ECUACIONES EMPLEADAS EN CINÉTICA

REACCIONES IRREVERSIBLES

1 COMPONENTE CINÉTICAMENTE ACTIVO

$v = kC_A^n$

n	FORMA DIFERENCIAL	FORMA INTEGRADA	$t_{1/2}$
n = 0	$-\frac{dC_A}{dt} = k_o$	$C_A = C_{Ao} - k_o t$	$C_{Ao} / 2k_o$
n = 1	$-\frac{dC_A}{dt} = k_1 C_A$ $\frac{dx_A}{dt} = k_1(1 - x_A)$ $\frac{dx}{dt} = k_1(a - x)$	$\ln (C_{Ao} / C_A) = k_1 t$ $-\ln(1-x_A) = k_1 t$ $\ln \frac{a}{a-x} = k_1 t$	$\ln 2 / k_1$
n = 2	$-\frac{dC_A}{dt} = k_2 C_A^2$ $\frac{dx_A}{dt} = k_2 C_{Ao}(1 - x_A)^2$ $\frac{dx}{dt} = k_2(a - x)^2$	$\frac{1}{C_A} - \frac{1}{C_{Ao}} = k_2 t$ $\frac{x_A}{1 - x_A} = C_{Ao} k_2 t$ $\frac{x}{a-x} = ak_2 t$	$1 / k_2 C_{Ao}$
$\forall\ n \neq 1$		$\frac{1}{n-1}\left(\frac{1}{C_A^{n-1}} - \frac{1}{C_{Ao}^{n-1}}\right) = k_n t$	$\frac{1}{n-1}\left[\frac{2^{n-1} - 1}{C_{Ao}^{n-1}}\right] = k_n t_{1/2}$

Nota: x_A = fracción de A convertida en productos, $0 < x_A < 1$
x = concentración de A consumida

2 COMPONENTES CINÉTICAMENTE ACTIVOS

$v = kC_A^n C_B^m$

n	Estequiometría	FORMA DIFERENCIAL	FORMA INTEGRADA
n = 2	$A + B \rightarrow P$	$\frac{dx}{dt} = k(a-x)(b-x)$ $\frac{dx_A}{dt} = kC_{Ao}(1-x_A)(K-x_A)$	$\frac{1}{a-b}\ln\frac{(a-x)b}{(b-x)a} = kt \quad a \neq b$ $-\frac{1}{a} + \frac{1}{(a-x)} = kt \quad a = b$ $\frac{1}{K-1}\ln\frac{K-x_A}{K(1-x_A)} = kC_{Ao}t$ $K = \frac{C_{Bo}}{C_{Ao}} \neq 1$ $\frac{x_A}{1-x_A} = kC_{Ao}t \quad C_{Ao} = C_{Bo}$
	$A + 2\,B \rightarrow P$	$\frac{dx}{dt} = k(a-x)(b-2x)$ $\frac{dx_A}{dt} = kC_{Ao}(1-x_A)(K-2x_A)$	$\ln\frac{(a-x)b}{(b-2x)a} = k(2a-b)t$ $b \neq 2a$ $\ln\frac{K-2x_A}{K(1-x_A)} = k(K-2)C_{Ao}t$ $K = \frac{C_{Bo}}{C_{Ao}} \neq 2$ $\frac{x}{a-x} = 2akt \quad b = 2a$ $\frac{x_A}{1-x_A} = 2kC_{Ao}t \quad K = 2$
	$A + z\,B \rightarrow P$	$\frac{dx}{dt} = k(a-x)(b-zx)$	$\ln\frac{(a-x)b}{(b-zx)a} = k(za-b)t \quad b \neq za$

n	Estequiometría	FORMA DIFERENCIAL	FORMA INTEGRADA
n = 3	A + B→P	$\frac{dx}{dt}=k(a-x)(b-x)^2$	$\frac{1}{(a-b)^2}\left[\frac{(a-b)x}{(b-x)b}+\ln\frac{(b-x)a}{(a-x)b}\right]=kt$ $\frac{1}{(a-x)^2}-\frac{1}{a^2}=2kt$ a = b
	A + 2 B→P	$\frac{dx}{dt}=k(a-x)(b-2x)^2$	$\frac{(2a-b)2x}{b(b-2x)}+\ln\frac{a(b-2x)}{b(a-x)}=k(2a-b)^2t$ $\frac{1}{(a-x)^2}-\frac{1}{a^2}=8kt$ 2a = b

