PFR

Mole Balance

$$\frac{dF_j}{dV} = R_j$$

Energy Balance (ideal gas or no ΔP):

$$\sum_j F_j \cdot C_{P_j} \cdot \frac{dT}{dV} = -\sum_i \Delta H_{rxn_i} \cdot r_i + \dot{q}$$

$$\dot{q} = U \cdot a \cdot \left(T_a - T\right)$$

Batch Reactor

Mole Balance

$$\frac{dn_j}{dt} = R_j \cdot V_R$$

Energy Balance (incompressible fluid or constant pressure):

$$\sum_j n_j \cdot C_{Pj} \cdot \frac{dT}{dt} = -\sum_i \Delta H_{rxn_i} \cdot r_i \cdot V_R + \dot{Q}$$

$$\dot{Q} = U \cdot A \cdot \left(T_a - T\right)$$

CSTR

Mole Balance

$$\frac{dn_j}{dt} = R_j \cdot V_R + F_{jf} - F_j$$

Energy Balance (incompressible fluid or no pressure drop)

$$\sum_j n_j \cdot C_{P_j} \cdot \frac{dT}{dt} = -\sum_i \Delta H_{rxn_i} \cdot r_i \cdot V_R + \sum_j F_{jf} \cdot \left(H_{jf} - H_j\right) + \dot{Q}$$

$$\dot{Q} = U \cdot A \cdot \left(T_a - T\right)$$

Arrhenius Equation

$$k_i = A_i \cdot e^{\left(\frac{-E_{A_i}}{R \cdot T}\right)}$$

Integrated Van't hoff equation

$$K_P(T) = K_P\left(T_R\right) \cdot e^{\left(\frac{-\Delta H_{rxn}}{R} \cdot \left(\frac{1}{T} - \frac{1}{T_R}\right)\right)}$$

Heat of Reaction

$$\Delta H_i = \Delta H_i(T_R) + \int_{T_R}^{T} \Delta C_{p_i} \cdot dT$$