ERQ II – Exercises

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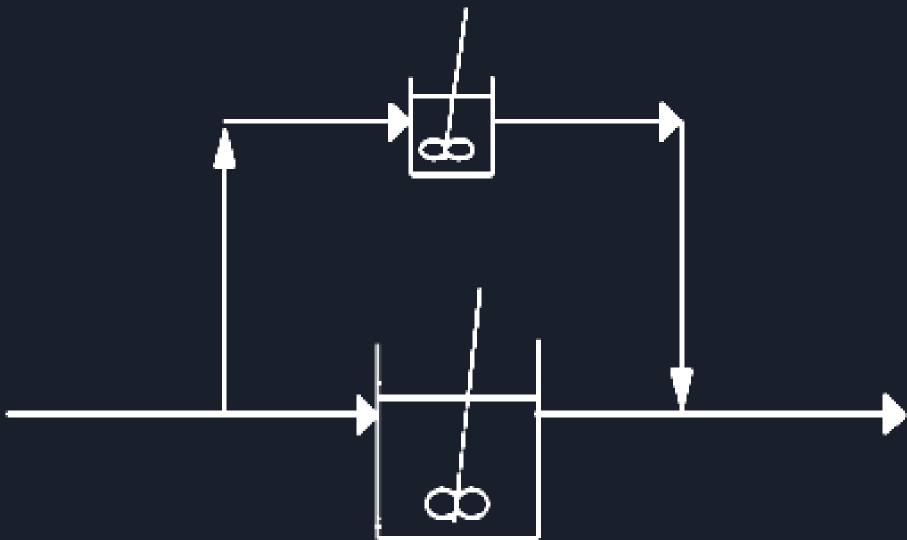
Conteúdo

Questão 2

Considere um reactor CSTR cujo comportamento não ideal pode ser modelado pela associação de reactores ideais em "by-pass", esquematizada na figura.



Transformadas de Laplace:

$f(s)$	$F(t)$
$\frac{1}{s-a}$	$e^{a\,t}$

Q2 a.

Escreva as equações do modelo que representa o escoamento no reactor.

Resposta

Reator	Volume	Caldal In	Caldal Out
1	$(1-\alpha)\,V$	$(1-\beta)\,\nu$	$(1-\beta)\,\nu$
2	$\alpha\,V$	$\beta\,\nu$	$\beta\,\nu$

R_1 :

$$(1-\beta)\,\nu\,C_{in,1} = (1-\beta)\,\nu\,C_{in} =$$

$$= (1-\beta)\,\nu\,C_{out,1} + (1-\alpha)\,V\,\frac{\mathrm{d}C_{out,1}}{\mathrm{d}t};$$

R_2 :

$$\beta\,\nu\,C_{in,2} = \beta\,\nu\,C_{in} = \beta\,\nu\,C_{out,2} + \alpha\,V\,\frac{\mathrm{d}C_{out,2}}{\mathrm{d}t};$$

Nó:

$$\nu\,C_{out} = \beta\,\nu\,C_{out,2} + (1-\beta)\,\nu\,C_{out,1}$$

Q2 b.

Deduza a expressão da distribuição de tempos de residência.

Resposta

$$E(t) = \mathcal{L}\, g(s);$$

$g(s)$:

$$g(s) = \bar{C}_{out}/\bar{C}_{in} = \mathcal{L}\, C_{out}/\,\mathcal{L}\, C_{in};$$

$$\nu\, C_{out} = \beta\, \nu\, C_{out,2} + (1-\beta)\, \nu\, C_{out,1} \implies$$

$$\implies C_{out} = \beta\, C_{out,2} + (1-\beta)\, C_{out,1} \implies$$

$$\implies \mathcal{L}\, C_{out} = \bar{C}_{out} = \beta\, \bar{C}_{out,2} + (1-\beta)\, \bar{C}_{out,1} \implies$$

$$\implies g(s) = \frac{\bar{C}_{out}}{\bar{C}_{in}} = \beta\, \frac{\bar{C}_{out,2}}{\bar{C}_{in}} + (1-\beta)\, \frac{\bar{C}_{out,1}}{\bar{C}_{in}};$$

$\bar{C}_{out,1}$:

$$(1-\beta)\, \nu\, C_{in} = (1-\beta)\, \nu\, C_{out,1} + (1-\alpha)\, V\, \frac{\mathrm{d}C_{out,1}}{\mathrm{d}t} \implies$$

$$\implies (1-\beta)\, C_{in} = (1-\beta)\, C_{out,1} + (1-\alpha)\tau\, \frac{\mathrm{d}C_{out,1}}{\mathrm{d}t} \implies$$

$$\implies \mathcal{L}\,((1-\beta)\, C_{in}) = (1-\beta)\, \bar{C}_{in} =$$

$$= \mathcal{L}\,((1-\beta)\, C_{out,1}) + \mathcal{L}\left((1-\alpha)\tau\, \frac{\mathrm{d}C_{out,1}}{\mathrm{d}t}\right) =$$

$$= (1-\beta)\, \bar{C}_{out,1} + (1-\alpha)\tau\, s\, \bar{C}_{out,1} \implies$$

$$\implies \frac{\bar{C}_{out,1}}{\bar{C}_{in}} = \frac{1-\beta}{1-\beta+(1-\alpha)\tau\, s};$$

