RESOLUÇÃO LISTA 1

PARTE A

(1) REAÇÃO SEQUENCIAL

$$A_0 \xrightarrow{k_0} A_1 \xrightarrow{k_1} A_2 \xrightarrow{k_2} \cdots A_m \xrightarrow{k_m} P$$

$A_0(0) = A_0 \qquad A_n(0) = 0 \qquad n = 1, 2, \ldots m$

CONDIÇÃO ESPECIAL: $k_n = k$ (IND. DE n)

RESOLUÇÃO

$$\begin{cases} \dfrac{dA_0}{dt} = -k_0 A_0 \\ A_0(0) = A_0 \end{cases}$$

$A_0(t) = A_0 e^{-k_0 t}$

ou

$A_0(t) = A_0 e^{-kt}$ pois $k_0 = k$

PARA A ESPÉCIE A_1 VALE:

$$\begin{cases} \dfrac{dA_1}{dt} = k_0 A_0(t) - k_1 A_1 = k A_0 e^{-kt} - k A_1 \\ A_1(0) = 0 \end{cases}$$

ASSIM

$A_1(t) = k A_0(t) \otimes e^{-kt}$

$A_1(t) = k A_0 e^{-kt} \otimes e^{-kt}$

EM TERMOS DA FRAÇÃO $F_1 = \frac{A_1}{A_0}$

$$F_1 = k e^{-kt} \otimes e^{-kt} = k \int_0^t e^{-k\tau} \cdot e^{-k(t-\tau)} d\tau$$

$$F_1 = kte^{-kt}$$

CONTINUANDO:

$$\begin{cases} \frac{dA_2}{dt} = k_1 A_1(t) - k_2 A_2 = k A_1(t) - k A_2 \\ A_2(0) = 0 \end{cases}$$

$$F_2 = \left(\frac{A_2}{A_0}\right) = k(kt)e^{-kt} \otimes e^{-kt}$$

$$F_2 = k^2 \int_0^t \tau e^{-k\tau} \cdot e^{-k(t-\tau)} d\tau$$

$$F_2 = k^2 e^{-kt} \int_0^t \tau \, d\tau = \frac{k^2 t^2}{1 \cdot 2} e^{-kt}$$

GENERALIZANDO

$$F_3 = \frac{(kt)^3}{1 \cdot 2 \cdot 3} e^{-kt}$$

$$\boxed{F_n = \frac{(kt)^n}{n!} e^{-kt}}$$

b) PONTO DE MÁXIMO $\quad F_n = \frac{(kt)^n}{n!} e^{-kt}$

$$\frac{dF_n}{dt} = \frac{k^n}{n!}\left(nt^{n-1} e^{-kt} - t^n k e^{-kt}\right) = 0$$

$$= \frac{(kt)^n}{n!}\left(\underbrace{\frac{n e^{-kt}}{t} - k e^{-kt}}_{0}\right) = 0$$

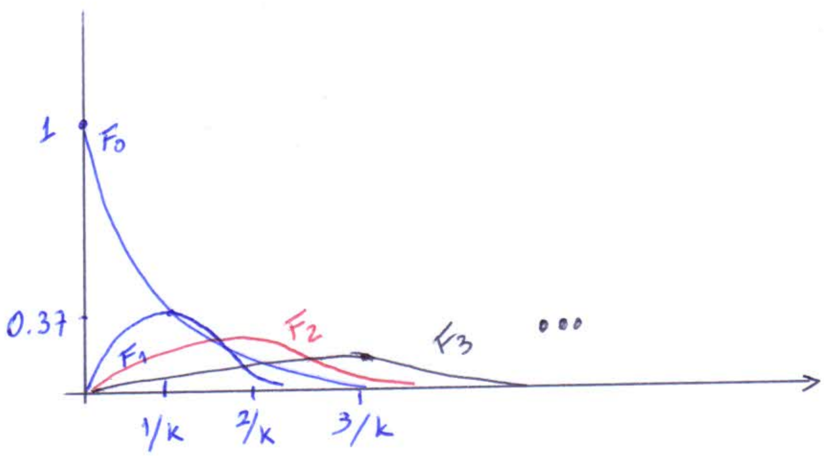
ASSIM: $\frac{n}{t} - k = 0$

$$\boxed{t_{max} = \frac{n}{k}}$$

$$F_n(t_{max}) = \left(\frac{\cancel{k} n}{\cancel{k}}\right)^n \frac{1}{n!} e^{-\cancel{k} n/\cancel{k}}$$

$$\boxed{F_n(t_{max}) = \frac{n^n}{n!} e^{-n}}$$

n	$F_n(t_{max})$	
0	1	1
1	e^{-1}	0.368
2	$2e^{-2}$	0.271
3	$\frac{9}{2}e^{-3}$	0.224
⋮		



