4th ed
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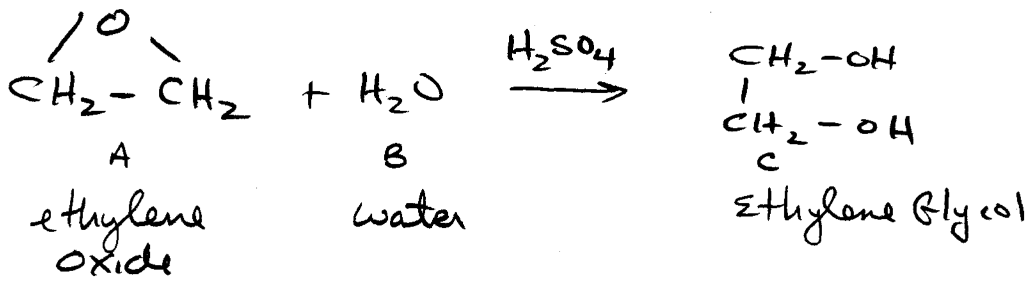
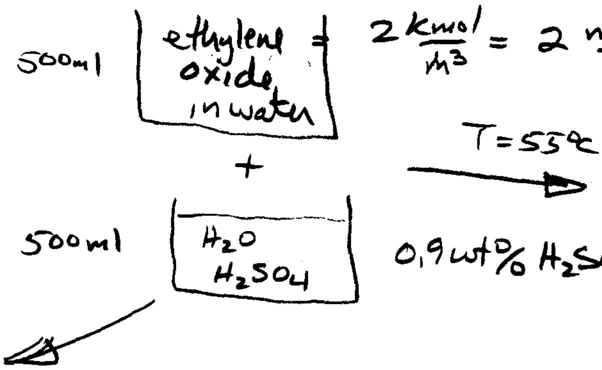
Example 4-1



"Hydrolyze ethylene oxide"

Lab experiment $V = 500ml$



$= 2 \frac{kmol}{m^3} = 2 \frac{mol}{L} = 2 M$

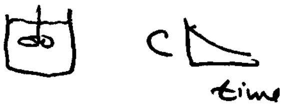
0.9 wt% H_2SO_4 (catalyst)

Data from lab C_C vs t (EG)

$T = 55°C$
first order in EO

A: Problem statement: find k

B. sketch



C. Identify

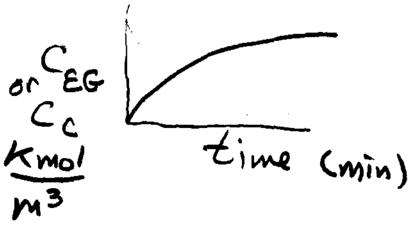
1) equations $\frac{dC_A}{dt} = r_A$ $V=$ constant

$r_A = -kC_A$

$X_A = \frac{N_{A0} - N_A}{N_{A0}}$

2) Variables Dependent: C_A, r_A also C_B & C_C
Independent: t

C 3) Knowns & unknowns



Unknowns
1) C_{EO} vs t or C_C vs t
2) k_A ?
3) $V = ?$

C 4 INPUTS & OUTPUTS — all fed at one time
C_{A_0} = needs to be calc.

C5 — No missing info

D. Assumptions & Approximations

1) - well-mixed, all reactants enter at one time
No side rxns, negligible filling time
Isothermal

Approximations
Why first order?

$r_A = -k' C_A C_B$ — C_B is in excess so it does not change by very much or $\Delta C_B << \Delta C_A$

$r_A \simeq -\underbrace{(k' C_{B_0})}_{k} C_A$

$C_B \simeq C_{B_0}$

E Specification

Equations — m.B.
— rxn rate
— stoic table to relate C to A (data)
or rewrite mole balance for