$\bar{C}_{out,2}$:

$$\beta\, \nu\, C_{in} = \beta\, \nu\, C_{out,2} + \alpha\, V\, \frac{\mathrm{d}C_{out,2}}{\mathrm{d}t} \implies$$

$$\implies \beta\, C_{in} = \beta\, C_{out,2} + \alpha\, \tau\, \frac{\mathrm{d}C_{out,2}}{\mathrm{d}t} \implies$$

$$\implies \mathcal{L}\,(\beta\, C_{in}) = \beta\, \bar{C}_{in} =$$

$$= \mathcal{L}\,(\beta\, C_{out,2}) + \mathcal{L}\left(\alpha\, \tau\, \frac{\mathrm{d}C_{out,2}}{\mathrm{d}t}\right) =$$

$$= \beta\, \bar{C}_{out,2} + \alpha\, \tau\, s\, \bar{C}_{out,2} \implies$$

$$\implies \frac{\bar{C}_{out,2}}{\bar{C}_{in}} = \frac{\beta}{\beta+\alpha\, \tau\, s};$$

$$\implies g(s) = \beta\, \frac{\beta}{\beta+\alpha\, \tau\, s} + (1-\beta)\, \frac{1-\beta}{1-\beta+(1-\alpha)\tau\, s} =$$

$$= \frac{\beta^2}{\alpha\, \tau} \left(\frac{1}{\frac{\beta}{\alpha\, \tau}+s}\right) + \frac{(1-\beta)^2}{(1-\alpha)\tau} \left(\frac{1}{\frac{1-\beta}{(1-\alpha)\tau}+s}\right) \implies$$

$$\implies \mathcal{L}\, g(s) = \frac{\beta^2}{\alpha\, \tau}\, \exp\left(-\frac{\beta}{\alpha\, \tau}\, t\right) + \frac{(1-\beta)^2}{(1-\alpha)\tau}\, \exp\left(-\frac{1-\beta}{(1-\alpha)\tau}\, t\right)$$

Q2 c.

Deduza a expressão da função cumulativa.

Resposta

Função culmulativa:

$$F(t) = \int_0^t E(t)\ \mathrm{d}t =$$

$$= \int_0^t \left(\frac{\beta^2}{\alpha\,\tau} \exp\left(-\frac{\beta}{\alpha\,\tau}\,t\right) + \frac{(1-\beta)^2}{(1-\alpha)\tau} \exp\left(-\frac{1-\beta}{(1-\alpha)\tau}\,t\right)\right)\ \mathrm{d}t =$$

$$= \frac{\beta^2}{\alpha\,\tau} \int_0^t \exp\left(-\frac{\beta}{\alpha\,\tau}\,t\right)\ \mathrm{d}t +$$

$$+ \frac{(1-\beta)^2}{(1-\alpha)\tau} \int_0^t \exp\left(-\frac{1-\beta}{(1-\alpha)\tau}\,t\right) \mathrm{d}t =$$

$$= \frac{\beta^2}{\alpha\,\tau}\,\frac{\alpha\,\tau}{\beta}\,\Delta - \exp\left(-\frac{\beta}{\alpha\,\tau}\,t\right)\Big|_0^t +$$

$$+ \frac{(1-\beta)^2}{(1-\alpha)\tau}\,\frac{(1-\alpha)\tau}{1-\beta}\,\Delta - \exp\left(-\frac{1-\beta}{(1-\alpha)\tau}\,t\right)\Big|_0^t =$$

$$= (\beta)\left(-\exp\left(-\frac{\beta}{\alpha\,\tau}\,t\right) + \exp 0\right) +$$

$$+ (1-\beta)\left(-\exp\left(-\frac{1-\beta}{(1-\alpha)\tau}\,t\right) + \exp 0\right) =$$

$$= \beta\left(-\exp\left(-\frac{\beta}{\alpha\,\tau}\,t\right) + 1\right) +$$

$$+ (1-\beta)\left(-\exp\left(-\frac{1-\beta}{(1-\alpha)\tau}\,t\right) + 1\right)$$

Q2 d.

Sabendo que no reactor é introduzido um traçador, por degrau, com uma concentração à entrada do reactor $C_0 = 0.1\,\mathrm{M}$, a um caudal volumétrico $10\,\mathrm{dm}^3/\mathrm{min}$, calcule o tempo ao fim do qual a concentração de traçador à saída é 95% da concentração à entrada.

- Volume do reactor: $1\,\mathrm{m}^3$;
- caudal de by-pass: 10% do caudal volumétrico à entrada;
- volume do by-pass: 20% do volume do reactor.