3 COMPONENTES CINÉTICAMENTE ACTIVOS

$v= kC_A^nC_B^mC_C^p$

n	Estequiometría	FORMA DIFERENCIAL	FORMA INTEGRADA
n = 3	A + B + C→P	$\frac{dx}{dt}=k(a-x)(b-x)(c-x)$	$\frac{1}{(a-b)(c-a)}\ln\frac{(a-x)}{a}+$ $\frac{1}{(b-a)(c-b)}\ln\frac{(b-x)}{b}+$ $\frac{1}{(c-a)(b-c)}\ln\frac{(c-x)}{c}=kt$

REACCIONES REVERSIBLES

n	Estequiometría	FORMA DIFERENCIAL	FORMA INTEGRADA	$t_{1/2}$
n = 1	$A \underset{k_2}{\overset{k_1}{\rightleftharpoons}} B$ $C_{Ao} = a$ $C_{Bo} = 0$	$\frac{dx}{dt} = k_1(a-x) - k_2x$ $\frac{dx}{dt} = (k_1+k_2)(x_e - x)$ $\frac{dx_A}{dt} = k_1\frac{(x_{Ae}-x_A)}{x_{Ae}}$	$\ln\frac{x_e}{x_e - x} = (k_1+k_2)t$ $\ln\frac{x_{Ae}}{x_{Ae}-x_A} = (k_1+k_2)t$ $K_e = \frac{k_1}{k_2} = \frac{x_e}{a-x_e} = \frac{x_{Ae}}{1-x_{Ae}}$	$t_{1/2} = \frac{\ln 2}{k_1+k_2}$
	$C_{Ao} = a$ $C_{Bo} = b$	$\frac{dx}{dt} = k_1(a-x) - k_2(b+x)$ $\frac{dx}{dt} = \frac{k_1(a+b)(x_e-x)}{b+x_e}$ $\frac{dx_A}{dt} = \frac{k_1(1+M)(x_{Ae}-x_A)}{M+x_{Ae}}$	$\ln\frac{x_e}{x_e-x} = \frac{k_1(a+b)}{(b+x_e)}t$ $\ln\frac{x_{Ae}}{x_{Ae}-x_A} = \frac{(1+M)}{(M+x_{Ae})}k_1t$	

$M = C_{Bo} / C_{Ao}$

$$K_e = \frac{k_1}{k_2} = \frac{b+x_e}{a-x_e} = \frac{M+x_{Ae}}{1-x_{Ae}}$$

n	Estequiometría	FORMA DIFERENCIAL	FORMA INTEGRADA
n = 2	$A + B \underset{k_2}{\overset{k_1}{\rightleftharpoons}} C + D$ $C_{Ao} = C_{Bo}$ $C_{Co} = C_{Do} = 0$	$\frac{dx_A}{dt} = k_1 C_{Ao}(1 - x_A)^2 - k_2 C_{Ao} x_A^2$ $\frac{dx_A}{dt} = (k_1 - k_2) C_{Ao}(m_1 - x_A)(m_2 - x_A)$ $m_1 = \frac{K_e + \sqrt{K_e}}{K_e - 1}$ $m_2 = \frac{K_e - \sqrt{K_e}}{K_e - 1}$	$\frac{1}{m_2 - m_1} \ln \frac{m_1(m_2 - x_A)}{m_2(m_1 - x_A)} = (k_1 - k_2) C_{Ao} t$
	$A + B \underset{k_2}{\overset{k_1}{\rightleftharpoons}} C$ $C_{Ao} = C_{Bo}$ $C_{Co} = 0$	$\frac{dx_A}{dt} = k_1 C_{Ao}(1 - x_A)^2 - k_2 x_A$ $\frac{dx_A}{dt} = k_1 C_{Ao}(m_1 - x_A)(m_2 - x_A)$ $m_{1,2} = \left(\frac{2K_e C_{Ao} + 1}{K_e C_{Ao}} \pm \sqrt{\left(\frac{2K_e C_{Ao} + 1}{C_{Ao} K_e} \right)^2 - 4} \right) / 2$	$\frac{1}{m_2 - m_1} \ln \frac{m_1(m_2 - x_A)}{m_2(m_1 - x_A)} = k_1 C_{Ao} t$