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RESEARCH ARTICLE

# Estimation of a higher probability collision for chemical reaction model

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## ABSTRACT

The paper explained and estimated collision probability for chemical reaction modeling in detail. To define the risk of a chemical process, it is vital to determine the probability of an event occurrence. Characterize the collision probability that a molecule may encounter along its lifetime. This characterization is intended to define a methodology to compute the associated collision. Analyzing the characteristics of data sets by the statistical method in regards to the main aspects relates to collision probability. An investigation of the impact of these features addressed. Approaches based on Minitab presented and status of particle collision probability determined mathematically. Results showed the status of collision probability based on the correlation of kinetic energy and rate of reaction associated with envisaged encounters. A comparison was made to define the best fit model. The study recommended accepted levels of collision probability for the occurrence of the chemical reaction.

***Keywords:*** chemical; collision; probability; reaction; rate; kinetic

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## 1. Introduction

Over the past decades, the desire to develop alternatives to traditional processes for the transformation of chemical substances from one material to another has resulted in the development of chemical process modelling which becomes essential in modern living standards. Chemical reaction or process modelling has widely inspired scientists and engineers. Chemical equations have been used to describe the chemical reactions[1]. These chemical reactions are usually characterized by a chemical change to produce a new product at a characteristic rate of reaction at certain process conditions.

To calculate the rate of reaction, here are important factors: (1) It is required energy to proceed the reaction forward, (2) Effective collision among molecules, and (3) Right orientation[1]. These factors are necessary for any reaction to occur otherwise nothing will happen.

The consideration of the geometry of the particles may discover events that are resulting in a collision or estimate a higher probability of collision associated with the event. It is important for the large particles as the uncertainty in positions does not reach small particles to make a difference for the tiny size particles. As the features of the particles are known more precisely, the importance of considering the actual shape of the particles will become more relevant.

The Information laboratory testing and measurement were taken from previous studies while chemical reaction modelling was theoretically considered[3,4]. The main features of available data need to be analyzed regarding accuracy to perform estimation of a collision among particles. MINITAB and mathematical models have been implemented for the seeking of experimental evaluation and the probability of collision among particles.

The purpose of the paper is to characterize the collision probability that a molecule may encounter along its lifetime. This characterization is intended to define a methodology to compute the associated collision and to identify strategies for allowance manoeuvres. We approximately know the orbital position and velocity of the particle's rotation in the process. These orbits can be propagated and compared with the free particles (with no collision).

The number of particles orbiting in the process is constrained to some rotational regimes of particular interest, these particle rotations, or orbits, including the large size orbits, are associated with a higher collision probability. That expectation imposes the need to estimate the eventual collision encounter and calculate the associated energy. However, the uncertainty associated with the particles and missing distance is one of the most relevant aspects of the evaluation of collision probability.

In addition, optimization of the probability of particles collision improves the energy consumption and increases the probability of a process yield.

A. Principle of chemical kinetics

The main concept of chemical kinetics is considered in the present study. The reaction type studied here is written as

$$A + B \longrightarrow C \tag{1}$$

For this particular reaction, the reaction rate , r, can be defined as (2):

$$r = - d[A] / dt = - d[B] /dt = d[C] / dt \tag{2}$$

Where [A],[B],and [C] are concentration of each species reaction rate on the concentration of reacting species is expressed by reaction law of the reaction [9]. Thus, the reaction rate is proportional to A and B concentrations; as a result, the kinetic reaction can be defined as (3):

$$r = k[A][B] \tag{3}$$

where k is the constant rate, In addition, k is a temperature dependent that can be described by Arrhenius equation (4):

$$k = A \exp(-E_a/RT) \tag{4}$$

The collision theory[4] provides an interpretation of Arrhenius equation by defining the specific empirical parameters required for a reactive encounter. In fact that the molecular kinetic energy is connected to thermal movement (the correlation of molecular speed with temperature and molecular mass[5]

## 2. Experimental and methodology

Minitab used to evaluate the significant effect on the reaction process. Also, it reduces the time of reaction. To apply the analysis, creating data sheet in Minitab is required. The graphs show that log concentration level is more bounded as it has no points outside the limits and is better distributed as it is closer to a straight line than the concentration level. In addition, all values of mean and standard deviation of each as well standard error of means given on the right corner of each graph.

