10.37 Chemical and Biological Reaction Engineering, Spring 2007
Prof. K. Dane Wittrup
Lecture 7: Batch Reactors

This lecture covers batch reactor equations, reactor sizing for constant volume and variable volume processes.

Batch Reactors

Run at non-steady state conditions

Which to choose? Batch vs. CSTR?

Figure 1. Schematics of a batch reactor and a CSTR.

	Batch	CSTR
Small Amount of Material	(small quantities)	(does not tie up equipment continuously)
Flexibility	+	-
Expensive Reactants	+	-
If product does not flow, Materials Handling (e.g. Polymers)	+	-
Do not have to shut down and clean, less down time	-	+
Captial costs? For size of reactor, for given conversion	+ (concentration stays higher longer)	-
Operability & Control (T, P, p4) e.g. Exothermic reaction	-	+ (Manipulate only one setpoint, steady state. You can control additional variables. Such as flow rates.)

Material Balance

$$\cancel{\text{In}}_{0} - \cancel{\text{Out}}_{0} + \text{Product} = \text{Accumulation}$$

$$r_A \mathrm{V} = \frac{dN_A}{dt}$$

Constant V, $r_A = \frac{dC_A}{dt}$

In terms of conversion, $C_{Ao}\frac{dX_A}{dt} = r_A$

Integrating, $t = \int_{C_{Ao}}^{C_A}\frac{dC_A}{r_A}$ or $t = C_{Ao}\int_0^{X_A}\frac{dX_A}{r_A}$

1st Order Reaction $A \xrightarrow{k} B$

$$-r_A = kC_A = kC_{Ao}(1-x_A)$$

$$t = C_{Ao}\int_0^{x_A}\frac{dx_A}{-kC_{Ao}(1-x_A)} \longrightarrow t = \frac{1}{k}\ln\left(\frac{1}{1-x_A}\right)$$

$$x_A = 1 - e^{-kt}$$

90% conversion $t_{90.0\%} = \frac{1}{k}\ln\left(\frac{1}{1-0.9}\right) = \frac{2.3}{k}$

(order of $\frac{1}{k}$)

2nd Order Reaction $A + A \xrightarrow{k} B$

$$-r_A = kC_A{}^2 = kC_{Ao}{}^2(1-X_A)^2$$

$$t = C_{Ao}\int_0^{X_A}\frac{dX_A}{-kC_{Ao}{}^2(1-X_A)^2} = \frac{1}{-kC_{Ao}}\int_0^{X_A}\frac{dX_A}{(1-X_A)^2}$$

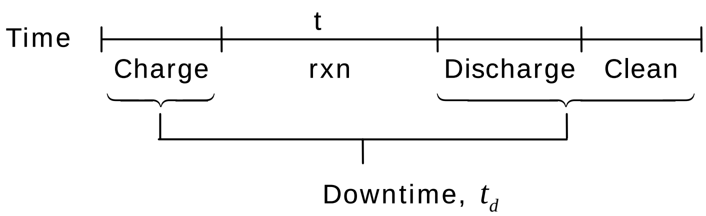
$$t = \frac{1}{kC_{Ao}}\frac{X_A}{1-X_A} \qquad X_A = \frac{kC_{Ao}t}{1+kC_{Ao}t}$$

If $k_{\text{first order}} = k_{\text{second order}}C_{Ao}$, which is faster?

	1	2	3	
1st order	0.63	0.86	0.95	$\}x_A$
2nd order	0.50	0.67	0.75	

For a given Damkohler number, 1st order is faster. The second order reaction has greater concentration dependence. Exponential approach (1st order) is faster.

Batch Cycle



How long should t be?
How high should X_A be?

Economic calculation: Compare economics of further conversion to a different use of equipment

Chemical consideration: Will product degrade? Assume product stable.

Product produced in one cycle $= X_A C_{Ao} \mathrm{V}$

$\mathrm{P_r}$(Rate of Production) $= \dfrac{X_A C_{Ao} \mathrm{V}}{t + t_d}$

What value of t will maximize $\mathrm{P_r}$?

If there is a maximum of $\mathrm{P_r}$ vs. t, $\dfrac{d\,\mathrm{P_r}}{dt} = 0$

Assume $t_d =$ constant. $0 = \dfrac{d\,\mathrm{P_r}}{dt} = C_{Ao} \mathrm{V} \dfrac{(t_{optimum} + t_d)\dfrac{dX_A}{dt} - X_A}{(t_{optimum} + t_d)^2}$

$$(t_{optimum} + t_d)\frac{dX_A}{dt} - X_A = 0$$

Now specify kinetics. There may be no optimum.

1st order $\quad X_A = 1 - e^{-kt}$

$$\frac{dX_A}{dt} = ke^{-kt}$$

$$(t_{optimum} + t_d)ke^{-kt_{optimum}} - (1 - e^{-kt_{optimum}}) = 0$$

Can numerically solve for $t_{optimum}$.

Semi-batch Reactor

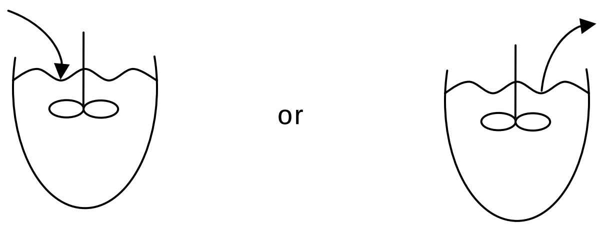


Figure 2. Schematics of two types of fed-batch reactors.

1) Why?

- To remove “poisonous” product
- Make room in reactor (expansion of product)
- If a reactant has a negative order effect on rate, add in small quantities
- Selectivity (control) $A + B \rightarrow$ Desired
  $A + A \rightarrow$ Byproduct

  Start with B, slowly feed A.

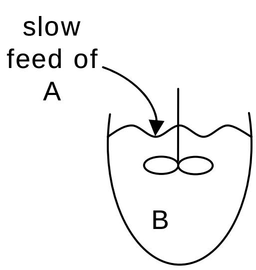


Figure 3. A fed-batch reactor with a slow feed of one reactant.

- To shift equilibrium, strip off product
- To control evolution of heat
- In biological cases
  Fed-batch - Feed in carbon source slowly to avoid overflow metabolism
  - (glucose)
  - O_2 sparingly soluble, must feed.

2) Balances

A Balance

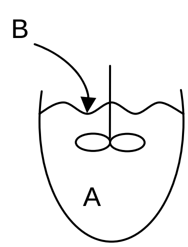


Figure 4. Fed-batch reactor with a feed of B.

In – Out + Product = Accumulation

$$r_A \mathrm{V}(t) = \frac{d(r_A \mathrm{V})}{dt}$$

$$r_A \mathrm{V}(t) = \mathrm{V}\frac{dC_A}{dt} + C_A \frac{d\mathrm{V}}{dt}$$

Liquid $\mathrm{V} = \mathrm{V}_0 + v_0 t$ ← flow

$$\frac{dC_A}{dt} = r_A - \underbrace{\frac{v_0}{\mathrm{V}_0} C_A}_{\text{dilution}}$$

B Balance

$$\frac{dC_B}{dt} = r_B + \underbrace{\frac{v_0}{\mathrm{V}_0} C_{Bo}}_{\text{Addition}} - \underbrace{\frac{v_0}{\mathrm{V}_0} C_B}_{\text{Dilution}}$$