ERQ II – Prática 1

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Conteúdo

Absorvancia Experimental

$$\int \mathrm{Abs}_i = (\boldsymbol{t_i} - \boldsymbol{t_{i-1}})\,\frac{\mathrm{Abs}_i + \mathrm{Abs}_{i-1}}{\mathbf{2}}$$

Distribuição de tempos de residência

$$\boldsymbol{E(t)} = \frac{\boldsymbol{C(t)}}{\int_0^\infty \boldsymbol{C(t)}\ \mathrm{d}\boldsymbol{t}} = \frac{\boldsymbol{\varepsilon\, A(t)}}{\int_0^\infty \boldsymbol{\varepsilon\, A(t)}\ \mathrm{d}\boldsymbol{t}} = \frac{\boldsymbol{A(t)}}{\int_0^\infty \boldsymbol{A(t)}\ \mathrm{d}\boldsymbol{t}}$$

$$\int_0^\infty \boldsymbol{E(t)}\ \mathrm{d}\boldsymbol{t} = \mathbf{1}$$

Função culmulativa de tempos de residência

$$\boldsymbol{F(t) = \int_0^t E(t)\ \mathrm{d}t = F_{i-1} + (t_i - t_{i-1})\,\frac{E_i + E_{i+1}}{2}}$$

Tempo espacial

$$\boldsymbol{\tau} = \int_0^\infty \boldsymbol{t}\, \boldsymbol{E}(\boldsymbol{t})\ \mathrm{d}\boldsymbol{t} = \sum (\boldsymbol{t}_i - \boldsymbol{t}_{i-1})\, \frac{\boldsymbol{t}_{m,i} - \boldsymbol{t}_{m,i-1}}{\mathbf{2}}$$

$$\boldsymbol{t}_m = \boldsymbol{t}\, \boldsymbol{E}(\boldsymbol{t})$$

Funções em tempo adimensional

$$\boldsymbol{\theta(t) = t/t_m; \quad E(\theta) = t_m\, E(t);}$$

$$\boldsymbol{F(\theta) = \int_0^{\theta} E(\theta)\, \mathrm{d}\theta = F_{i-1} + (\theta_i - \theta_{i-1})\, \frac{E_i + E_{i-1}}{2}}$$

II – Prática 2

$$\boldsymbol{X}_{\boldsymbol{exp}} = \mathbf{1} - \frac{\mathrm{Abs}_{est}}{\mathrm{Abs}_0}; \quad \boldsymbol{v}_0 = \frac{\boldsymbol{V}_{\boldsymbol{m}}}{\boldsymbol{t}}; \quad \boldsymbol{\tau} = \frac{\boldsymbol{V}_{\boldsymbol{ativo}}}{\boldsymbol{v}_0}; \quad \boldsymbol{k} = \left(\left(\boldsymbol{X}_{\boldsymbol{exp}}^{-1} - 1 \right) \boldsymbol{\tau} \right)^{-1}$$

Modelo de Segregação

$$\boldsymbol{X} = \mathbf{1} - \exp\left(-\boldsymbol{k}\,\boldsymbol{t}\right)$$

$$\bar{\boldsymbol{X}} = \int_{\mathbf{0}}^{\infty} \boldsymbol{X}\,\boldsymbol{E}(\boldsymbol{t})\ \mathrm{d}\boldsymbol{t} = \boldsymbol{\Delta t}\frac{(\boldsymbol{X}\,\boldsymbol{E}(\boldsymbol{t}))_{\boldsymbol{i}} + (\boldsymbol{X}\,\boldsymbol{E}(\boldsymbol{t}))_{\boldsymbol{i-1}}}{\mathbf{2}}$$

Modelo de Máxima Mistura

$$\boldsymbol{X_i = X_{i-1} + \left(-k\,(1 - X_{i-1}) + \frac{E_{i-1}(\lambda)\,X_{i-1}}{1 - F_{i-1}(\lambda)}\right)\Delta\lambda}$$

$$\begin{aligned}
&\frac{\mathrm{d}x}{\mathrm{d}\lambda} = \frac{r_A}{C_{A,0}} + \frac{E\,X}{1 - F} \implies \\
&\implies \frac{\Delta X}{\Delta\lambda} = \frac{X_i - X_{i-1}}{\Delta\lambda} = \frac{-k\,C_{A,0}\,(1 - X_{i-1})}{C_{A,0}} + \frac{E_{i-1}(\lambda)\,X_{i-1}}{1 - F_{i-1}(\lambda)} \implies \\
&\implies X_i = X_{i-1} + \left(-k\,(1 - X_{i-1}) + \frac{E_{i-1}(\lambda)\,X_{i-1}}{1 - F_{i-1}(\lambda)}\right)\Delta\lambda
\end{aligned}$$

Segregação

$$\boldsymbol{k} = \frac{\mathrm{Abs}_0/\mathrm{Abs}_{est} - 1}{\boldsymbol{\tau}}$$

$$\boldsymbol{X_i = \Delta t\,\frac{(X * E_{calc})_i + (X * E_{calc})_{i-1}}{2}}$$

III – Prática 3

$$\frac{\boldsymbol{N_{Ac}}}{\boldsymbol{N_{C9}}} = \boldsymbol{Fr}\,\frac{\boldsymbol{A_{Ac}}}{\boldsymbol{A_{C9}}} \implies \boldsymbol{N_{Ac}} = \boldsymbol{Fr}\,\boldsymbol{N_{C9}}\,\frac{\boldsymbol{A_{Ac}}}{\boldsymbol{A_{C9}}}$$

$$CH_3OOCC_2H_5 + CH_3OH \longrightarrow CH_3OOCH_3 + CH_3CH_2OH$$

$$\boldsymbol{\ln \frac{1}{1 - X} = \frac{W}{V}\, k'_{ap}\, t}$$

$$-\, r_A = k'_{ap}\, C_A = k'_{ap}\, C_{A,0}(1 - X); \quad \frac{\mathrm{d}N_A}{\mathrm{d}t} = W\, r_A \implies$$

$$\implies -r_A = \frac{N_{A,0}}{W}\,\frac{\mathrm{d}X}{\mathrm{d}t} = k'_{ap}\, C_{A,0}(1 - X) \implies$$

$$\implies \int \frac{\mathrm{d}X}{1 - X} = \ln \frac{1}{1 - X} = \int \frac{W}{N_{A,0}} k'_{ap}\, C_{A,0}\, \mathrm{d}t = \frac{W}{N_{A,0}/C_{A,0}} k'_{ap} \int \mathrm{d}t = \frac{W}{V_A} k'_{ap}\, t$$

Pellet P

$$\boldsymbol{k'}_{\boldsymbol{Ap}} = \text{Declive}\frac{\boldsymbol{V_A}}{\boldsymbol{W}}$$

$$X = 1 - \frac{N_{Ac,t}}{N_{Ac,0}}$$