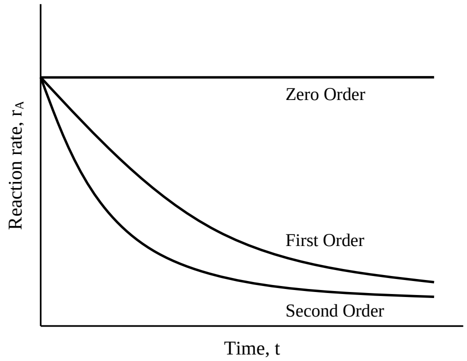
CHAPTER 2

2.1 The reaction is zero order with respect to the reactant.

2.2



Zero order expression: $r_A = - k$

First order expression: $r_A = - k [A]$

Second order expression: $r_A = - k [A]^2$

2.3

t, h	NO3, mg/L	Ln(NO3)	r_A	Ln($-r_A$)
0.0	30.0	3.40		
0.5	23.3	3.15	-13.40	2.60
1.0	19.0	2.94	-8.60	2.15
1.5	15.3	2.73	-7.40	2.00
2.0	11.0	2.40	-8.60	2.15
2.5	8.3	2.12	-5.40	1.69
3.0	7.0	1.95	-2.60	0.96
3.5	6.3	1.84	-1.40	0.34
4.0	5.7	1.74	-1.20	0.18
4.5	5.3	1.67	-0.80	-0.22
7.75	4.7	1.55	-0.18	-1.69

Figure 1 is a plot of NO_3 concentration versus time. The section of the curve between each time interval is assumed to be a straight line, and the rates are calculated from the slope of that section. So, r_A = d(NO3)/dt = (30-23.3)/(0-0.5) = -13.40 for the first interval and so on. Figure 2 is a plot of ln($-r_A$) versus ln(NO_3). The last 2 data points were excluded from plot, as the curve was almost horizontal showing minimal conversion. The slope of the best fit line is 1.54. So the order of the reaction is 1.54.

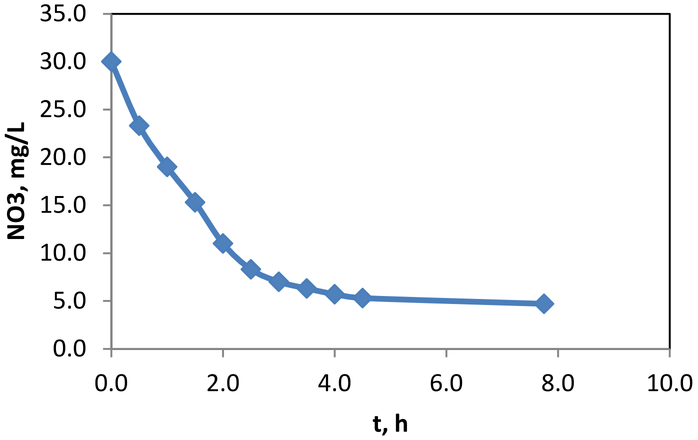


Figure 1. NO_3 versus Time curve.

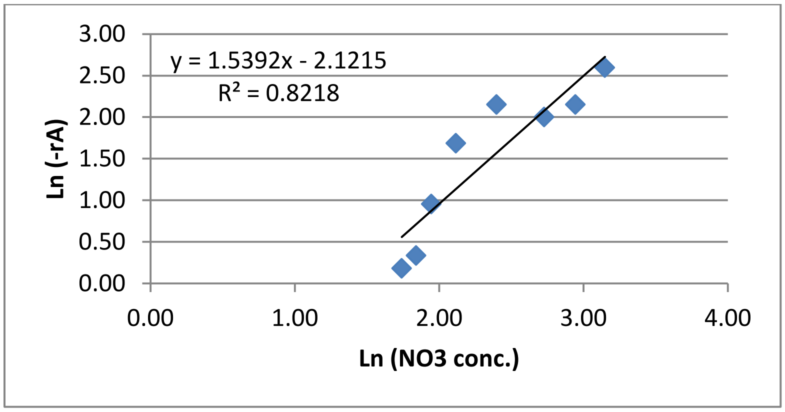


Figure 2.

2.4 Q = 500 m^3/d, k = 0.23 d^{-1}, $[A_o]$ = 150 mg/L

After 90% conversion, $[A_t]$ = 150 (1-0.90) = 15 mg/L

(a) 1st order reaction in PFR

$kt = \ln \{[A_o]/[A_t]\}$

or, $0.23t = \ln \{150/15\} = 2.3026$

or, $\mathbf{t = 10\ d}$

$V = Q \times t = (500\ m^3/d) \times 10\ d = \mathbf{5000\ m^3}$

(b) 1st order reaction in CSTR

$kt = \{[A_o]/[A_t]\} - 1$

$0.23t = \{150/15\} - 1 = 9$

or, $t = 39.13\ d$

$V = Q \times t = (500\ m^3/d) \times 39.13\ d = \mathbf{19{,}565\ m^3}$

(c) Option (a) is better. The PFR requires a much lower volume to carry out the same conversion. Volume required for CSTR is almost four times that of the PFR.

