Apéndice G

Formulario para la Parte I

Estequiometría:

$$\boxed{n_j = n_{j0} + \frac{\nu_j}{-\nu_i} \cdot (n_{i0} - n_i)} \quad (1.2)$$

$$\boxed{n_{rl} = n_{rl0}(1 - f_{rl})} \quad (1.5)$$

$$\boxed{n_j = n_{j0} + \frac{\nu_j}{-\nu_{rl}} \cdot n_{rl0} f_{rl}} \quad (1.6)$$

$$\boxed{n_i = n_{i0} + \nu_i\, \xi} \quad (1.8)$$

$$\begin{aligned} n_T &= n_{T0} + \frac{\Delta\nu}{-\nu_{rl}}\,(n_{rl0} - n_{rl}) \\ &= n_{T0} + \frac{\Delta\nu}{-\nu_{rl}}\, n_{rl0}\, f_{rl} \end{aligned} \quad (1.14)$$

$$\boxed{n_i = n_{i0} + \sum_{r=1}^{n_{rxn}} \nu_{ir}\, \xi_r} \quad (1.19)$$

$$\xi_r = \frac{n_{i0}\, f_{ir}}{(-\nu_{ir})} \quad (1.23)$$

$$-\sum \nu_{ir}\, \xi_r = n_{i0}\, f_i \quad (1.24)$$

$$n_T = n_{T0} + \sum \Delta\nu_r\, \xi_r \quad (1.26)$$

NOTA: En las ecuaciones anteriores se puede sustituir; n por C para líquidos (ξ por ξ^*); y n por F para gases (ξ por ξ').

Equilibrio:

$$\boxed{K_C = \frac{C_R{}^r\, C_S{}^s \ldots}{C_A{}^a\, C_B{}^b \ldots}} \quad (2.10)$$

$$\boxed{K_P = \frac{p_R{}^r\, p_S{}^s \ldots}{p_A{}^a\, p_B{}^b \ldots}} \quad (2.9)$$

Para SOLUCIÓN NUMÉRICA, <u>modificar</u> Ecs. 2.10 y 2.9

$$\boxed{\ln K \equiv \frac{-\Delta G}{R_g T}} \quad (2.5)$$

Ec. de van´t Hoff (ΔH-cte y por mol de rxn):

$$\boxed{K_P \simeq K_{P\,ref}\, e^{\frac{-\Delta H_{\text{cte}}}{R_g}\left(\frac{1}{T} - \frac{1}{T_{ref}}\right)}} \quad (2.17)$$

Cinética (1 rxn):

$$\boxed{\boldsymbol{r_i} \equiv \frac{1}{V}\frac{\mathrm{d}n_i}{\mathrm{d}t}} \quad (3.1)$$

$$\boxed{\boldsymbol{r} \equiv \frac{1}{\nu_i}\frac{1}{V}\frac{\mathrm{d}n_i}{\mathrm{d}t} = \frac{1}{V}\frac{\mathrm{d}\xi}{\mathrm{d}t}} \quad (3.5 \text{ y } 3.6)$$

$$\boxed{\boldsymbol{r_i} = \nu_i\, \boldsymbol{r}} \quad (3.19)$$

Relacionar velocidades (r es reacción; i y j componentes):

$$\boxed{\boldsymbol{r_i} = \sum_{r=1}^{n_{rxn}} \boldsymbol{r_{ir}}} \quad (4.20)$$

$$\boxed{\boldsymbol{r_{jr}} = \frac{\nu_{jr}}{\nu_{ir}}\boldsymbol{r_{ir}}} \quad (4.22)$$

$$\boxed{\boldsymbol{r_i} = \sum_{r=1}^{n_{rxn}} \nu_{ir}\, \boldsymbol{r_r}} \quad (4.23)$$

