

A First Course on Kinetics and Reaction Engineering

Unit 32. Ideal Semi-Batch Reactors

Definitions

semi-batch operation - while reaction is occurring, at least one, but not all, reagent flows into or out of the reactor.

Nomenclature

ΔH_j	heat of reaction j
$\Delta H_{latent,i}$	latent heat associated with any phase change that occurs when species i is added to or removed from a semi-batch reactor
$\nu_{i,j}$	stoichiometric coefficient of species i in reaction j ; value is positive for products and negative for reactants
ρ_i	density of pure species i
C_i	concentration of species i
$\hat{C}_{p,i}$	constant pressure specific molar heat capacity of species i
M_i	molecular weight of species i
P	pressure, a subscript denotes a partial pressure of that species and an additional asterisk denotes the saturation vapor pressure of that species
\dot{Q}	net heat input into a reactor through its walls or the walls of a submerged cooling coil
T	temperature; a subscripted e denotes the (external) temperature of the heat transfer media
V	volume within which reaction takes place, not necessarily the volume of the entire reactor; a superscripted zero denotes the volume at the start of processing
\dot{V}	inlet volumetric flow rate
\dot{W}	net rate at which mechanical work is done by a reactor system on its surroundings through shafts and moving boundaries
h_i	Henry's law constant for species i
\hat{h}_i	specific enthalpy of species i at the instantaneously prevailing conditions within the reactor, the additional subscript "stream" denotes the specific enthalpy of species i at the instantaneously prevailing input or outlet stream conditions
n_i	moles of species i
\dot{n}_i	molar flow rate of species i
r_j	the generalized rate of reaction j
t	time
x_i	liquid phase mole fraction of species i

Equations

$$\frac{dn_i}{dt} = \dot{n}_i + V \sum_{\substack{j=all \\ \text{reactions}}} v_{i,j} r_j \quad (32.1)$$

$$\begin{aligned} \dot{Q} - \dot{W} = & \sum_{\substack{i=all \\ \text{species}}} \dot{n}_i (\hat{h}_i - \hat{h}_{i,stream}) \\ & + \frac{dT}{dt} \sum_{\substack{i=all \\ \text{species}}} (n_i \hat{C}_{p,i}) + V \sum_{\substack{j=all \\ \text{reactions}}} (r_j \Delta H_j) - \frac{dP}{dt} V - P \frac{dV}{dt} \end{aligned} \quad (32.2)$$

$$\dot{n}_i (\hat{h}_i - \hat{h}_{i,stream}) = \dot{n}_i \left(\int_{T_{stream}}^T \hat{C}_{p,i} dT + \Delta H_{latent,i} \right) \quad (32.3)$$

$$P_i = x_i P_i^* \quad (32.4)$$

$$P_i h_i = C_i \quad (32.5)$$

$$V(t) = \sum_{\substack{i=all \\ \text{species}}} \frac{n_i(t) M_i}{\rho_i} \quad (32.6)$$

$$V(t) = V^0 + \dot{V}t \quad (32.7)$$