Resposta

$t : C(t) = 0.95\, C_0;$

Tracador em Degrau: $F(t) = \dfrac{C(t)}{C_0};$

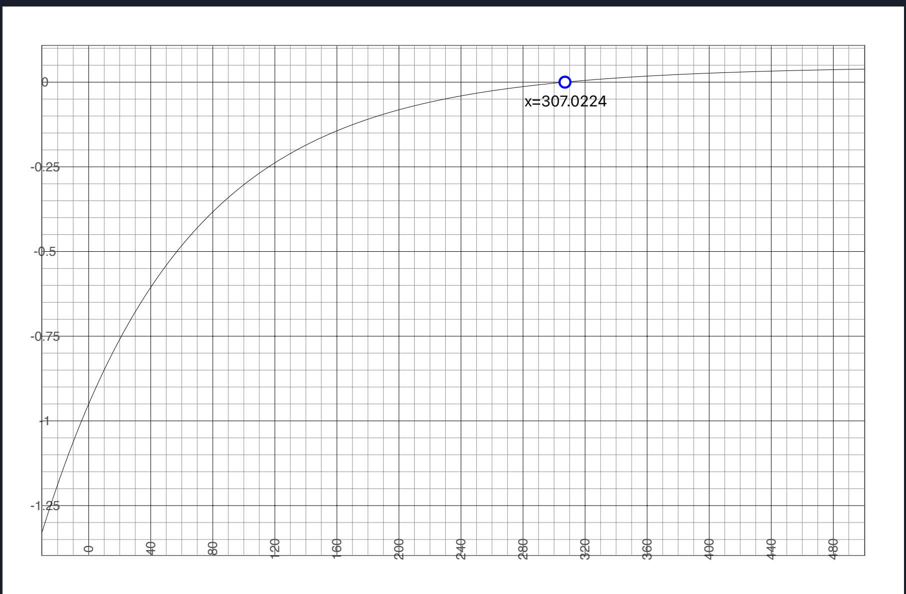
Normalização da curva C:

$$\begin{cases} \alpha = 20\% \\ \beta = 10\% \end{cases}$$

$$F(t) = \frac{C(t)}{C_0} = \frac{0.95\, C_0}{C_0} = 0.95 =$$

$$= \beta \left(-\exp\left(-\frac{\beta}{\alpha\,\tau}\, t \right) + 1 \right) +$$
$$+ (1-\beta) \left(-\exp\left(-\frac{1-\beta}{(1-\alpha)\tau}\, t \right) + 1 \right)$$
$$= 0.1 \left(-\exp\left(-\frac{0.1}{0.2\,\frac{1000}{10}}\, t \right) + 1 \right) +$$
$$+ (1-0.1) \left(-\exp\left(-\frac{1-0.1}{(1-0.2)\frac{1000}{10}}\, t \right) + 1 \right) \cong$$
$$\cong -\exp\left(-\frac{t}{200} \right) - \exp\left(-\frac{9\,t}{800} \right) + 1 \implies$$

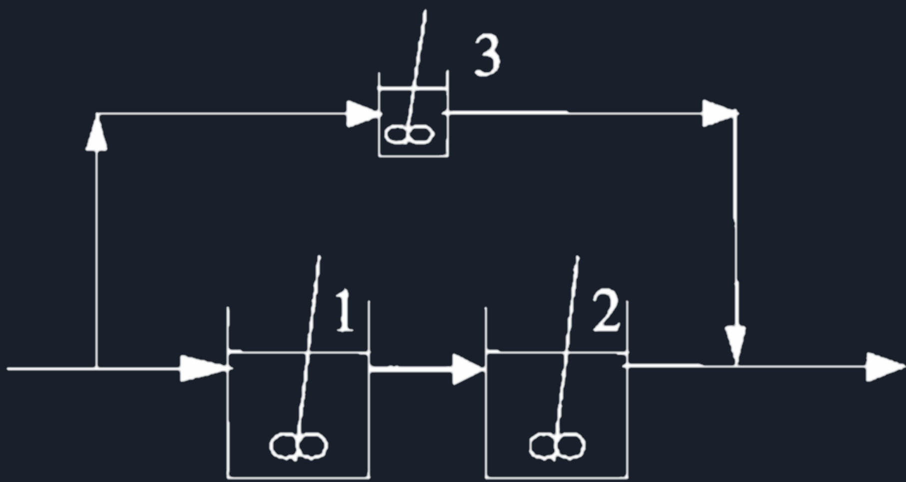
$$\implies f(t) = -\exp\left(-\frac{t}{200} \right) - \exp\left(-\frac{9\,t}{800} \right) + 0.05$$



$t \cong 307.022\,\mathrm{min}$

Questão 4

Considere um reactor contínuo cujo comportamento não ideal pode ser modelado pela associação de reactores ideais esquematizada na figura.



