# REB Equation Summary

## *Stoichiometry, Composition and State Equations*

$$n_i = n_{i,0} + \sum_{j'} \nu_{i,j'} \xi_{j'} \qquad \dot{n}_i = \dot{n}_{i,in} + \sum_{j'} \nu_{i,j'} \dot{\xi}_{j'} \qquad f_i = \frac{n_{i,0} - n_i}{n_{i,0}} \qquad f_i = \frac{\dot{n}_{i,in} - \dot{n}_i}{\dot{n}_{i,in}}$$

$$\frac{n_{lr,0}}{\left|\nu_{lr}\right|} < \frac{n_{nlr,0}}{\left|\nu_{nlr}\right|} \qquad \frac{\dot{n}_{lr,in}}{\left|\nu_{lr}\right|} < \frac{\dot{n}_{nlr,in}}{\left|\nu_{nlr}\right|} \qquad g_i = \frac{f_i}{f_{i,eq}} = \frac{\frac{n_{i,0} - n_i}{n_{i,0}}}{\frac{n_{i,0} - n_{i,eq}}{n_{i,0}}} = \frac{n_{i,0} - n_i}{n_{i,0} - n_{i,eq}}$$

$$g_i = \frac{\dot{n}_{i,in} - \dot{n}_i}{\dot{n}_{i,in} - \dot{n}_{i,eq}} \qquad Y_{D/i} = \frac{n_D}{n_{i,0}} \qquad Y_{D/i} = \frac{\dot{n}_D}{\dot{n}_{i,in}} \qquad Y'_{D/i} = \frac{\nu_{i,j}}{\nu_{D,j}} \frac{n_D}{n_{i,in}} \qquad Y'_{D/i} = \frac{\nu_{i,j}}{\nu_{D,j}} \frac{\dot{n}_D}{\dot{n}_{i,in}}$$

$$S_{D/U} = \frac{n_D}{n_U} \qquad S_{D/U} = \frac{\dot{n}_D}{\dot{n}_U} \qquad PV = RT \sum_i n_i \qquad P\dot{V} = RT \sum_i \dot{n}_i \qquad \rho_{liq} = \text{ constant}$$

$$C_i = \frac{n_i}{V} \qquad C_i = \frac{\dot{n}_i}{\dot{V}} \qquad P_i = \frac{n_i}{\sum_i n_i} P = \frac{n_i RT}{V} = C_i RT \qquad P_i = \frac{\dot{n}_i}{\sum_i \dot{n}_i} P = \frac{\dot{n}_i RT}{\dot{V}} = C_i RT$$

## *Rates, Rate Expressions and Reaction Mechanisms*

$$r_j = \frac{1}{V} \frac{d\Xi_j}{dt} \qquad r_{i,j} = \nu_{i,j} r_j \qquad r_j = r_{j,f} - r_{j,r} \qquad k_j = k_{0,j} \exp\left(\frac{-E_j}{RT}\right)$$

$$K_j = \frac{k_{j,f}}{k_{j,r}} \qquad \left\{ 1 - \frac{\prod_i C_i^{\nu_i,j}}{K_{j,c}} \right\} \Bigg|_{equilibrium} = 0 \qquad \left\{ 1 - \frac{\prod_i P_i^{\nu_i,j}}{K_{j,p}} \right\} \Bigg|_{equilibrium} = 0$$

$$r_j = k_{j,f} \prod_{i_r} C_{i_r}^{-\nu_{i_r,j}} - k_{j,r} \prod_{i_p} C_{i_p}^{\nu_{i_p,j}} \qquad r_j = k_{j,f} \prod_{i_r} P_{i_r}^{-\nu_{i_r,j}} - k_{j,r} \prod_{i_p} P_{i_p}^{\nu_{i_p,j}}$$

## *Thermodynamics*

$$\Delta H_j^0\Big|_{T=298K} = \sum_i \left( \nu_{i,j} \Delta H_{f,i}^0\Big|_{T=298K} \right) \qquad \Delta H_j^0\Big|_{T=298K} = \sum_i \left( -\nu_{i,j} \Delta H_{c,i}^0\Big|_{T=298K} \right)$$

$$\Delta H_j^0 = \Delta H_j^0\Big|_{T=298K} + \sum_i \left( \nu_{i,j} \int_{298\ \mathrm{K}}^{T} \hat{C}_{p,i} dT \right) \qquad \Delta G_j^0\Big|_{T=298K} = \sum_i \left( \nu_{i,j} \Delta G_{f,i}^0\Big|_{T=298K} \right)$$

$$K_j\Big|_{T=298K} = \exp\left( \frac{-\Delta G_j^0\Big|_{T=298K}}{R(298\ \mathrm{K})} \right) \qquad K_j = K_j\Big|_{T=298K} \exp\left\{ \frac{1}{R} \int_{298K}^{T} \frac{\Delta H_j^0}{T^2} dT \right\}$$

$$K_j = \exp\left( \frac{-\Delta G_j^0}{RT} \right) = \exp\left( \frac{\Delta S_j^0}{R} \right) \exp\left( \frac{-\Delta H_j^0}{RT} \right) \qquad K_j = K_{0,j} \exp\left( \frac{-\Delta H_j}{RT} \right)$$

***Ideal Reactors***

***Processes***

***Non-Ideal Reactors***