

ChE 43200: Chemical Reaction Engineering

Exam #1 Equation Sheet

$$R = 8.314 \text{ J/(mol}\cdot\text{K)} = 1.98 \text{ kcal/(mol}\cdot\text{K)}$$

$$PV = nRT$$

Pressure Conversion

Temperature

$$1 \text{ atm} = 760 \text{ torr} = 1 \text{ bar} = 14 \text{ psi}$$

$$K = ^\circ\text{C} + 273.15$$

$$x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

$$C_i = \frac{N_i}{V}$$

Base Kinetics

general
mole balance
applicable to
all reactors

$$\left\{ \begin{aligned} \frac{dN_j}{dt} &= F_{j,0} - F_j + \sum v_j r_j V \\ k(T) &= k_0 \exp\left(-\frac{E_a}{RT}\right) \\ X &= \frac{C_{i0} - C_i}{C_{i0}} \end{aligned} \right. \quad \text{Stoichiometric coefficient.}$$

$$\Delta T_{\text{Adiabatic}} = T_2 - T_1 = -\frac{\Delta H_R}{NC_{p,\text{products}}}$$

$$\ln(K_{298}) = -\frac{\Delta G_{298}}{RT}$$

$$\ln(K_{eq}) = \ln(K_{298}) - \frac{\Delta H_{R,298}}{R} \left(\frac{1}{T} - \frac{1}{298K} \right)$$

$$K_{eq} = \prod K_i, \quad i = P, \gamma, y \quad \Rightarrow K_{eq} = K_P \cdot K_R \cdot K_y$$

Flow Material Balances

For equations of variable
density for CSTR & PFR
refer slide no. 51 & 53
from chp. 3.

$$\tau = \frac{V}{v} \leftarrow \text{volumetric flowrate (m}^3/\text{s) or (m}^3/\text{min)}$$

$$\left\{ \begin{aligned} \text{CSTR: } C_{i0} - C_i &= \tau r_i \\ \text{PFR: } \frac{dC_i}{d\tau} &= r_i \end{aligned} \right. \quad \text{These equations are valid for constant density systems}$$

$$\text{Batch} \left\{ \begin{aligned} \frac{dC_i}{dt} &= r_i \rightarrow \text{const. density system} \\ \frac{1}{V} \cdot \frac{dN_i}{dt} &= r_i \rightarrow \text{variable density system.} \end{aligned} \right.$$