The values obtained from the probability distribution plots demonstrate the effects on the process based on the values of P-Value.

An experiment consists of a series of numbered steps with specific parameter values conducted previously. The aim of using the experimental data was to develop a mathematical model of an underlying random process. First, creating a relationship among variables by visualizing the data set, and defining the probability distributions which can be utilized as a probabilistic model. Then select the distribution that fits the data set. Finally, the using the model to determine the desired probability. A statistical technique could be used to estimate the mathematical model. To get an impression of the data set, we use Minitab to visualize the data in form of a plot.

**Table 1.** Experimental data collection of reaction.

| No. | $[A]_t$ (mM) | Time (s) |
|---|---|---|
| 1 | 0.0731 | 3 |
| 2 | 0.0728 | 4 |
| 3 | 0.0681 | 5 |
| 4 | 0.0582 | 6 |
| 5 | 0.0511 | 7 |
| 6 | 0.0448 | 8 |
| 7 | 0.0404 | 9 |
| 8 | 0.0339 | 10 |
| 9 | 0.0217 | 11 |
| 10 | 0.0143 | 12 |

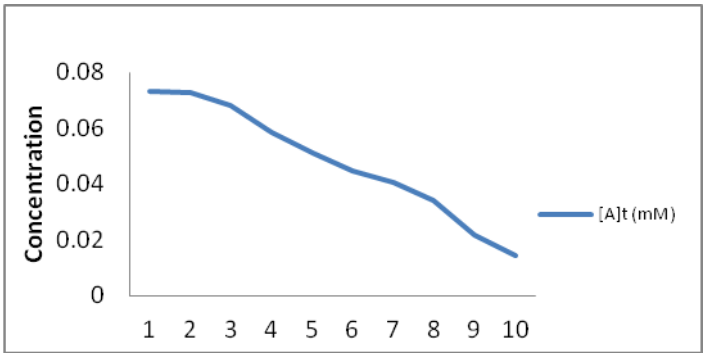


**Figure 1.** The linear plot of concentration (mM) versus time (s).

The rate constant and y-intercept of approximately 0.0068 $S^{-1}$ and 0.0735 respectively illustrated on **Figure 1**.

The graph shows the range and data points. Normal distribution used as a probabilistic model. Also, fit Lognormal and Weibull distribution.