c) PARA O PRODUTO P VALE

A CONSERVAÇÃO:

$$P = A_0 \left(1 - \sum_{n=0}^{m} F_n \right)$$

$$P = A_0 \left(1 - \sum_{n=0}^{m} \frac{(kt)^n}{n!} e^{-kt} \right)$$

$$\underbrace{\lim_{m \to \infty} \sum_{n=0}^{m} \frac{(kt)^n}{n!} e^{-kt}}_{=1} = e^{-kt} \cdot \underbrace{\sum_{n=0}^{\infty} \frac{(kt)^n}{n!}}_{e^{kt}}$$

ASSIM

$$\lim_{m \to \infty} P = A_0 (1 - 1) = 0$$

PRODUTO NUNCA SE FORMA POIS A CADEIA É INFINITA!

② REAGENTE $R = A(t)$

$$\left\{\begin{array}{l} A \xrightarrow{k_0} P_0 \\ A \xrightarrow{k_1} P_1 \\ A \xrightarrow{k_2} P_2 \\ A \xrightarrow{k_n} P_n \end{array}\right.$$

$$k(n) = k_0 \, r^n$$

$$r = k_0/k < 1$$

ou seja

$$k > k_0$$

SOLUÇÃO

$$-\frac{dA}{dt} = (k_0 + k_1 + \dots)A = \left(\sum_{n=0}^{\infty} k(n)\right) A$$

$$\sum_{n=0}^{\infty} k(n) = k_0 \underbrace{\sum_{n=0}^{\infty} r^n}_{\text{GEOMÉTRICA}} = \frac{k_0}{1-r} = \frac{k_0 k}{k-k_0} = \xi$$

$r < 1$

Assim

$$A(t) = A_0 \, e^{-\xi t} \quad \text{ou} \quad \boxed{A(t) = A_0 \, e^{-\left(\frac{k_0 k}{k-k_0}\right)t}}$$

PARA OS PRODUTOS P_n vale

$$\frac{dP_n}{dt} = k_n A(t) \qquad P_n(0) = 0$$

ou $$P_n = k_n \int_0^t A(t)\,dt$$

$$A(t) = A_0 e^{-\xi t}$$

$$P_n = \left(\frac{k_n}{\xi}\right) A_0 \left(1 - e^{-\xi t}\right)$$

ASSIM $$\sum_{n=0}^{\infty} P_n = \frac{A_0}{\xi}\left(1 - e^{-\xi t}\right) \underbrace{\sum_{n=0}^{\infty} k_0 r^n}_{\xi}$$

$$= \frac{A_0}{\cancel{\xi}}\left(1 - e^{-\xi t}\right) \cdot \cancel{\xi}$$

$$\sum_{n=0}^{\infty} P_n = A_0\left(1 - e^{-\xi t}\right); \qquad \xi = \frac{k_0 k}{k - k_0}$$

$$k > k_0$$

③ $A \xrightarrow{k_1} P$

$2A \xrightarrow{k_2} Q$

a) $$\begin{cases} A(0) = A_0 \\ \underbrace{-\dfrac{dA}{dt} = k_1 A + 2k_2 A^2} \end{cases}$$

EQ. RICCATI C/

COEF. CONST.

MÉTOD. BERNOULLI

$A^{-1} = z$ (MUDANÇA VARIÁVEL)

$$\begin{cases} z(0) = 1/A_0 \\ \dfrac{dz}{dt} = k_1 z + 2k_2 \end{cases}$$

$$z(t) = A_0^{-1} e^{k_1 t} + \frac{2k_2}{k_1}\left(e^{k_1 t} - 1\right)$$

ou

$$A(t) = \frac{e^{-k_1 t}}{A_0^{-1} + \left(\frac{2k_2}{k_1}\right)\left(1 - e^{-k_1 t}\right)}$$

b) $x_Q = \dfrac{Q}{Q + P}$

CONTUDO: $P = k_1 \int_0^t A(\tau)\, d\tau$

$$Q = 2k_2 \int_0^t A^2(\tau)\, d\tau$$

CONSERVAÇÃO

$$A_0 - A = P + Q$$

ASSIM $\left(\dfrac{Q}{P}\right) = \dfrac{A_0 - A - k_1 \int_0^t A(\tau)\, d\tau}{k_1 \int_0^t A(\tau)\, d\tau}$

ou $\left(\dfrac{Q}{P} + 1\right) = \dfrac{A_0 - A}{k_1 \int_0^t A(\tau)\, d\tau}$

