Stoichiometric Table for Batch Reactors

Reaction stoichiometry and conversion control how N_T changes in the system

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

Species	*Initial Amount* (mol)	*Change* (mol)	*Remaining* (mol)
A	N_{A0}	$-(N_{A0}X_A)$	$N_A = (N_{A0} - N_{A0}X_A)$
B	N_{B0}	$-\frac{b}{a}(N_{A0}X_A)$	$N_B = (N_{B0} - \frac{b}{a}N_{A0}X_A)$
C	N_{C0}	$\frac{c}{a}(N_{A0}X_A)$	$N_C = (N_{C0} + \frac{c}{a}N_{A0}X_A)$
D	N_{D0}	$\frac{d}{a}(N_{A0}X_A)$	$N_D = (N_{D0} + \frac{d}{a}N_{A0}X_A)$
I (inert)	N_{I0}	0	$N_I = N_{I0}$
Total	N_{T0}		$N_T = N_{T0} + \delta N_{A0}X_A$

δ = increase in the total number of moles per mole of A reacted

$$\delta = \frac{d}{a} + \frac{c}{a} - \frac{b}{a} - 1$$

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Stoichiometric Table for Flow Reactors

Reaction: $A + \frac{b}{a}B \rightarrow \frac{c}{a}C + \frac{d}{a}D$

Define $\theta_i = F_{i0} / F_{A0}$ (Limiting reagent A)

Species	*Feed Flow Rate* (mol/s)	*Change within Reactor* (mol/s)	*Effluent Rate from Reactor* (mol/s)
A	F_{A0}	$-(F_{A0}X_A)$	$F_A = F_{A0}(1 - X_A)$
B	$F_{B0} = \theta_B F_{A0}$	$-\frac{b}{a}(F_{A0}X_A)$	$F_B = F_{A0}(\theta_B - \frac{b}{a}X_A)$
C	$F_{C0} = \theta_C F_{A0}$	$\frac{c}{a}(F_{A0}X_A)$	$F_C = F_{A0}(\theta_C + \frac{c}{a}X_A)$
D	$F_{D0} = \theta_D F_{A0}$	$\frac{d}{a}(F_{A0}X_A)$	$F_D = F_{A0}(\theta_D + \frac{d}{a}X_A)$
I (inert)	$F_{I0} = \theta_I F_{A0}$	-	$F_I = F_{I0}$
Total	$F_{T0} = F_{A0}(1 + \theta_B + \theta_C + \theta_D + \theta_I)$	$\delta F_{A0}X_A$	$F_T = F_{T0} + \delta F_{A0}X_A$

Note the similarity between flow and batch reactor stoichiometric tables

$$\delta = \frac{d}{a} + \frac{c}{a} - \frac{b}{a} - 1$$

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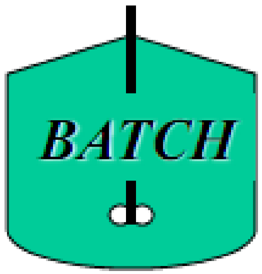
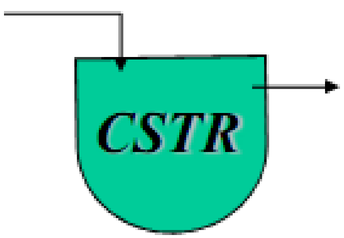
Design Equation in Terms of Conversion (limiting reactant A)

IDEAL REACTOR	DIFFERENTIAL FORM	ALGEBRAIC FORM	INTEGRAL FORM
	$N_{A0}\frac{dX_A}{dt} = (-r_A)V$		$t = N_{A0}\int_0^{X_A}\frac{dX'_A}{-r_A V}$
		$V = \frac{F_{A0}(X_A)}{(-r_A)}$	
	$F_{A0}\frac{dX_A}{dV} = (-r_A)$		$V = F_{A0}\int_0^{X_A}\frac{dX'_A}{-r_A}$

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Summary - Design Equations of Ideal Reactors

	Differential Equation	Algebraic Equation	Integral Equation	Remarks
Batch (well-mixed)	$\frac{dN_j}{dt} = (r_j)V$		$t = \int_{N_{j0}}^{N_j} \frac{dN'_j}{(r_j)V}$	Conc. changes with time but is uniform within the reactor. Reaction rate varies with time.
CSTR (well-mixed at steady-state)		$V = \frac{F_{j0} - F_j}{-(r_j)}$		Conc. inside reactor is uniform. (r_j) is constant. Exit conc = conc inside reactor.
PFR (steady-state flow; well-mixed radially)	$\frac{dF_j}{dV} = r_j$		$V = \int_{F_{j0}}^{F_j} \frac{dF'_j}{(r_j)}$	Concentration and hence reaction rates vary spatially (with length).