

## **Non-Linear Dynamical Behaviour of a Specific Reaction Kinetics**

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**Abstract.** Chemical reaction kinetics plays an important role in many applied mathematical modeling and simulation to arrive at definite relation between different components in the reaction. Most of the medical research activities try to explain the medicines and the side effects in their products. Here we attempt to model the non-linear dynamical behavior of the oxidation of p-anisaldehyde. Experimental details and the model fitted are given in the paper.

**Keywords:** oxidation, irreversible reaction, method of least square, exponential curve fit, temperature and time component in the concentration.

### **1. Introduction**

A rate equation characterizes the rate of reaction and its form may either be suggested by theoretical considerations or simply by the result of an empirical curve-fitting procedure. In any case, the value can only found by experiment; predictive methods are inadequate at present. There are two procedures for analyzing kinetic data, the integral and differential methods. In the integral method of analysis we guess a particular form of rate equation and after appropriate integration and mathematical manipulation, predict that the plot of a certain concentration function versus time should yield a straight line. The data are plotted and if reasonably good straight line is obtained then the rate equation is said to satisfactorily fit the data. In the differential method of analysis we test the fit of the rate expression to the data directly and without any integration. There are advantages and disadvantages to each method<sup>7</sup>. A chemical process is a one where the identity of molecules is changed consequently; it involves rupture and formation of chemical bonds. Thiyagarajan<sup>10</sup> has presented a stochastic approach to chemical reaction kinetics. He has

given an approximation to the equilibrium distribution using the method of Dunstan<sup>9</sup> (1981) and presented a deterministic limit of a stochastic model of chemical reaction kinetics.

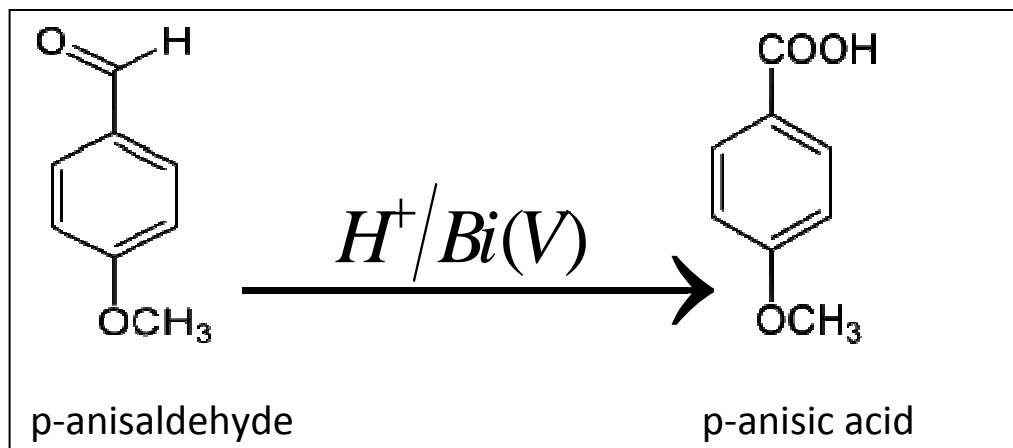
We can give the following reasons for formulating chemical kinetics in stochastic framework. A basic reason is that the process is in fact statistical in nature. The concentration or the number of molecules in the system is an integer-valued random variable. The mean of this distribution will be the observed concentration and the variance will supply a measure of the inherent statistical aspects help us to predict rates from molecular properties. There are number of reactions for which the deterministic is not adequate and stochastic models must in fact be used, for example, many reactions in the field of polymer chemistry such as distribution of chain length, the distribution of copolymeric composition, diffusion controlled reaction etc.,

At low concentration a stochastic model must be used to give an accurate representation of the process. But no attempt has been used to analyze a number of common reactions but the results are difficult to handle algebraically. Thus we tried to fit probability distribution for the reactions.

