

CINÈTICA QUÍMICA, VELOCITATS DE REACCIÓ:

$A + 2B \rightarrow \text{productes.}$

$t = 0 \quad [A] = [A]_0 \quad \text{i} \quad [B] = [B]_0$

$t = t' \quad [A] = [A]_{0-x} \quad \text{i} \quad [B] = [B]_{0-x/2}$

tornant a la mecànica de les equacions de velocitat, tenim que
 $dx/dt = k \cdot ([A]_{0-x}) \cdot ([B]_{0-x/2})^2 \quad (*)$

recordem que en àcid-base també usem els constants de velocitat "k" i segueixen el mateix criteri quan a exponents:

$aA + bB \rightarrow cC + dD \quad K = \text{ctnt d'equilibri} = \frac{[C]^c \cdot [D]^d}{[A]^a \cdot [B]^b}$

(*) se resol usant el mètode de les *integrals racionals*:

tenim $dx / ([A]_{0-x}) \cdot ([B]_{0-x/2})^2 = k \cdot dt$ llavors

$$\int \frac{dx}{(A_0 - x)(B_0 - \frac{x}{2})^2} = \int k \cdot dt$$

Que resoldrem usant les integrals racionals:

$$\frac{M}{(A_0 - x)} + \frac{N}{(B_0 - \frac{x}{2})} + \frac{Q}{(B_0 - \frac{x}{2})^2} =$$

$$\frac{M(B_0 - \frac{x}{2})^2}{(A_0 - x)(B_0 - \frac{x}{2})^2} + \frac{N(A_0 - x)(B_0 - \frac{x}{2})}{(A_0 - x)(B_0 - \frac{x}{2})^2} + \frac{Q(A_0 - x)}{(A_0 - x)(B_0 - \frac{x}{2})^2}$$

$$1 = M(B_0 - \frac{x}{2})^2 + N(A_0 - x)(B_0 - \frac{x}{2}) + Q(A_0 - x)$$

Ara toca dilucidar M, N, Q:

$$x = A_0 : 1 = M \cdot (B_0 - \frac{A_0}{2})^2 \quad M = \frac{1}{(B_0 - \frac{A_0}{2})^2}$$

$$\left(B_0 - \frac{x}{2}\right) = 0 \quad x = 2B_0 \quad 1 = Q \cdot (A_0 - 2B_0) \quad Q = \frac{1}{(A_0 - 2B_0)}$$

I suposem $x = C_0$:

$$1 = \frac{1}{\left(B_0 - \frac{A_0}{2}\right)^2} \cdot \left(B_0 - \frac{C_0}{2}\right)^2 + N \cdot (A_0 - C_0) \left(B_0 - \frac{C_0}{2}\right) +$$

$$\frac{1}{(A_0 - 2B_0)} \cdot (A_0 - C_0)$$

$$N \cdot (A_0 - C_0) \left(B_0 - \frac{C_0}{2}\right) = 1 - \frac{1}{\left(B_0 - \frac{A_0}{2}\right)^2} \cdot \left(B_0 - \frac{C_0}{2}\right)^2 -$$

$$\frac{1}{(A_0 - 2B_0)} \cdot (A_0 - C_0)$$

$$N \cdot (A_0 - C_0) \left(B_0 - \frac{C_0}{2}\right) = 1 - \frac{\left(B_0 - \frac{C_0}{2}\right)^2 \cdot (A_0 - 2B_0) - (A_0 - C_0) \cdot \left(B_0 - \frac{A_0}{2}\right)^2}{\left(B_0 - \frac{A_0}{2}\right)^2 \cdot (A_0 - 2B_0)}$$

$$N \cdot (A_0 - C_0) \left(B_0 - \frac{C_0}{2}\right) =$$

$$\frac{\left(B_0 - \frac{A_0}{2}\right)^2 \cdot (A_0 - 2B_0) - \left(B_0 - \frac{C_0}{2}\right)^2 \cdot (A_0 - 2B_0) - (A_0 - C_0) \cdot \left(B_0 - \frac{A_0}{2}\right)^2}{\left(B_0 - \frac{A_0}{2}\right)^2 \cdot (A_0 - 2B_0)}$$

$$N = \frac{\left(B_0 - \frac{A_0}{2}\right)^2 \cdot (A_0 - 2B_0) - \left(B_0 - \frac{C_0}{2}\right)^2 \cdot (A_0 - 2B_0) - (A_0 - C_0) \cdot \left(B_0 - \frac{A_0}{2}\right)^2}{(A_0 - C_0) \left(B_0 - \frac{C_0}{2}\right) \cdot \left(B_0 - \frac{A_0}{2}\right)^2 \cdot (A_0 - 2B_0)}$$

Aleshores:

$$\int \frac{dx}{(A_0 - x) \left(B_0 - \frac{x}{2}\right)^2} = \frac{1}{\left(B_0 - \frac{A_0}{2}\right)^2} \cdot \log(A_0 - x) +$$

$$\frac{\left(B_0 - \frac{A_0}{2}\right)^2 \cdot (A_0 - 2B_0) - \left(B_0 - \frac{C_0}{2}\right)^2 \cdot (A_0 - 2B_0) - (A_0 - C_0) \cdot \left(B_0 - \frac{A_0}{2}\right)^2}{(A_0 - C_0) \left(B_0 - \frac{C_0}{2}\right) \cdot \left(B_0 - \frac{A_0}{2}\right)^2 \cdot (A_0 - 2B_0)} \cdot \log\left(B_0 - \frac{x}{2}\right) +$$

$$\frac{1}{(A_0 - 2B_0)} \cdot (-2) \cdot \left(B_0 - \frac{x}{2}\right)^{-1}$$

$$\int \frac{dx}{\left(B_0 - \frac{x}{2}\right)^2} = \int (-2) \cdot \left(B_0 - \frac{x}{2}\right)^{-2} dx = (-2) \cdot \left(B_0 - \frac{x}{2}\right)^{-1}$$