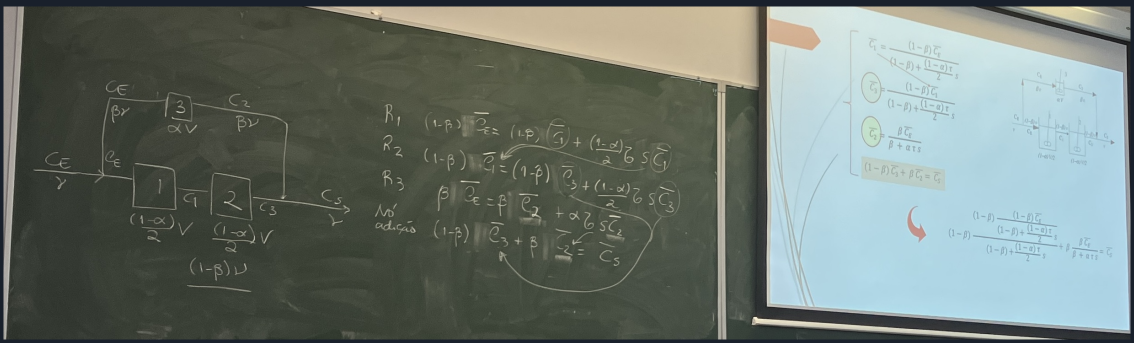
Transformadas de Laplace:

$f(s)$	$F(t)$
$\frac{1}{s-a}$	$e^{a\,t}$
$\frac{1}{(s-a)^2}$	$t\,e^{a\,t}$

Q4 a.

Escreva as equações do modelo que representa o escoamento no reactor, tendo em conta que os tanques 1 e 2 são iguais.

Resposta



Reator	Volume	Caldal In	Caldal Out
1	$\alpha\,V$	$\beta\,\nu$	$\beta\,\nu$
2	$(1-\alpha)\,V/2$	$(1-\beta)\,\nu$	$(1-\beta)\,\nu$
3	$(1-\alpha)\,V/2$	$(1-\beta)\,\nu$	$(1-\beta)\,\nu$

R_1 :

$$(1-\beta)\,\nu\,C_{in,1} = (1-\beta)\,\nu\,C_{in} =$$
$$= (1-\beta)\,\nu\,C_{out,1} + (1-\alpha)\,\frac{V}{2}\,\frac{\mathrm{d}C_{out,1}}{\mathrm{d}t};$$

R_2 :

$$(1-\beta)\,\nu\,C_{in,2} = (1-\beta)\,\nu\,C_{out,1} =$$
$$= (1-\beta)\,\nu\,C_{out,2} + (1-\alpha)\,\frac{V}{2}\,\frac{\mathrm{d}C_{out,2}}{\mathrm{d}t};$$

R_3 :

$$\beta\,\nu\,C_{in,3} = \beta\,\nu\,C_{in} = \beta\,\nu\,C_{out,3} + \alpha\,V\,\frac{\mathrm{d}C_{out,3}}{\mathrm{d}t};$$

Nó :

$$\nu\,C_{out} = (1-\beta)\,\nu\,C_{out,2} + \beta\,\nu\,C_{out,3}$$

Q4 b.

Deduza a expressão da distribuição de tempos de residência.

Resposta

$E(t) = \mathcal{L}\, g(s);$

$g(s):$

$$
\begin{aligned}
& g(s) = \bar{C}_{out}/\bar{C}_{in} = \mathcal{L}\, C_{out}/\, \mathcal{L}\, C_{in}; \\
& \nu\, C_{out} = (1-\beta)\, \nu\, C_{out,2} + \beta\, \nu\, C_{out,3} \implies \\
& \implies C_{out} = (1-\beta)\, C_{out,2} + \beta\, C_{out,3} \implies \\
& \implies \mathcal{L}\, C_{out} = \bar{C}_{out} = \\
& = \mathcal{L}\left((1-\beta)\, C_{out,2}\right) + \mathcal{L}\left(\beta\, C_{out,3}\right) = \\
& = (1-\beta)\, \bar{C}_{out,2} + \beta\, \bar{C}_{out,3} \implies \\
& \implies g(s) = (1-\beta)\, \frac{\bar{C}_{out,2}}{\bar{C}_{in}} + \beta\, \frac{\bar{C}_{out,3}}{\bar{C}_{in}};
\end{aligned}
$$

$\bar{C}_{out,3}/\bar{C}_{in}:$

$$
\begin{aligned}
& \beta\, \nu\, C_{in} = \beta\, \nu\, C_{out,3} + \alpha\, V\, \frac{\mathrm{d}C_{out,3}}{\mathrm{d}t} \implies \\
& \implies \beta\, C_{in} = \beta\, C_{out,3} + \alpha\, \tau\, \frac{\mathrm{d}C_{out,3}}{\mathrm{d}t} \implies \\
& \implies \mathcal{L}\left(\beta\, C_{in}\right) = \beta\, \bar{C}_{in} = \\
& = \mathcal{L}\left(\beta\, C_{out,3}\right) + \mathcal{L}\left(\alpha\, \tau\, \frac{\mathrm{d}C_{out,3}}{\mathrm{d}t}\right) = \beta\, \bar{C}_{out,3} + \alpha\, \tau\, s\, \bar{C}_{out,3} \implies \\
& \implies \frac{\bar{C}_{out,3}}{\bar{C}_{in}} = \frac{\beta}{\beta + \alpha\, \tau\, s};
\end{aligned}
$$