Ec. de Arrhenius:

$$\boxed{k = A\, e^{\frac{-E_A}{R_g T}}} \quad (3.22)$$

Tiempo Espacial:

$$\boxed{\tau \equiv \frac{V_R}{\dot{\mathcal{V}}_0}} \quad (4.1)$$

Tiempo de Residencia (R. Continuos):

$$t_1 = \int_0^{V_{R1}} \frac{\mathrm{d}V_R}{\dot{\mathcal{V}}} \quad (4.2)$$

Relación Flujo-Concentración:

$$F_i = \dot{\mathcal{V}}\, C_i$$

<u>ECUACIONES DE DISEÑO</u>

R. por Lotes (para V_{R1}-cte):

$$\boxed{t_1 = C_{rl0} \int_0^{f_{rl1}} \frac{\mathrm{d}f_{rl}}{(-\boldsymbol{r}_{rl})}} \quad (4.7)$$

$$\boxed{\frac{\mathrm{d}f_{rl}}{\mathrm{d}t} = \frac{(-\boldsymbol{r}_{rl})}{C_{rl0}}} \quad (7.16)$$

$$\boxed{\frac{\mathrm{d}C_i}{\mathrm{d}t} = \boldsymbol{r_i}} \quad (4.8)$$

Si V_{R1}-variable $[P_{CTE}]$:

$$t_1 = C_{rl0} \int_0^{f_{rl1}} \frac{\mathrm{d}f_{rl}}{(-\boldsymbol{r}_{rl})(1 + \delta_{rl} f_{rl})(\frac{T}{T_0})}$$

R. de Tanque Agitado (k reactores en serie), $\tau_k = \frac{V_{Rk}}{\dot{\mathcal{V}}_0}$:

$$\boxed{\tau_k = \frac{V_{Rk}}{\dot{\mathcal{V}}_0} = \frac{C_{rl0}\,(f_{rl\,k} - f_{rl\,k-1})}{(-\boldsymbol{r}_{rl})_k}} \quad (4.11)$$

$$\boxed{V_{Rk} = \frac{F_{ik} - F_{ik-1}}{(\boldsymbol{r}_i)_k}} \quad (4.12)$$

Para líquidos (varias rxnes):

$$\tau_k = \frac{V_{Rk}}{\dot{\mathcal{V}}_0} = \frac{C_{ik} - C_{ik-1}}{(\boldsymbol{r}_i)_k} \quad (4.13)$$

Para SOLUCIÓN NUMÉRICA, <u>modificar</u> Ecs.4.11, 4.12 y 4.13

$$[\mathbf{A} - \mathbf{B}] \times 10^0 = 0$$

R. de Flujo Pistón:

$$\boxed{\tau_1 = C_{rl0} \int_0^{f_{rl1}} \frac{\mathrm{d}f_{rl}}{(-\boldsymbol{r}_{rl})}} \tag{4.17}$$

$$\boxed{\frac{\mathrm{d}f_{rl}}{\mathrm{d}\tau} = \frac{(-\boldsymbol{r_{rl}})}{C_{rl0}}} \tag{7.39}$$

$$\boxed{\frac{\mathrm{d}F_i}{\mathrm{d}V_R} = \boldsymbol{r_i}} \tag{4.18}$$

Para líquidos (varias rxnes):

$$\frac{\mathrm{d}C_i}{\mathrm{d}\tau} = \boldsymbol{r_i} \tag{4.19}$$

Para gases ideales:

$$\boxed{\delta_{rl} = \frac{y_{rl0}\,\Delta\nu}{-\nu_{rl}}} \tag{6.9}$$

$$\boxed{\dot{\mathcal{V}} = \dot{\mathcal{V}}_0\ (1 + \delta_{rl}\, f_{rl})\left(\frac{T}{T_0}\right)\left(\frac{P_{T0}}{P_T}\right)} \tag{6.12}$$