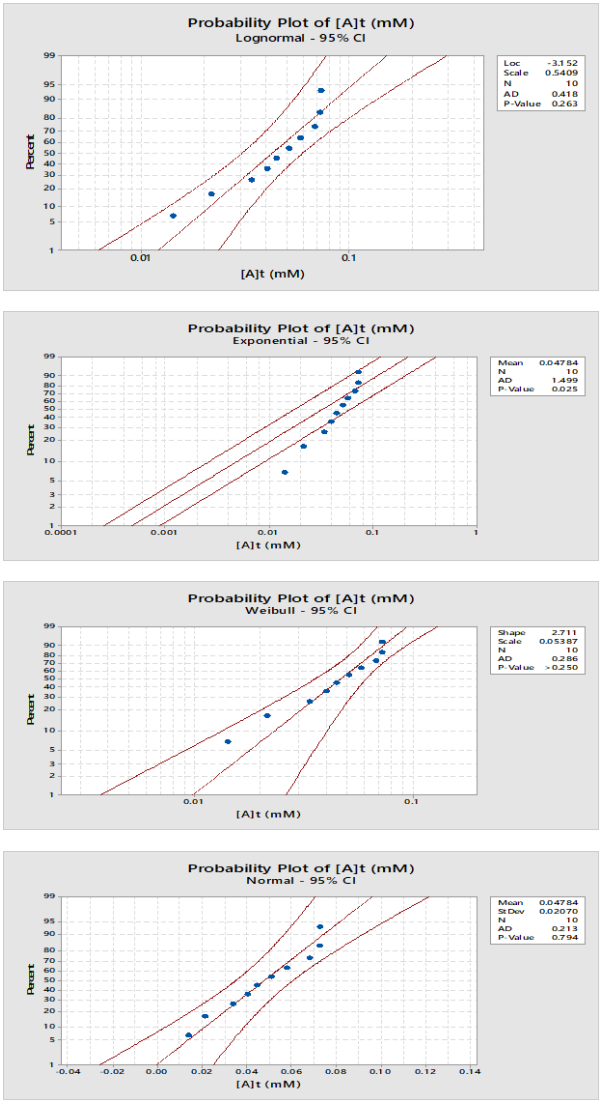


**Figure 2.** The probability distributions of the chemical concentration (mM).

The graph constructed the concentration levels with time. The process analysis implemented using Minitab or Designing of the Experiment DOE, which save time and money, to evaluate the fate of the process reaction and investigate the vital factors that have a significant impact on the process is a useful technique. A number of probability distributions that are most likely to fit the chosen data set illustrated **Figure 1**, an estimation of their parameters, and selection of the most adequate model achieved.

The experimental design observed the changes in concentration at different period of time **Figure 1**.

The experimental design showed that there will be not a harm effect with p-value greater than (> 0.05). From above graph, the probability distribution of chemical reaction designed by several plots as (i.e. lognormal, exponential, well bull, and Normal). However, blue dots between red curves described the fate of best fit plot. Therefore, lognormal, wellbull, and normal distribution probability plots illustrated a good results as the blue dots constructed between two red curves but the normal plot gives the best fit model due to the P-value = 0.792 and low standard deviation compared to lognormal and wellbull plots 0.263 and 0.025 respectively.

The probability plots describe the given values of concentration, the value of f(x), the probability density. Although the random variable may vary with time, A possible normal data distribution. The normal distribution plots show a good points distribution which results from a log and Weibull distributions, however, more consistency among the blue dots through the line that results from normal distribution than other probability plots (lognormal, exponential, and Weibull distributions) was noticed. Therefore, the graph demonstrates that

the experimental data are normally distributed. The following summary report presents the number of defects per unit for the given data.

The given regression fitted equation by Minitab describes the relationship between concentrations versus time is obtained through (5):

$$Y = b_0 + b_1 x + b_3x^2 + \ldots + b_m x^{m-1} \quad (5)$$

It is more common that a model process relationship among the variables is postulated based on the principles of the process thermodynamics or theoretical principles. In 2020, a report written by Altuwair used the regression model to estimate the risk probability[12]. It is known from the experimental data that the concentration of the reactant x is linearly related to the concentration of products Y as (6):

$$Y = ax \quad (6)$$

In the reaction, a is the parameter describing the proportionality among the concentrations. However, a statistical regression model was used for parameters estimation of the model based on a former set of experimental data where there is one dependent variable and one independent variable. In general, the mathematical model is: Y = f (x, a) where Y is a single dependent variable , x is the independent variable, a is a model parameter. Therefore, the fitted model is:

$Y = 0.08628 - 0.002910 x - 0.000258 x^2$

Parameters functions are: $B_0$= 0.08628, $B_1$= 0.002910, and

$B_3$ = 0.000258

Also, regression analysis used to determine the error of the dependent variable Y. The variance is the residual sum of squares, $S_R = \sum(yi - f(x_{1i} \ldots x_{li} ; a_1, \ldots, a_m)$.To measure the extent to which the model has captured the variation in the data, R-squared can be statistically analyzed. Then R-sq is the ratio of variance independent variable y-measurements that are described by the model to the overall variance of the y-measurements, the R-sq can be written regarding $S_R$ and $S_D$.

$$R^2 = 1 - S_R / S_D \quad (7)$$

$S_R$ is the residual sum of squared, $S_D$ is the corrected sum of squared Forgiven data, if the model fits the data well, this equation used to predict the concentration for a value of time or find the settings for the time that corresponds to the desired value for concentration. R-sq equals 98.14% which is the variation of concentration accounted by the regression model. It indicates that the variables are highly correlated. Therefore, the number of defects per unit is stable. The main objective of stability analysis is finding the desired area to design the optimal mechanism regarding collision probability.