$\bar{C}_{out,2}/\bar{C}_{in}:$

$$
\begin{aligned}
& (1-\beta)\, \nu\, C_{out,1} = (1-\beta)\, \nu\, C_{out,2} + (1-\alpha)\, \frac{V}{2}\, \frac{\mathrm{d}C_{out,2}}{\mathrm{d}t} \implies \\
& \implies (1-\beta)\, C_{out,1} = (1-\beta)\, C_{out,2} + \frac{1-\alpha}{2}\, \tau\, \frac{\mathrm{d}C_{out,2}}{\mathrm{d}t} \implies \\
& \implies \mathcal{L}\left((1-\beta)\, C_{out,1}\right) = (1-\beta)\, \bar{C}_{out,1} = \\
& = \mathcal{L}\left((1-\beta)\, C_{out,2}\right) + \mathcal{L}\left(\frac{1-\alpha}{2}\, \tau\, \frac{\mathrm{d}C_{out,2}}{\mathrm{d}t}\right) = \\
& = (1-\beta)\, \bar{C}_{out,2} + \frac{1-\alpha}{2}\, \tau\, s\, \bar{C}_{out,2} \implies \\
& \implies \frac{\bar{C}_{out,2}}{\bar{C}_{in}} = \frac{(1-\beta)}{(1-\beta) + \frac{(1-\alpha)\tau}{2}\, s}\, \frac{\bar{C}_{out,1}}{\bar{C}_{in}};
\end{aligned}
$$

$\bar{C}_{out,1}/\bar{C}_{in}:$

$$
\begin{aligned}
& (1-\beta)\, \nu\, C_{in} = (1-\beta)\, \nu\, C_{out,1} + (1-\alpha)\, \frac{V}{2}\, \frac{\mathrm{d}C_{out,1}}{\mathrm{d}t} \implies \\
& \implies (1-\beta)\, C_{in} = (1-\beta)\, C_{out,1} + \frac{1-\alpha}{2}\, \tau\, \frac{\mathrm{d}C_{out,1}}{\mathrm{d}t} \implies \\
& \implies \mathcal{L}\left((1-\beta)\, C_{in}\right) = (1-\beta)\, \bar{C}_{in} = \\
& = \mathcal{L}\, (1-\beta)\, C_{out,1} + \mathcal{L}\left(\frac{1-\alpha}{2}\, \tau\, \frac{\mathrm{d}C_{out,1}}{\mathrm{d}t}\right) = \\
& = (1-\beta)\, \bar{C}_{out,1} + \frac{1-\alpha}{2}\, \tau\, s\, \bar{C}_{out,1} \implies \\
& \implies \frac{\bar{C}_{out,1}}{\bar{C}_{in}} = \frac{(1-\beta)}{(1-\beta) + \frac{(1-\alpha)\,\tau}{2}\, s} \implies
\end{aligned}
$$

$$
\begin{aligned}
& \implies \frac{\bar{C}_{out,2}}{\bar{C}_{in}} = \frac{(1-\beta)}{(1-\beta) + \frac{(1-\alpha)\tau}{2}\, s}\, \frac{\bar{C}_{out,1}}{\bar{C}_{in}} = \\
& = \left(\frac{(1-\beta)}{(1-\beta) + \frac{(1-\alpha)\,\tau}{2}\, s}\right)^2;
\end{aligned}
$$

$$
\begin{aligned}
& \implies g(s) = \\
& = (1-\beta)\left(\frac{(1-\beta)}{(1-\beta) + \frac{(1-\alpha)\,\tau}{2}\, s}\right)^2 + \beta\left(\frac{\beta}{\beta + \alpha\,\tau\, s}\right) = \\
& = \frac{(1-\beta)^3}{\left(\frac{(1-\alpha)\,\tau}{2}\right)^2}\, \frac{1}{\left(\frac{(1-\beta)\,2}{(1-\alpha)\,\tau} + s\right)^2} + \frac{\beta^2}{\alpha\,\tau}\, \frac{1}{\frac{\beta}{\alpha\,\tau} + s} \implies
\end{aligned}
$$

$$
\begin{aligned}
& \implies E(t) = \mathcal{L}\, g(s) = \\
& = \frac{(1-\beta)^3\, 4}{(1-\alpha)^2\, \tau^2}\, t\, \exp\left(-\frac{(1-\beta)\, 2}{(1-\alpha)\,\tau}\, t\right) + \frac{\beta^2}{\alpha\,\tau}\, \exp\left(-\frac{\beta}{\alpha\,\tau}\, t\right)
\end{aligned}
$$

Q4 c.