$$\boxed{\dot{\mathcal{V}} = \dot{\mathcal{V}}_0\ \left(\frac{\sum F_i}{\sum F_{i0}}\right)\left(\frac{T}{T_0}\right)\left(\frac{P_{T0}}{P_T}\right)} \tag{6.11}$$

$$\boxed{C_i = \left(\frac{C_{i0} + \frac{\nu_i}{(-\nu_{rl})}\, C_{rl0}\, f_{rl}}{1 + \delta_{rl}\, f_{rl}}\right)\left(\frac{T_0}{T}\right)\left(\frac{P_T}{P_{T0}}\right)} \tag{6.19}$$

$$\boxed{C_i = \left(\frac{F_i}{F_T}\right) C_T = \left(\frac{F_i}{F_T}\right) \frac{P_T}{R_g\, T}} \tag{6.20}$$

Calor de Reacción de referido a ...

$$\Delta H_{jr} = \Delta H_{ir} \frac{|\nu_{ir}|}{|\nu_{jr}|} = \frac{\Delta H_r}{|\nu_{jr}|} \tag{7.1}$$

<u>NOTA</u>: En las ecuaciones que se presenta a continuación si aparece rl se refiere a una reacción; si aparece F_i se refiere a gases mientras que si aparece ρ a líquidos.

OPERACIÓN ADIABÁTICA (sólo si propiedades constantes):

$$\boxed{T = T_0 - \frac{\Delta H_{rl}\, C_{rl0}\, f_{rl}}{\rho\, C_P}} \Rrightarrow T = T_0 + m\, f_{rl} \tag{7.5}$$

$$\boxed{T = T_0 - \frac{\Delta H_{rl}\, F_{rl0}\, f_{rl}}{\sum F_i\, C_{P\,i}}} \Rrightarrow T = T_0 + \frac{f_{rl}}{b + m\, f_{rl}} \tag{7.6}$$

$$\boxed{T = T_0 - \frac{\sum_{r=1}^{n_{rxn}} \Delta H_r \xi_r^*}{\rho\, C_P}} \Rrightarrow T = b + \sum^{\text{indep}} m_i C_i \tag{7.7}$$

$$\boxed{T = T_0 - \frac{\sum_{r=1}^{n_{rxn}} \Delta H_r \xi_r^{'}}{\sum F_i\, C_{P\,i}}} \Rrightarrow T = b + \frac{\sum^{\text{indep}} m_i F_i}{b_2 + \sum^{\text{indep}} m_{2i} F_i}$$

OPERACIÓN CON INTERCAMBIO
Reactor por Lotes:

$$\boxed{\frac{\mathrm{d}T}{\mathrm{d}t} = \frac{\dot{Q}_{tr}}{V_{R1}\,\rho\, C_P} - \frac{\Delta H_{rl}\,(-\boldsymbol{r_{rl}})}{\rho\, C_P}} \tag{7.15}$$

$$\boxed{\frac{\mathrm{d}T}{\mathrm{d}t} = \frac{\dot{Q}_{tr}}{V_{R1}\,\rho\, C_P} - \sum_{r=1}^{n_{rxn}} \frac{\Delta H_r \boldsymbol{r_r}}{\rho\, C_P}} \tag{7.13}$$

Si T_C es constante (Lotes y Tanque):

$$\dot{Q}_{tr} = UA\,(T_C^{sat} - T) \tag{7.17}$$

$$= \dot{m}_{cond}\,\lambda_{vap} \qquad \text{si } T_C^{sat} > T \tag{7.18}$$

$$= -\dot{m}_{evap}\,\lambda_{vap} \qquad \text{si } T_C^{sat} < T \tag{7.19}$$

Si T_C cambia (Lotes y Tanque):

$$\dot{Q}_{tr} = -\dot{\mathcal{V}}_C\,\rho_C\, C_{P\,C}\,(T_{C1} - T_{C0}) \tag{7.21 y 7.22}$$

$$= \dot{\mathcal{V}}_C\,\rho_C\, C_{P\,C}\,(T_{C0} - T)\left(1 - e^{-\frac{UA}{\dot{\mathcal{V}}_C\,\rho_C\, C_{P\,C}}}\right)$$

