A First Course on Kinetics and Reaction Engineering
Unit 11. Laboratory Reactors

Definitions

perfectly mixed batch reactor (batch reactor) - a chemical reactor (as defined in Unit 1) with no material flow in or out and with perfectly uniform composition and temperature throughout.

continuously stirred tank reactor (CSTR, perfectly mixed flow reactor) - a chemical reactor (as defined in Unit 1) with material flow in and out and with perfectly uniform composition and temperature within.

plug flow reactor (PFR) - tube or pipe with uniform fluid velocity across its diameter that is used as a chemical reactor (as defined in Unit 1)

adiabatic reactor - a chemical reactor (as defined in Unit 1) that has no heat added or removed during operation

isothermal reactor - a chemical reactor (as defined in Unit 1) where the temperature is the uniform throughout.

steady-state reactor - a chemical reactor (as defined in Unit 1) where the temperature, flow and composition at each location within the reactor is invariant over time

age function - an expression used to calculate the fraction of the fluid leaving a reactor with a residence time less than a given value

residence time distribution function (age distribution function) - an expression used to calculate the fraction of the fluid leaving a reactor with a residence time within a given differential time span

stimulus - change in the inlet concentration of a tracer applied at the inlet to a reactor

response - outlet concentration of a tracer as a function of time following the application of a stimulus

tracer - an easily detectable material that flows through a reactor as a part of the total fluid flow

step change stimulus - a stimulus (as defined above) where the concentration of tracer instantaneously jumps from one value to another

impulse stimulus - a stimulus (as defined above) where a small amount of tracer is instantaneously injected into the fluid at the inlet to a reactor

fluid element - a very small, hypothetical, amount of fluid that stays together as a unit for the whole time it is inside a reactor system

Nomenclature

λ	age (or residence time) of a fluid element leaving a reactor
ρ_{fluid}	fluid density
A	cross-sectional area available to flow inside a PFR
D	inside diameter of a PFR
$F(\lambda)$	age function equal to the fraction of the fluid leaving a reactor with an age less than λ
L	length of a PFR

$\dot{M}$	total mass flow rate
V	reactor volume within which reaction takes place
V_{PFR}	internal volume of a PFR
$dF(\lambda)$	residence time distribution function equal to the fraction of the fluid leaving a reactor with an age between between λ and $\lambda + d\lambda$
m	mass of tracer, a subscript denotes what part of the tracer or the time at which it was measured
n_i	moles of species i
$\dot{n}_i$	molar flow rate of species i
$r_{i,j}$	rate per unit volume of reaction j with respect to species i
t	time, a subscripted 0 denotes the time at which a stimulus was applied and a prime denotes the time at which a sample was taken
$\overline{t}$	average fluid residence time in a reactor
v	linear velocity of flowing fluid
w	mass fraction, a subscripted 0 denotes before application of a stimulus, a subscripted f denotes after application of a stimulus, a subscripted t denotes the time at which it was measured and a subscripted out denotes it was measured at the reactor outlet
y	dummy variable used to integrate over a range of ages
z	axial distance from the inlet to a PFR

Equations

$$\frac{dn_i}{dt} = Vr_{i,j} \tag{11.1}$$

$$\dot{n}_i - \dot{n}_i^0 = Vr_{i,j} \tag{11.2}$$

$$\frac{d\dot{n}_i}{dz} = \frac{\pi D^2}{4} r_{i,j} \tag{11.3}$$

$$dF(\lambda) = F(\lambda + d\lambda) - F(\lambda) \tag{11.4}$$

$$F(\lambda) = \int_{y=0}^{y=\lambda} dF(y) \tag{11.5}$$

$$m_{sample} w_{t'} = m_{young} w_f + m_{aged} w_0 \tag{11.6}$$

$$m_{sample} w_{t'} = m_{sample} F(t' - t_0) w_f + m_{sample} \left[1 - F(t' - t_0)\right] w_0 \tag{11.7}$$

$$F\left(t'-t_0\right)=F\left(\lambda\right)=\frac{w_{t'}-w_0}{w_f-w_0} \tag{11.8}$$

$$m_{t'}=\dot{M}\int_{t_0}^{t'}\left(w_{out}\left(t\right)-w_0\right)dt \tag{11.9}$$

$$F\left(t'-t_0\right)=F\left(\lambda\right)=\frac{\dot{M}\int_{t_0}^{t'}\left(w_{out}\left(t\right)-w_0\right)dt}{m_{tot}} \tag{11.10}$$

$$m_{tot}=\dot{M}\int_{t_0}^{\infty}\left(w_{out}\left(t\right)-w_0\right)dt \tag{11.11}$$

$$\dot{M}w_f=\dot{M}w_{out}+\rho_{fluid}V_{fluid}\frac{dw_{out}}{dt} \tag{11.12}$$

$$w_{out}\left(0\right)=w_0 \tag{11.13}$$

$$\bar{t}=\frac{\rho_{fluid}V_{fluid}}{\dot{M}} \tag{11.14}$$

$$w_{out}\left(t\right)=w_f-\left(w_f-w_0\right)\exp\left\{\frac{-t}{\bar{t}}\right\} \tag{11.15}$$

$$F_{CSTR}\left(\lambda\right)=1-\exp\left\{\frac{-\lambda}{\bar{t}}\right\} \tag{11.16}$$

$$v=\frac{\dot{M}}{\rho_{fluid}A} \tag{11.17}$$

$$t_{\text{travel distance L}}=\frac{L}{v}=\frac{L}{\frac{\dot{M}}{\rho_{fluid}A}}=\frac{\rho_{fluid}AL}{\dot{M}}=\frac{\rho_{fluid}V_{PFR}}{\dot{M}}=\bar{t} \tag{11.18}$$

$$\begin{gathered}F_{PFR}\left(\lambda\right)=0\text{ for }\lambda<\bar{t}\\F_{PFR}\left(\lambda\right)=1\text{ for }\lambda\ge\bar{t}\end{gathered} \tag{11.19}$$