Deduza e expressão da função cumulativa.

Resposta

$$F(t)=\int_0^t E(t)\ \mathrm{d}t=$$
$$=\int_0^t \frac{(1-\beta)^3\,4}{(1-\alpha)^2\,\tau^2}\,t\ \exp\left(-\frac{(1-\beta)\,2}{(1-\alpha)\,\tau}\,t\right)\ \mathrm{d}t+$$
$$+\int_0^t \frac{\beta^2}{\alpha\,\tau}\ \exp\left(-\frac{\beta}{\alpha\,\tau}\,t\right)\ \mathrm{d}t=$$
$$=\frac{(1-\beta)^3\,4}{(1-\alpha)^2\,\tau^2}\int_0^t t\ \exp\left(-\frac{(1-\beta)\,2}{(1-\alpha)\,\tau}\,t\right)\ \mathrm{d}t+$$
$$+\frac{\beta^2}{\alpha\,\tau}\,\frac{\alpha\,\tau}{\beta}\,\Delta\left(-\exp\left(-\frac{\beta}{\alpha\,\tau}\,t\right)\right)\Big|_0^t=$$
$$=\frac{(1-\beta)^3\,4}{(1-\alpha)^2\,\tau^2}\int_0^t t\ \exp\left(-\frac{(1-\beta)\,2}{(1-\alpha)\,\tau}\,t\right)\ \mathrm{d}t+$$
$$+\beta\left(-\exp\left(-\frac{\beta}{\alpha\,\tau}\,t\right)+\exp 0\right);$$

Primitiva:

$$\mathrm{d}\left(t\ \exp\left(-\frac{(1-\beta)\,2}{(1-\alpha)\,\tau}\,t\right)\right)=$$
$$=\exp\left(-\frac{(1-\beta)\,2}{(1-\alpha)\,\tau}\,t\right)+$$
$$+t\left(-\frac{(1-\beta)\,2}{(1-\alpha)\,\tau}\right)\ \exp\left(-\frac{(1-\beta)\,2}{(1-\alpha)\,\tau}\,t\right)\implies$$
$$\implies\mathcal{P}\left(\mathrm{d}\left(t\ \exp\left(-\frac{(1-\beta)\,2}{(1-\alpha)\,\tau}\,t\right)\right)\right)=t\ \exp\left(-\frac{(1-\beta)\,2}{(1-\alpha)\,\tau}\,t\right)=$$
$$=\mathcal{P}\left(\exp\left(-\frac{(1-\beta)\,2}{(1-\alpha)\,\tau}\,t\right)\right)+$$
$$+\mathcal{P}\left(t\left(-\frac{(1-\beta)\,2}{(1-\alpha)\,\tau}\right)\ \exp\left(-\frac{(1-\beta)\,2}{(1-\alpha)\,\tau}\,t\right)\right)=$$
$$=-\frac{(1-\alpha)\,\tau}{(1-\beta)\,2}\exp\left(-\frac{(1-\beta)\,2}{(1-\alpha)\,\tau}\,t\right)+$$
$$-\frac{(1-\beta)\,2}{(1-\alpha)\,\tau}\,\mathcal{P}\left(t\ \exp\left(-\frac{(1-\beta)\,2}{(1-\alpha)\,\tau}\,t\right)\right)\implies$$
$$\implies\mathcal{P}\left(t\ \exp\left(-\frac{(1-\beta)\,2}{(1-\alpha)\,\tau}\,t\right)\right)=$$
$$=-\frac{(1-\alpha)\,\tau}{(1-\beta)\,2}\left(t+\frac{(1-\alpha)\,\tau}{(1-\beta)\,2}\right)\exp\left(-\frac{(1-\beta)\,2}{(1-\alpha)\,\tau}\,t\right)\implies$$

$$\implies F(t)=\frac{(1-\beta)^3\,4}{(1-\alpha)^2\,\tau^2}*$$
$$*\,\Delta\left(-\frac{(1-\alpha)\,\tau}{(1-\beta)\,2}\left(t+\frac{(1-\alpha)\,\tau}{(1-\beta)\,2}\right)\exp\left(-\frac{(1-\beta)\,2}{(1-\alpha)\,\tau}\,t\right)\right)\Big|_0^t+$$
$$+\beta\left(-\exp\left(-\frac{\beta}{\alpha\,\tau}\,t\right)+1\right)=$$
$$=\frac{(1-\beta)^3\,4}{(1-\alpha)^2\,\tau^2}*$$
$$*\left(-\frac{(1-\alpha)\,\tau}{(1-\beta)\,2}\left(t+\frac{(1-\alpha)\,\tau}{(1-\beta)\,2}\right)\exp\left(-\frac{(1-\beta)\,2}{(1-\alpha)\,\tau}\,t\right)+\right.$$
$$\left.+\left(\frac{(1-\alpha)\,\tau}{(1-\beta)\,2}\right)^2\exp 0\right)+$$
$$+\beta\left(-\exp\left(-\frac{\beta}{\alpha\,\tau}\,t\right)+1\right)=$$
$$=(1-\beta)\left(-\left(t\,\frac{(1-\beta)\,2}{(1-\alpha)\,\tau}+1\right)\exp\left(-\frac{(1-\beta)\,2}{(1-\alpha)\,\tau}\,t\right)+1\right)+$$
$$+\beta\left(-\exp\left(-\frac{\beta}{\alpha\,\tau}\,t\right)+1\right)$$

Q4 d.

