ATENOLOL EPOXIDE REACTION DATA ANALYSIS IN BATCH REACTOR

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Abstract
In this paper Integral method of analysis of data for Batch reactor is used to find the rate and order of reaction of Atenolol epoxide. The integral method is useful for fitting simple chemical reactions. This method puts a particular rate equation to test by integrating and comparing the predicted C versus t curve with experimental C versus t data. If the fit is unsatisfactory, another rate equation is tested. The key raw materials required to produce Atenolol epoxide are Parahydroxyphenylacetamide (PHPA) and Epichlorohydrine (EPH). Firstly, the order and rate with respect to reactant i.e. PHPA is tested and then overall order and rate of equation is evaluated with Integral method of analysis of data. The integrated rate law depends on the kinetics. Since the reaction is being carried out in a batch reactor, the volume of reactor is assumed constant throughout the reaction. The theoretical and actual rates of reaction are then compared for various concentrations of reactant.

Keywords: Batch reactor, Irreversible bimolecular-type second order reaction, Theoretical rate constant, Integral method of analysis, Experimental rate.

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1. ATENOLOL EPOXIDE

Atenolol Epoxide is produced by condensing PHPA and EPH, the reaction is being carried out in a one litre, 3 mouthed round bottom flask at isothermal conditions and with constant stirring [1].

PHPA + EPH $\longrightarrow$ ATENOLOL EPOXIDE

Concentrations versus time data are obtained for reactants and integrated method for finding the rate law are checked for first and second order reactions.

2. COMPARISON BETWEEN THEORETICAL AND ACTUAL RATE, FOR CHANGE IN CONCENTRATION DATA

Various batches with change in concentration of key reactant PHPA were carried out and their order and rate of reaction was calculated. Further the theoretical rate was calculated and experimental rate was found by integral method of analysis data.[2]
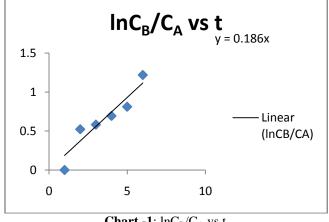
3. FOR 60 GM PHPA BATCH

3.1 Overall Order

Overall order is sum of order with respect to each reactant, i.e. sum of orders of both the reactants[2]. Both reactants are first order therefore, overall order is second order, which can be proved with integral method of analysis.

Plot a graph of $\ln C_B/C_A$ vs time and $\ln C_B C_{A0}/C_A C_{B0}$ vs time.[2]

Table -1: $\ln C_B/C_A$ data

Time(hours)	C_A in moles/liter	C_B in moles/liter	$\ln C_B/C_A$
0	0.6622	1.1166	0.5224
2	0.5764	1.03098	0.5814
4	0.4543	0.9088	0.6933
6	0.368	0.828	0.8109
8	0.191	0.6455	1.2177

Chart -1: $\ln C_B/C_A$ vs t

From graph it can be seen that, slope= $(C_{B0}-C_{A0})k=0.186$, value of k can be calculated, k=0.409 L/molhr.[3]

$$-r_A = 0.409\ C_A C_B \qquad (1)$$

Therefore, straight line in graph proves that the concentration vs time data fits to second order kinetics.

3.2 Theoretical rate

$$-r_A = -\frac{dC_A}{dt} = -\frac{(0.191 - 0.6622)}{(8 - 0)} = 0.0589 \ mol/Lhr$$

$$0.0589 = k_{th} C_A C_B$$

Where k_{th}=theoretical rate constant

$$0.0589 = k_{th} \ (0.4266)(0.8858)$$

$$k_{th} = 0.156 \ L/molhr$$

Calculating theoretical rates at various time during reaction.

At 0 hr
$$-r_1 = 0.156(0.662)(1.1166) = 0.1153 \ mol/Lhr$$

At 2 hr
$$-r_2 = 0.156(0.576)(1.0309) = 0.09269 \ mol/Lhr$$

At 4 hr
$$-r_3 = 0.156(0.4543)(0.9088) = 0.0644 \ mol/Lhr$$

At 6 hr
$$-r_4 = 0.156(0.368)(0.828) = 0.0475 \ mol/Lhr$$

At 8 hr
$$-r_5 = 0.156(0.191)(0.6455) = 0.0192 \ mol/Lhr$$

3.3 Actual Rate or Experimental Rate

From graph

$$-r_A = 0.409 \ C_A C_B$$

$$k_{ex} = 0.409 \ \frac{L}{molhr}$$

Where k_{ex}= experimental rate constant

Calculating experimental rates at various time during reaction[3]

At 0 hr
$$r_1 = 0.409(0.662)(1.1166) = 0.303 \ mol/Lhr$$

At 2 hr
$$-r_2 = 0.409(0.576)(1.0309) = 0.2430 \ mol/Lhr$$

At 4 hr
$$-r_3 = 0.409(0.4543)(0.9088) = 0.1688 \ mol/Lhr$$

At 6 hr
$$-r_4 = 0.409(0.368)(0.828) = 0.1246 \ mol/Lhr$$

At 8 hr
$$-r_5 = 0.409(0.191)(0.6455) = 0.05042 \ mol/Lhr$$

Table-2: Comparison between theoretical and experimental rate

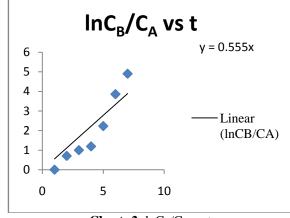| Time (hr)	Theoretical rate (mol/Lhr)	Experimental rate (mol/Lhr)
0	0.1153	0.303
2	0.0926	0.2430
4	0.0644	0.1688
6	0.0475	0.1246
8	0.0192	0.05042

4. FOR 50 GM PHPA BATCH

4.1 Overall Order

Overall order is sum of order with respect to each reactant, i.e. sum of orders of both the reactants[4]. Both reactants are first order therefore; overall order is second order, which can be proved with integral method of analysis.