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Batch Reactors

$$\frac{d(C_A V)}{\partial t} = r_A V$$

$r_A = -kC_A$ liquid phase

$$\frac{d(C_A V)}{dt} = -kC_A V$$ V = constant

$$\int \frac{dC_A}{C_A} = \int k\,dt$$

$$\ln C_A \Big|_{C_{A0}}^{C_A} = -kt$$

$\ln C_A / C_{A0} = -kt$ (Go to page 4)

or

$X_A = (N_{A0} - N_A)/N_{A0}$ Skip

$N_A = N_{A0} - N_{A0} X_A$

for constant volume $V = V_0$

$$\frac{N_A}{V} = \frac{N_{A0}}{V} - \frac{N_{A0}}{V} X_A \rightarrow C_A = C_{A0} - C_{A0} X_A$$

$$\ln (1 - X_A) C_{A0} - \ln C_{A0} = -kt$$

$$\ln \left[1 - X_A\right] = -kt$$

Reaction time t_R time to achieve a conversion X

$t_R = t = \frac{1}{k} \ln\left(\frac{1}{1 - X_A}\right)$ first order

Solution (continued)

Relate C_A to C_c ← data

C_A ← equation – MB & rate

Stoic table

Species	initial	change	final
A	N_{A0}	$-N_{A0}X_A$	$N_A = N_{A0}(1-X_A)$
B	N_{B0}	$-N_{A0}X_A$	$N_B = N_{B0} - N_{A0}X_A$
C	0	$+N_{A0}X_A$	$N_c = N_{A0}X_A$

$\frac{N_c}{V} = \frac{N_{A0}}{V} X_A$ since $V = V_0$ $C_c = C_{A0} X_A$

$C_A = C_{A0} - C_{A0} X_A = C_{A0} - C_c$

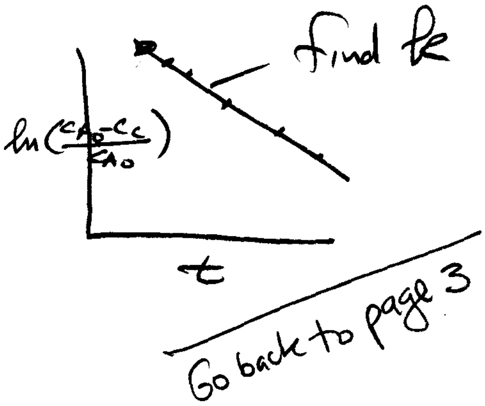
$C_{A0} = 1\,\text{mol A}/L = \frac{\frac{2\,\text{mol A}}{L}\,0.5L + 0.\cancel{5}^{0}L}{(0.5L + 0.5L)}$

Rewrite table

t (min)	C_c (mol/L)	$(C_{A0} - C_c)/C_{A0}$
0	0.0	
↓	↓	
10	0.957	

$$\ln \frac{C_A}{C_{A0}} = -kt$$

$$\ln\left(\frac{C_{A0} - C_c}{C_{A0}}\right) = -kt$$



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Book give result for $r_A = -kC_A^2$

$$t_R = \frac{x_A}{kC_{A_0}(1-x_A)} \quad \text{equ 4-5}$$

$r_A = -kC_A$

$$t_R = \frac{1}{k}\ln\left(\frac{1}{1-x_A}\right)$$

Note difference in units of k

$$k_{\text{second order}} [=] \frac{1}{s}\,\frac{L}{mol}$$

$$r = -kC_A [=] \frac{1}{s}\,\frac{L}{mol}\left(\frac{mol}{L}\right)^2 [=] \frac{mol}{s\,L}$$

$$k_{\text{first order}} [=] \frac{1}{s}$$

Batch times - cycle times

$$t_{total} = \overset{\text{Agitation}}{\underset{\substack{\uparrow \\ 1.5-3\text{hr}}}{\text{fill }\overset{\neq}{\text{time}}}} + \underset{\substack{\uparrow \\ 0.2-2\text{hr}}}{\text{heating}} + \text{Reacting time} + \overset{0.5\text{hr}}{\text{drain time}} + \overset{1\text{hr}}{\text{clean time}}$$

modified p151 equation

$$t_{total} = 3\text{-}6\text{hr} + t_{Reaction}$$

See example 4-1 for finding k from Batch data

Good Example of Problem Solving algorithm