Sabendo que o reactor real tem um volume de $1\,\mathrm{m}^3$ e que são introduzidos, por impulso, $6\,\mathrm{mol}$ de um tracador, determine o valor da concentração máxima de tracador. à saída do reactor.

- Caudal volumétrico da alimentação: $20\,\mathrm{dm}^3/\mathrm{min}$;
- caudal de by-pass: 5% do caudal volumétrico à entrada;
- volume do reciclo: 8% do volume activo;
- volumes mortos: 12% do volume do reactor.

Resposta

Traçador por impulso:

$$\frac{\mathrm{d}C}{\mathrm{d}t} = \frac{N}{\nu}\,\frac{\mathrm{d}E(t)}{\mathrm{d}t};$$

$$\begin{cases} \beta = 0.05; \quad (1-\beta) = 0.95 \\ \alpha = 0.08; \quad (1-\alpha) = 0.92 \\ V_m = 0.12 * 1000\,\mathrm{dm}^3 = 120\,\mathrm{dm}^3 \\ V = (1000-120)\,\mathrm{dm}^3 = 880\,\mathrm{dm}^3 \\ \nu = 20\,\mathrm{dm}^3/\mathrm{min} \\ \tau = \frac{880}{20}\mathrm{min} = 44\,\mathrm{min} \\ N = 6\,\mathrm{mol} \\ t = 21\,\mathrm{min} \end{cases}$$

$$\implies \frac{\mathrm{d}C}{\mathrm{d}t} = 0 =$$

$$= \frac{N}{\nu}\left(\frac{(1-\beta)^3\,4}{(1-\alpha)^2\,\tau^2}\left(1 - \frac{(1-\beta)\,2}{(1-\alpha)\,\tau}\,t\right)\exp\left(-\frac{(1-\beta)\,2}{(1-\alpha)\,\tau}\,t\right)\right.$$

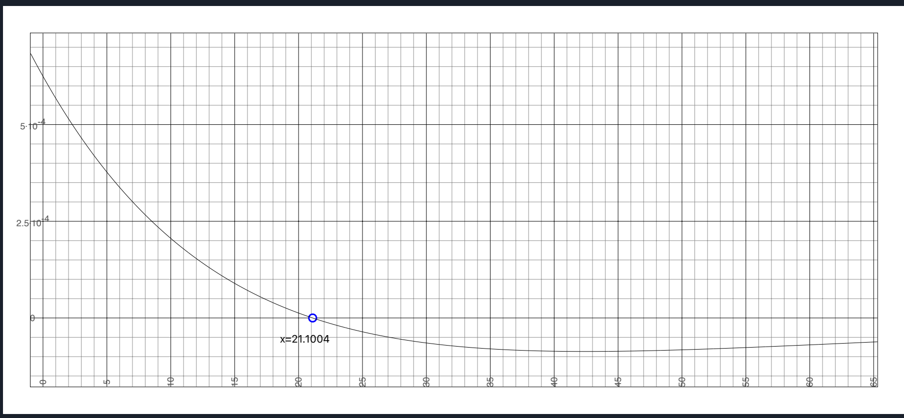
$$\left. - \frac{\beta^3}{\alpha^2\,\tau^2}\,\exp\left(-\frac{\beta}{\alpha\,\tau}\,t\right)\right) =$$

$$= \frac{6}{20}\left(\frac{0.95^3 * 4}{0.92^2 * 44^2}\left(1 - \frac{0.95*2}{0.92*44}\,t\right)\exp\left(-\frac{0.95*2}{0.92*44}\,t\right)\right.$$

$$\left. - \frac{0.05^3}{0.08^2 * 44^2}\,\exp\left(-\frac{0.05}{0.08*44}\,t\right)\right) =$$

$$= \left(6.279\,\mathrm{E}^{-4} - 2.947\,\mathrm{E}^{-5}\,t\right)\exp\left(-4.694\,\mathrm{E}^{-2}\,t\right)$$

$$- 3.027\,\mathrm{E}^{-6}\,\exp\left(-1.420\,\mathrm{E}^{-2}\,t\right)$$



$t = 21.100\,\mathrm{min};$

$$C \cong \frac{N}{\nu}E(21.100) \cong$$

$$\cong \frac{6}{20}\left(\frac{0.95^3 * 4}{0.92^2 * 44^2}\,21.100\,\exp\left(-\frac{0.95*2}{0.92*44}\,21.100\right) + \right.$$

