A First Course on Kinetics and Reaction Engineering
Unit 15. Integral Data Analysis

Definitions

half-life - time required for the concentration of a reactant to decrease to one-half of its initial value

Nomenclature

α	kinetic reaction order with respect to the reactant
τ	space time (average residence time)
C_i	molar concentration of species i, a superscripted 0 denotes the reactor inlet concentration of species i
D	inside diameter of a PFR
L	length of a PFR
P	total pressure, a subscripted i denotes the partial pressure of species i
R	ideal gas constant
SV	space velocity
T	absolute temperature
V	volume within which the reaction is taking place
$\dot{V}$	volumetric flow rate, a superscripted 0 denotes the inlet volumetric flow rate
k	rate coefficient
n_i	moles of reagent i, i = tot denotes the total moles, a superscripted 0 denotes the moles at time zero
$\dot{n}_i$	molar flow rate of species i, i = tot denotes the total molar flow rate, a superscripted 0 denotes the molar flow rate at the reactor inlet
$r_{i,j}$	rate of reaction j with respect to species i (rate of generation of species i via reaction j); j may be omitted if only one reaction is taking place
t	time
$t_{1/2}$	half-life
y_i	mole fraction of species i
z	axial distance along the length of a PFR, measured from the inlet

Equations

$$\frac{dn_i}{dt} = Vr_{i,j} \tag{15.1}$$

$$\frac{d\dot{n}_i}{dz} = \frac{\pi D^2}{4} r_{i,j} \tag{15.2}$$

$$C_i = \frac{\dot{n}_i}{\dot{V}} \tag{15.3}$$

$$\dot{V}^0 = \dot{V} \qquad \text{(incompressible liquids)} \tag{15.4}$$

$$\dot{V} = \frac{\dot{n}_{tot} RT}{P} \qquad \text{(ideal gas)} \tag{15.5}$$

$$\dot{n}_{tot} = \sum_{\substack{i=all\\species}} \dot{n}_i \tag{15.6}$$

$$y_i = \frac{\dot{n}_i}{\dot{n}_{tot}} \tag{15.7}$$

$$P_i = y_i P = \frac{\dot{n}_i P}{\dot{n}_{tot}} \tag{15.8}$$

$$\tau = \frac{V}{\dot{V}^0} \tag{15.9}$$

$$SV = \frac{1}{\tau} = \frac{\dot{V}^0}{V} \tag{15.10}$$

$$C_i = \frac{n_i}{V} \tag{15.11}$$

$$P_i = \frac{n_i RT}{V} \tag{15.12}$$

$$P = \frac{n_{tot} RT}{V} \tag{15.13}$$

$$r_A = -k\left(C_A\right)^\alpha \tag{15.14}$$

$$\frac{dn_A}{dt} = -kV\left(C_A\right)^\alpha \tag{15.15}$$

$$\frac{dn_A}{dt} = -kV\left(\frac{n_A}{V}\right)^\alpha = -kV^{1-\alpha} n_A^\alpha \tag{15.16}$$

$$t_{1/2} = \frac{0.693}{k} \qquad \text{(first order kinetics)} \qquad (15.17)$$

$$t_{1/2} = \frac{\left(2^{\alpha-1} - 1\right)}{k\left(\alpha - 1\right)\left(C_A^0\right)^{\alpha-1}} \qquad (\alpha \neq 1) \qquad (15.18)$$

$$\ln\left(t_{1/2}\right) = \ln\left(\frac{\left(2^{\alpha-1} - 1\right)}{k\left(\alpha - 1\right)}\right) + \left(1 - \alpha\right)\ln\left(C_A^0\right) \qquad (\alpha \neq 1) \qquad (15.19)$$