$$\left(\frac{Q}{P} + 1\right)_\infty = \frac{A_0 - A(\infty)}{k_1 \int_0^\infty A(\tau)\, d\tau} \quad ; \quad A(\infty) = 0$$

$$\left(\frac{Q + P}{P}\right) = \frac{1}{x_P} = \frac{A_0}{k_1 \int_0^\infty A(\tau)\, d\tau}$$

$$x_P = \left(\frac{k_1}{A_0}\right)\int_0^{\infty} A(\tau)\,d\tau$$

$$x_Q = 1 - x_P$$

$$x_Q = 1 - \left(\frac{k_1}{A_0}\right)\int_0^{\infty} A(\tau)\,d\tau$$

MAS $\displaystyle\int_0^{\infty} A(\tau)\,d\tau = \frac{A_0}{2k_2}\ln 2$ (MOSTRAR)

CONCLUINDO

$$\boxed{x_Q = 1 - \frac{k_1}{2k_2}\ln 2}$$

$$\boxed{x_P = \frac{k_1}{2k_2}\ln 2}$$

USAR

$$z = e^{-k_1 t}$$

$$-k_1 e^{-k_1 t}\,dt = dz$$

$$\int_0^{\infty} A(\tau)\,d\tau = \frac{1}{k_1}\int_0^{1}\frac{dz}{A_0^{-1}\alpha(1-z)}$$

$$\alpha = \frac{2k_2}{k_1}$$

$$\int_0^{\infty} A(\tau)\,d\tau = \left(\frac{1}{k_1}\right)\frac{A_0}{\alpha}\ln 2$$

$$\int_0^{\infty} A(\tau)\,d\tau = \frac{A_0}{2k_2}\ln 2$$

4 REAÇÃO SEQUENCIAL COM ETAPAS AUTOCATALÍTICAS

$$A \xrightarrow{k_1} B \xrightarrow{k_2} C$$

$A(0) = A_0$

$B(0) = B_0$

$C(0) = C_0$

c/ $A_0 \gg B_0 \simeq C_0$

$$-\frac{dA}{dt} = k_1 A \cdot B$$

$$-\frac{dB}{dt} = k_2 B \cdot C - k_1 A \cdot B$$

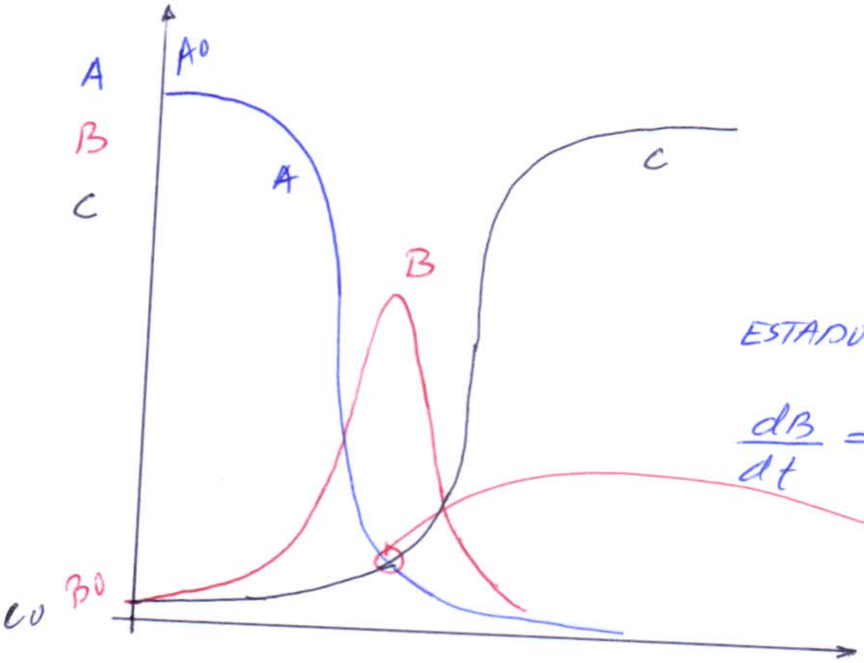
$$+\frac{dC}{dt} = k_2 BC$$

CONSERVAÇÃO

$$A + B + C = A_0 + B_0 + C_0$$

ou

$$dA + dB + dC = 0$$



A e C : SIGMOIDAIS

B : BANDA TIPO GAUSSIANA AFINADA

ESTADO ESTACIONÁRIO ?

$$\frac{dB}{dt} = 0 \Rightarrow k_2 \cancel{B} C \simeq k_1 A \cancel{B}$$

PONTO NÃO UMA REGIÃO

NÃO HÁ ESTADO-ESTACIONÁRIO !