Reactores de Tanque Agitado (7.26 a 7.29):

$$\boxed{\dot{\mathcal{V}}_0\,\rho\, C_P\,(T_k - T_{k-1}) = \dot{Q}_{tr_k} - \Delta H_{rl}\,\dot{\mathcal{V}}_0\, C_{rl0}\,(f_{rl\,k} - f_{rl\,k-1})}$$

$$T_k = \frac{UA\,T_{C\,k} + \dot{\mathcal{V}}_0\,\rho\, C_P\, T_{k-1} - \Delta H_{rl}\,\dot{\mathcal{V}}_0\, C_{rl0}\,(f_{rl\,k} - f_{rl\,k-1})}{\dot{\mathcal{V}}_0\,\rho\, C_P + UA}$$

$$\boxed{\dot{\mathcal{V}}_0\,\rho\, C_P\,(T_k - T_{k-1}) = \dot{Q}_{tr_k} - \sum_{r=1}^{n_{rxn}} \Delta H_r ({\xi'}_{rk} - {\xi'}_{r\,k-1})}$$

$$T_k = \frac{UA\,T_{C\,k} + \dot{\mathcal{V}}_0\,\rho\, C_P\, T_{k-1} - \sum_{r=1}^{n_{rxn}} \Delta H_r ({\xi'}_{rk} - {\xi'}_{r\,k-1})}{\dot{\mathcal{V}}_0\,\rho\, C_P + U\,A}$$

Reactores Tubulares:

$$\boxed{\frac{\mathrm{d}T}{\mathrm{d}\tau} = \frac{\frac{4}{D}\, U\,(T_C - T) - \Delta H_{rl}\,(-\boldsymbol{r_{rl}})}{\rho\, C_P}} \tag{7.37}$$

$$\boxed{\frac{\mathrm{d}T}{\mathrm{d}\tau} = \frac{\frac{4}{D}\,\dot{\mathcal{V}}_0\, U\,(T_C - T) - \dot{\mathcal{V}}_0\,\Delta H_{rl}\,(-\boldsymbol{r_{rl}})}{\sum F_i\, C_{P\,i}}} \tag{7.38}$$

$$\boxed{\frac{\mathrm{d}T}{\mathrm{d}\tau} = \frac{\frac{4}{D}\, U\,(T_C - T) - \sum_{r=1}^{n_{rxn}} \Delta H_r\, \boldsymbol{r_r}}{\rho\, C_P}} \tag{7.40}$$

$$\boxed{\frac{\mathrm{d}T}{\mathrm{d}V_R} = \frac{\frac{4}{D}\, U\,(T_C - T) - \sum_{r=1}^{n_{rxn}} \Delta H_r\, \boldsymbol{r_r}}{\sum F_i\, C_{P\,i}}} \tag{7.41}$$

$$\boxed{\frac{\mathrm{d}T_C}{\mathrm{d}V_R} = \begin{cases} -\dfrac{\frac{4}{D}\, U\,(T_C - T)}{F_C\, C_{P\,C}} & \text{concurrente.} \\[2ex] +\dfrac{\frac{4}{D}\, U\,(T_C - T)}{F_C\, C_{P\,C}} & \text{contracorriente.} \end{cases}} \tag{7.45}$$

Si calentamiento uniforme: $\frac{4}{D}\, U\,(T_C - T) \Rrightarrow \frac{\dot{Q}_{tr}}{V_{R1}}$

Si se requiere en Ec. 7.45: $\mathrm{d}V_R \Rrightarrow \dot{\mathcal{V}}_0\,\mathrm{d}\tau$ y/o $F_C \Rrightarrow \mathcal{V}_C\,\rho_C$

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