$$\left. + \frac{0.05^2}{0.08*44}\,\exp\left(-\frac{0.05}{0.08*44}\,21.100\right)\right) \cong$$

$$\cong 8.435\,\mathrm{E}^{-3}\,\mathrm{M}$$

Questão 13

A reacção elementar A $\longrightarrow$ B é conduzida, na fase gasosa, num reactor multitubular de leito fixo, consistindo em 100 tubos de $2\,\mathrm{m}$ de comprimento e $2\,\mathrm{cm}$ de diâmetro da secção recta, cheios com um catalisador sólido, poroso, na forma de pellets esféricas de $5\,\mathrm{mm}$ de diâmetro. O reagente A é alimentado puro a um caudal de $100\,\mathrm{dm/min}$, à temperatura de $373\,\mathrm{K}$ e à pressão de $6\,\mathrm{atm}$

Dados:

- $\rho_P = 1.3\,\mathrm{g/cm^3}$
- Coeficiente de Difusão externo: $D_A = 2.7\,\mathrm{E}^{-7}\,\mathrm{m^2/s}$
- Viscosidade Cinemática: $\nu = 4\,\mathrm{E}^{-6}\,\mathrm{m^2/s}$
- $\varepsilon_B = 0.45$
- Difusidade efetiva intraparticular: $D_e = 1.3\,\mathrm{E}^{-8}\,\mathrm{m^2/s}$
- Constante cinética: $k' = 0.023\,\mathrm{dm^3\,g^{-1}\,(cat)\,min^{-1}}$
- $R \cong 8.206\,\mathrm{E}^{-2}\,\mathrm{dm^3\,atm\,mol^{-1}\,K^{-1}}$

Formulas:

$$\boldsymbol{Sh = 1.0\,Re^{1/2}\,Sc^{1/3} = \frac{k_c\,d_P}{D_A}\,\frac{1}{(1/\varepsilon_b)-1};}$$

$$\boldsymbol{Re = \frac{u\,d_P}{\nu\,(1-\varepsilon_b)}; Sc = \frac{\nu}{D_A};}$$

$$\boldsymbol{\phi = R\sqrt{\frac{k'\,\rho_P}{D_e}}; \eta = \frac{3}{\phi^2}(\phi\,\coth\phi - 1)}$$

Perfil de concentração de pellet: $\rho = \frac{\sinh(\phi\,\lambda)}{\lambda\,\cosh\phi}$

Q13 a.

Calcule o valor da constante cinética aparente, que observaria no caso da ausência de limitações difusionais externas.

Resposta

$$k'_{ap} = \eta\, k' = \left(\frac{3}{\phi^2}(\phi\,\coth\phi - 1)\right) k';$$

$$\phi = R\sqrt{\frac{k'\,\rho_P}{D_e}} \cong$$

$$\cong 8.206\,\mathrm{E}^{-2}\,\mathrm{dm}^3\,\mathrm{atm}\,\mathrm{mol}^{-1}\,\mathrm{K}^{-1}\sqrt{\frac{0.023\,\mathrm{E}^{-3}\,\frac{\mathrm{m}^3}{\mathrm{min}}\,\frac{\mathrm{min}}{60\,\mathrm{s}} * 1.300\,\mathrm{E}^3\,\mathrm{m}^2/\mathrm{s}}{1.300\,\mathrm{E}^{-8}\,\mathrm{m}^2/\mathrm{s}}} \cong$$

$$\cong 16.066 \implies$$

$$\implies k'_{ap} = \frac{3}{\phi^2}(\phi\,\coth\phi - 1)\,k' \cong$$

$$\cong \frac{3}{(16.066)^2}\,(16.066\,\coth 16.066 - 1)\,\frac{0.023}{60} \cong 6.712\,\mathrm{E}^{-5}\,\mathrm{L/sec\,g}$$

Q13 b.

Calcule o valor do coeficiente de transferência de massa.

Resposta

$$Sh = Re^{1/2}\,Sc^{1/3} = \left(\frac{u\,d_P}{\nu\,(1-\varepsilon_b)}\right)^{1/2}\left(\frac{\nu}{D_a}\right)^{1/3};$$

$$u = \frac{\nu_{tubos}}{A_c} = \frac{(\nu/N_{tubos})}{(\varepsilon_b\,\pi\,D^2/4)} = \frac{(\nu/60*100)}{(0.45\,\pi\,0.02^2/4)} \cong$$
$$\cong \nu\,1.179 \implies$$

$$\implies Sh = \left(\frac{u\,d_P}{\nu\,(1-\varepsilon_b)}\right)^{1/2}\left(\frac{\nu}{D_a}\right)^{1/3}$$

Q13 c.

Calcule o valor da constante cinética realmente observada.

Q13 d.

Diga, justificando a sua resposta, se o reactor se encontra em regime cinético, difusional interno, difusional externo ou misto.

Q13 e.

Calcule a conversão à saída do reactor.

Q13 f.

Determine o valor da concentração de A no centro das pellets, à saída do reactor.