A First Course on Kinetics and Reaction Engineering

Unit 14. Differential Data Analysis

Definitions

forward differences - approximation of a derivative at point k based on the quantity values at point k and point $k + 1$

backward differences - approximation of a derivative at point k based on the quantity values at point k and point $k - 1$

central differences - approximation of a derivative at point k as the average of forward and backward differences

initial rate - instantaneous rate of a reaction, as defined in Unit 4, immediately after a batch reactor has been charged

Nomenclature

D	inside diameter of a PFR
L	length of a PFR
V	reaction volume
n_i	moles of reagent i
$(n_i)_k$	moles of reagent i for data point k
$\dot{n}_i$	molar flow rate of reagent i
$r_{i,j}$	rate of reaction j with respect to reagent i
t	time
z	axial distance along the length of a PFR, measured from the inlet

Equations

$$\frac{dn_i}{dt} = Vr_{i,j} \tag{14.1}$$

$$\frac{dn_i}{dt} \approx \left.\frac{\Delta n_i}{\Delta t}\right|_{(t,n_i)} \tag{14.2}$$

$$\left.\frac{dn_i}{dt}\right|_k \approx \frac{\left(n_i\right)_{k+1} - \left(n_i\right)_k}{\left(t\right)_{k+1} - \left(t\right)_k} \tag{14.3}$$

$$\left.\frac{dn_i}{dt}\right|_k \approx \frac{\left(n_i\right)_k - \left(n_i\right)_{k-1}}{\left(t\right)_k - \left(t\right)_{k-1}} \tag{14.4}$$

$$\left.\frac{dn_i}{dt}\right|_k \approx \left(\frac{1}{2}\right)\left(\frac{\left(n_i\right)_{k+1}-\left(n_i\right)_k}{\left(t\right)_{k+1}-\left(t\right)_k}+\frac{\left(n_i\right)_k-\left(n_i\right)_{k-1}}{\left(t\right)_k-\left(t\right)_{k-1}}\right) \tag{14.5}$$

$$\frac{d\dot{n}_i}{dz}=\frac{\pi D^2}{4}r_{i,j} \tag{14.6}$$

$$\frac{d\dot{n}_i}{dz}\approx\frac{\Delta\dot{n}_i}{\Delta z}=\frac{\left.\dot{n}_i\right|_{outlet}-\left.\dot{n}_i\right|_{inlet}}{L} \tag{14.7}$$