A First Course on Kinetics and Reaction Engineering
Unit 27. Analysis of Transient Plug Flow Reactors

Definitions

discretization - dividing the range of a spatial variable, such as the axial position in a PFR, into some number of smaller intervals

discretization point - the value of a spatial variable, such as the axial position in a PFR, at the boundary between two discretization intervals

finite differences - approximations where a derivative is taken to equal the ratio of a finite change in the dependent variable (e. g. the change between two discretization points) to the change in the independent variable

front - a distinct change in the value of one or more variables at a single axial position; the axial position at which the change appears increases monotonically giving the appearance that the change is moving along the length of the reactor

break through - the point in time when a front reaches the outlet of the reactor

Nomenclature

ΔH_j	heat of reaction j
$\nu_{i,j}$	stoichiometric coefficient of species i in reaction j; value is positive for products and negative for reactants
$\hat{C}_{p,i}$	constant pressure specific molar heat capacity of species i
D	inside diameter of a PFR; a subscripted p denotes a particle diameter
P	pressure, a subscripted i denotes the partial pressure of species i
T	temperature; a subscripted e denotes the (external) temperature of the heat transfer media
U	overall heat transfer coefficient for heat transfer through the wall of a tubular reactor
$\dot{V}$	volumetric flow rate; a superscripted zero denotes the value at the reactor inlet
$\dot{n}_i$	molar flow rate of species i; a superscripted zero denotes the value at the reactor inlet
r_j	the generalized rate of reaction j
t	time
z	axial distance from the inlet to a PFR

Equations

$$\frac{\partial \dot{n}_i}{\partial z} = \frac{\pi D^2}{4} \sum_{\substack{j=all \\ reactions}} \nu_{i,j} r_j - \frac{\pi D^2}{4\dot{V}} \frac{\partial \dot{n}_i}{\partial t} + \frac{\pi D^2 \dot{n}_i}{4\dot{V}^2} \frac{\partial \dot{V}}{\partial t} \tag{27.1}$$

$$\pi DU\left(T_e - T\right) = \left(\sum_{\substack{i=all \\ species}} \dot{n}_i \hat{C}_{pi}\right)\frac{\partial T}{\partial z} + \frac{\pi D^2}{4}\sum_{\substack{j=all \\ reactions}}\left(r_j \Delta H_j\right) + \frac{\pi D^2}{4\dot{V}}\sum_{\substack{i=all \\ species}}\left(\dot{n}_i \hat{C}_{pi}\right)\frac{\partial T}{\partial t} - \frac{\pi D^2}{4}\frac{\partial P}{\partial t} \tag{27.2}$$

$$\frac{\partial \dot{n}_i}{\partial z} \cong \frac{\Delta \dot{n}_i}{\Delta z} \tag{27.3}$$

$$\frac{\partial T}{\partial z} = \frac{\Delta T}{\Delta z} \tag{27.4}$$

$$\frac{\partial \dot{n}_i}{\partial t} \cong \frac{\Delta \dot{n}_i}{\Delta t} \tag{27.5}$$

$$\frac{\partial T}{\partial t} = \frac{\Delta T}{\Delta t} \tag{27.6}$$