2.5 $[A_o] = 0.25$ mol/L, $t = 20$ min

After 85% conversion, $[A_t] = 0.25\ (1-0.85) = 0.0375$ mol/L

(a) Zero order reaction in Batch reactor

$kt = [A_o] - [A_t]$

or, $k\ (20\ min) = 0.25\ mol/L - 0.0375\ mol/L = 0.2125\ mol/L$

or, $\mathbf{k = 0.0106\ min^{-1}}$

(b) First order reaction in Batch reactor

$kt = \ln \{[A_o]/[A_t]\}$

or, $k\ (20\ min) = \ln \{0.25/0.0375\} = 1.897$

or, $\mathbf{k = 0.0949\ min^{-1}}$

2.6 Assume first order reaction. Usually at zero order reactions, the difference in efficiency is minimal between a CSTR and a PFR. At higher order reactions, the difference is more prominent. Calculate the detention time and flow rates for a CSTR and PFR to achieve the same conversion and select the better design.

$[A_o]$ = 145 mg/L, V = 50 m^3

After 90% conversion, $[A_t]$ = 145 (1-0.9) = 14.5 mg/L

Consider 1st order reaction in CSTR

$kt = \{[A_o]/[A_t]\} - 1 = (145/14.5) - 1 = 9.0$

Consider 1st order reaction in PFR

$kt = \ln \{[A_o]/[A_t]\} = \ln \{145/14.5\} = 2.3$

Since k is the same for both reactors, therefore detention time required for PFR is much lower than that required for a CSTR. Also, Q = V/t. With a lower value of t, PFR will be able to process higher flow rates than a CSTR. The engineer should select a PFR.

2.7 Given, $r_A = - 1.2 [A]$ mg/L.h

First order reaction in a CSTR, V = 60 m^3, k = 1.2 h^{-1}

After 95% conversion, $[A_t] = (1- 0.95) [A_o] = 0.05 [A_o]$

(a) 1st order reaction in CSTR

$kt = \{[A_o]/[A_t]\} - 1$

or, $1.2t = \{[A_o]/0.05[A_o]\} - 1 = 19$

or, t = 15.83 h

Q = V/t = 60 m^3/15.83 h = **3.79 m^3/h**

(b) After 90% conversion, $[A_t] = (1- 0.90) [A_o] = 0.1 [A_o]$

1st order reaction in CSTR

$kt = \{[A_o]/[A_t]\} - 1$

or, $1.2t = \{[A_o]/0.1[A_o]\} - 1 = 9$

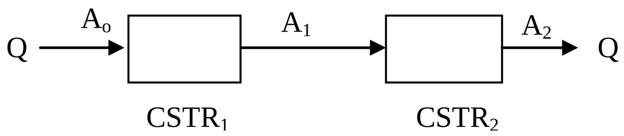
or, t = 7.5 h

V = Q x t = 3.79 x 7.5 = 28.43 m^3 ≈ **29 m^3**

For 90% conversion efficiency, a smaller reactor volume of 29 m^3 is sufficient.

2.8 Detention time, $t = 1.5$ d in each reactor

Therefore, reactors are of equal volume



Given, $k = 0.45\ d^{-1}$, $A_o = 1500$ mg/L

1st order reaction in $CSTR_1$

$kt = \{[A_o]/[A_1]\} - 1$

or, $(0.45\ d^{-1})\ (1.5\ d) = \{1500/\ A_1\} - 1$

or, $A_1 = 895.52$ mg/L

A_1 = effluent from $CSTR_1$ = influent to $CSTR_2$

For $CSTR_2$, $kt = \{[A_1]/[A_2]\} - 1$

or, $(0.45\ d^{-1})\ (1.5\ d) = \{895.52/\ A_2\} - 1$

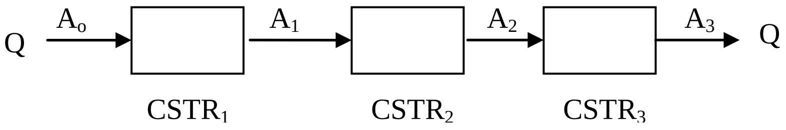
or, $\mathbf{A_2 = 534.64}$ **mg/L**

Overall conversion efficiency = $\{(A_o - A_2)/A_o\}$x 100%

= $\{(1500 - 534.64)/1500\}$ x 100%

= **64.36 %**

2.9



From Problem 2-8, $k = 0.45\ d^{-1}$, $t = 1.5$ d, $A_o = 1500$ mg/L, $A_2 = 534.64$ mg/L

For $CSTR_3$, $kt = \{[A_2]/[A_3]\} - 1$

or, $(0.45\ d^{-1})\ (1.5\ d) = \{534.64/A_3\} - 1$

or, $A_3 = 319.19$ mg/L

Overall conversion efficiency $= \{(A_o - A_3)/A_o\} \times 100\%$

$= \{(1500 - 319.19)/1500\} \times 100\%$

$= 78.72\%$

Adding a third reactor in series increases the overall conversion efficiency from 64.36% to 78.72%. A cost-benefit analysis needs to be done to determine the benefits of achieving a higher conversion versus the cost of adding another reactor.

2.13 In order to increase the conversion efficiency, we have to add reactors in series. Adding reactors in parallel will increase the capacity or volumetric flow rate, but will not increase the conversion efficiency.