Antifungal activity of p-anisaldehyde was investigated on Candida strains. p-anisaldehyde (4-methoxybenzaldehyde), an extract from Pimpinella anisum seeds, is a very common digestive herb of north India<sup>1</sup> used as insecticide<sup>2</sup>. Also oxidation of p-anisaldehyde is very useful in production of medicinally and chemically important p-anisic acid (p-methoxy benzoic acid) is a part of cresol class antiseptic compounds. It is also used as an insect repellent and ovicide. Anisole, anisic acid, and their derivatives are also widely used in chemical reaction as intermediates to obtain target materials such as dyes, pharmaceuticals, perfumes, photo initiators and agrochemicals<sup>3</sup>. Anisic acid is a phenolic acid, an organic molecule commonly found in anis-seed, a common food spice. Anisic acid is occasionally found in human biofluids. Anisic acid has been characterized as a classical non-competitive inhibitor of the oxidation of L-3, 4-dihydroxyphenylalanine (L-DOPA), and the hydroxylation of L-tyrosine catalyzed by tyrosinase<sup>4</sup>. Additionally, anisic acid is a metabolite of aniracetam, a cognition enhancer<sup>7</sup> and acts as a natural preservative, with mould inhibitor properties<sup>6</sup>.

## 2. Our Model-Experimental Part

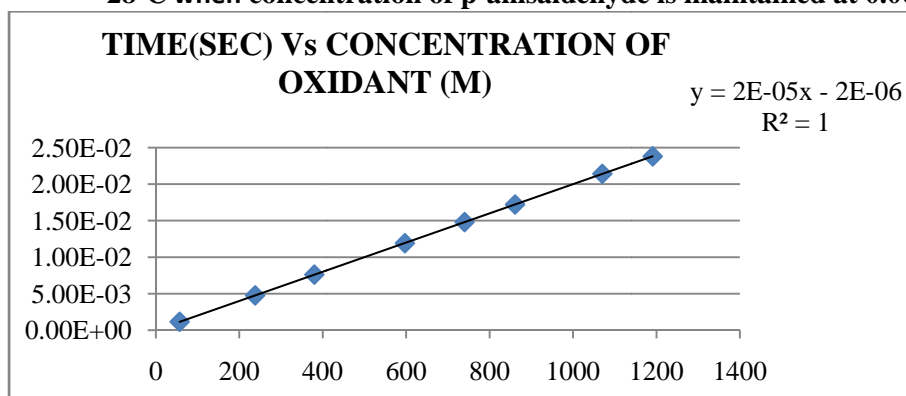
The kinetics of oxidation of p-anisaldehyde by Bi(v) has been measured in aqueous acetic acid medium (50–50% v/v) in the presence of  $\text{HClO}_4$  (0.10–1.00 mol dm<sup>-3</sup>) at constant ionic strength at room the temperature. The reactions has been found to obey the rate law and acid-dependent reaction path. The progress of the reaction was studied titrimetrically by titrating the liberated iodine against standard solution of sodium thio sulphate using starch as indicator.



**Figure 1: Oxidation reaction of p-anisaldehyde to p-anisic acid**

### 3. Data Analysis

A plot of time Vs concentration of oxidant for oxidation of p-anisaldehyde at 28°C when concentration of p-anisaldehyde is maintained at 0.001M



**Figure 2: Kinetic data for oxidation of p-anisaldehyde at 28°C when concentration of p-anisaldehyde is maintained at 0.001M**

TIME ( Sec.)	CONCENTRATION OF OXIDANT (M)
57	1.14E-03
238	4.76E-03
380	7.60E-03
597	1.19E-02
740	1.48E-02
861	1.72E-02
1070	2.14E-02
1191	2.38E-02

log t	[Concentration of oxidant]	[Concentration] × log t	[Concentration] <sup>2</sup>
1.755875	1.14E-03	2.00E-03	1.30E-06
2.376577	4.76E-03	1.13E-02	2.27E-05
2.579784	7.60E-03	1.96E-02	5.78E-05
2.775974	1.19E-02	3.31E-02	1.43E-04
2.869232	1.48E-02	4.25E-02	2.19E-04
2.935003	1.72E-02	5.05E-02	2.97E-04
3.029384	2.14E-02	6.48E-02	4.58E-04
3.075912	2.38E-02	7.33E-02	5.67E-04
Σ=	21.39774	1.03E-01	2.97E-01

$y = 48.446 e^{-4.7196x}$  where y is the time in seconds and x is the concentration

#### 4. Conclusion

We find the exponential model fits better than the linear model for the oxidation kinetics of p-anisaldehyde. We also study the probabilistic aspect of reaction kinetics process.

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