Plot a graph of lnC_B/C_A vs time and $ln \ C_B C_{A0}/C_A C_{B0}$ vs time.

Table -3: lnC_B/C_A and $ln \ C_B C_{A0}/C_A C_{B0}$ data

Time(hours)	C_A in moles/liter	C_B in moles/liter	lnC_B/C_A
0	0.5518	1.11660	0.70472
2	0.3297	0.89450	0.99808
4	0.2466	0.81142	0.19101
6	0.0682	0.63305	2.22722
8	0.00424	0.56903	4.89937

Chart -2: lnC_B/C_A vs t

From graph it can be seen that slope= $(C_{B0}-C_{A0})k=0.555$, value of k can be calculated, k=0.982L/molhr.[4]

$$-r_A = 0.982 \ C_A C_B \qquad (2)$$

Therefore, straight line in graph proves that the concentration vs time data fits to second order kinetics.

4.2 Theoretical Rate

$$-r_A = -\frac{dC_A}{dt} = -\frac{(0.00424 - 0.551)}{(8 - 0)}$$
$$= 0.06844 \ mol/Lhr$$

$$0.06844 = k_{th} C_A C_B$$

Where k_{th}=theoretical rate constant

$$0.06844 = k_{th} (0.278)(0.8428)$$

$$k_{th} = 0.2921 \, L/molhr$$

Calculating theoretical rates at various time during reaction.

4.3 Actual Rate or Experimental Rate

From graph

$$-r_A = 0.982 \, C_A C_B$$

$$k_{ex} = 0.982 \frac{L}{molhr}$$

Where k_{ex}= experimental rate constant

Calculating experimental rates at various time during reaction.[5]

Table-4: Comparison between theoretical and experimental rates

Time (hr)	Theoretical rate (mol/Lhr)	Experimental rate (mol/Lhr)
0	0.1799	0.605
2	0.0861	0.2896
4	0.0584	0.1964
6	0.0126	0.0424
8	0.0007	0.0023

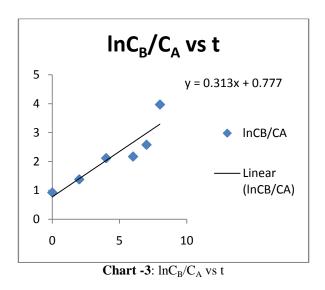## 5. FOR 40 GM PHPA BATCH

5.1 Overall Order

Overall order is sum of order with respect to each reactant, i.e. sum of orders of both the reactants[6]. Both reactants are first order therefore; overall order is second order, which can be proved with integral method of analysis.

Plot a graph of $\ln C_B/C_A$ vs time and $\ln C_B C_{A0}/C_A C_{B0}$ vs time.

Table-5: $\ln C_B/C_A$ and $\ln C_B C_{A0}/C_A C_{B0}$ data

Time(hours)	C_A in moles/liter	C_B in moles/liter	$\ln C_B/C_A$	$\ln(C_B C_{A0}/C_A C_{B0})$
0	0.4420	1.1166	0.926734	0
2	0.2268	0.9019	1.380435	0.453701
4	0.0927	0.7689	2.115592	1.188859
6	0.0871	0.763	2.170201	1.243467
8	0.0130	0.688	3.968839	3.042106

Chart -3: $\ln C_B/C_A$ vs t

From both graphs we can see slope= $(C_{B0}-C_{A0})k=0.313$, value of k can be calculated, k=0.464 L/molhr.[7]

$$-r_A=0.464 \, C_A C_B \qquad (3)$$

Therefore, straight line in both graphs proves that the concentration vs time data fits to second order kinetics.

5.2 Theoretical Rate

$$-r_A = -\frac{dC_A}{dt} = -\frac{(0.0130 - 0.4420)}{(8 - 0)} = 0.0536 \, mol/Lhr$$

$$0.0536 = k_{th} C_A C_B$$

Where k_{th}=theoretical rate constant

$$0.0536 = k_{th} (0.2275)(0.9023)$$

$$k_{th} = 0.2612 \, L/molhr$$

Calculating theoretical rates at various time during reaction.

5.3 Actual Rate or Experimental Rate

From graph

$$-r_A = 0.464 \, C_A C_B$$

$$k_{ex} = 0.464 \frac{L}{molhr}$$

Where k_{ex}= experimental rate constant

Calculating experimental rates at various time during reaction.[8]

Table-6: Comparison between theoretical and experimental rates

Time (hr)	Theoretical rate (mol/Lhr)	Experimental rate (mol/Lhr)
0	0.1289	0.2291
2	0.0534	0.0949
4	0.0186	0.0331

6	0.0173	0.0308
8	0.0023	0.0042

6. RESULTS AND CONCLUSIONS

Overall order of reaction is second order, proved using integral method of analysis. This method is also used to find the overall rate equation and the value of rate constant. The reaction of Atenolol epoxide is a homogeneous reaction with no catalyst used. The concentrations versus time data are used to find the order of reaction.Comparison of theoretical and experimental rates is done. Concentration of reactant decreases as reaction proceeds with time. Effect of concentration of reactant is studied by varying the concentrations of PHPA. The batch with 60 gm PHPA used shows that the reactant remains unreacted as compared to 50 gm batch.

7. ABBREVIATIONS AND NOMENCLATURE

PHPA- Parahydroxyphenylacetamide
EPH- Epichlorohydrine
C_{A0}-Initial concentration of reactant A
C_{B0}- Initial concentration of reactant B
C_A- Concentration of A
C_B- Concentration of B
X_A- Fractional Conversion of A
r_i- Reaction rate of component i

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