{A0}X$
			$F_T = F_{T0} + \delta F_{A0}X$

Flow system: column 5 (concentration)

$$C_A = \frac{F_A}{v} = \frac{F_{A0}(1-X)}{v} = \frac{F_{A0}(1-X)}{v_0(1+\varepsilon X)}\left(\frac{T_0}{T}\right)\frac{P}{P_0} = C_{A0}\left(\frac{1-X}{1+\varepsilon X}\right)\frac{T_0}{T}\left(\frac{P}{P_0}\right)$$

$$C_B = \frac{F_B}{v} = \frac{F_{A0}[\Theta_B-(b/a)X]}{v} = \frac{F_{A0}[\Theta_B-(b/a)X]}{v_0(1+\varepsilon X)}\left(\frac{T_0}{T}\right)\frac{P}{P_0} = C_{A0}\left(\frac{\Theta_B-(b/a)X}{1+\varepsilon X}\right)\frac{T_0}{T}\left(\frac{P}{P_0}\right)$$

$$C_C = \frac{F_C}{v} = \frac{F_{A0}[\Theta_C+(c/a)X]}{v} = \frac{F_{A0}[\Theta_C+(c/a)X]}{v_0(1+\varepsilon X)}\left(\frac{T_0}{T}\right)\frac{P}{P_0} = C_{A0}\left(\frac{\Theta_C+(c/a)X}{1+\varepsilon X}\right)\frac{T_0}{T}\left(\frac{P}{P_0}\right)$$

$$C_D = \frac{F_D}{v} = \frac{F_{A0}[\Theta_D+(d/a)X]}{v} = \frac{F_{A0}[\Theta_D+(d/a)X]}{v_0(1+\varepsilon X)}\left(\frac{T_0}{T}\right)\frac{P}{P_0} = C_{A0}\left(\frac{\Theta_D+(d/a)X}{1+\varepsilon X}\right)\frac{T_0}{T}\left(\frac{P}{P_0}\right)$$

$$C_I = \frac{F_I}{v} = \frac{F_{A0}\Theta_I}{v} = \frac{F_{A0}\Theta_I}{v_0(1+\varepsilon X)}\left(\frac{T_0}{T}\right)\frac{P}{P_0} = \frac{C_{A0}\Theta_I}{1+\varepsilon X}\left(\frac{T_0}{T}\right)\frac{P}{P_0}$$

(Derived in the previous class)

Example

A mixture of 28% SO_2 and air, 72% are added into a flow reactor at $P_0 = 1485\,\text{kPa}$ and $T_0 = 500K$

$$\begin{aligned} 2SO_2 + O_2 &\leftrightharpoons 2SO_3 \\ A + \tfrac{1}{2}B &\leftrightharpoons C \end{aligned}$$

The reaction takes place isothermally, and with no pressure drop. Express the outlet concentrations of ALL species as a function of conversion, X, only.

Use the table provided to lay out your answer.

Where we left off ...

Assuming isothermal behaviour, and no pressure drop

Species	**Concentrations**
A $= SO_2$	$C_A = C_{A0}\left(\dfrac{1-X}{1+\epsilon X}\right)$
B $= O_2$	$C_B = C_{A0}\left(\dfrac{\Theta_B - \frac{1}{2}X}{1+\epsilon X}\right)$
C $= SO_2$	$C_C = C_{A0}\left(\dfrac{\Theta_C + \frac{1}{1}X}{1+\epsilon X}\right)$
I $= N_2$	$C_I = C_{A0}\left(\dfrac{\Theta_I}{1+\epsilon X}\right)$

Unknowns

C_A0

ϵ

Θ_B

Θ_C

Θ_I

Concentration profile with conversion