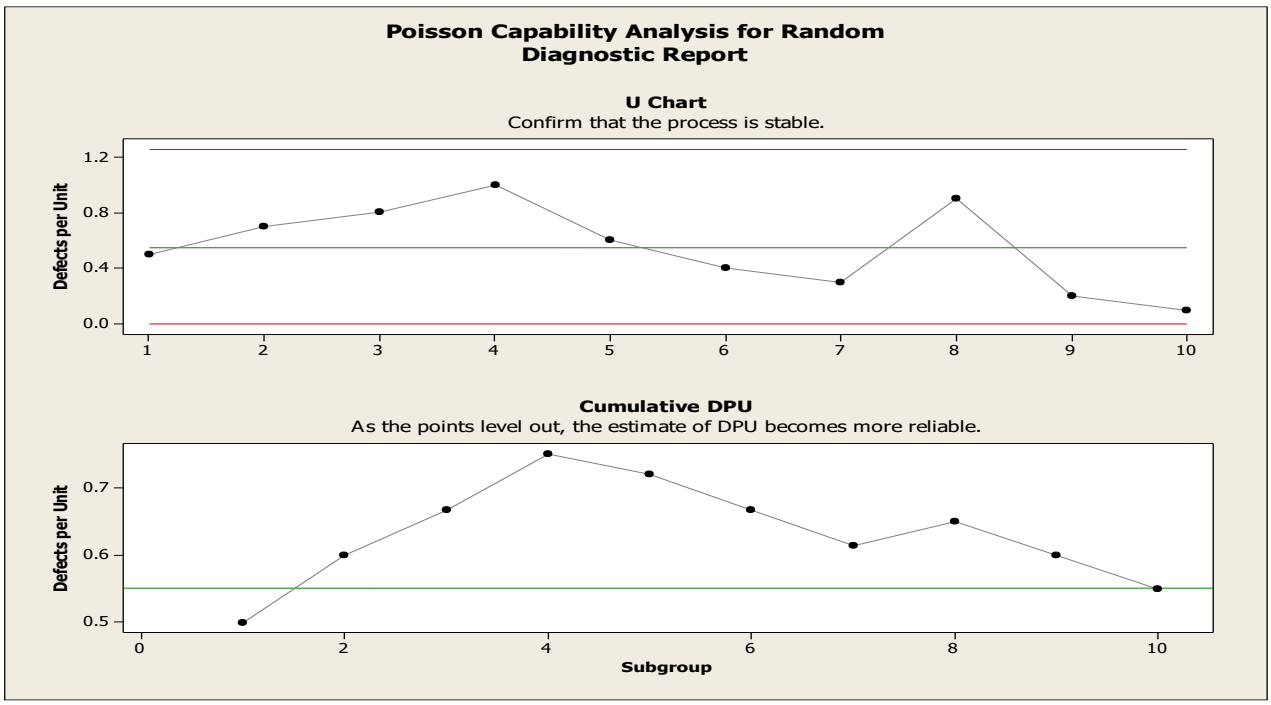


**Figure 3.** Stability of the points.

Plots derived from the integrated rate for different reaction orders can be used to determine the rate constant k.

**Table 2.** The measurement of rate constant.

| [A]t (mM) | time (s) | k |
|---|---|---|
| 0.0731 | 3 | 0.024366667 |
| 0.0728 | 4 | 0.0182 |
| 0.0681 | 5 | 0.01362 |
| 0.0582 | 6 | 0.0097 |
| 0.0511 | 7 | 0.0073 |
| 0.0448 | 8 | 0.0056 |
| 0.0404 | 9 | 0.004488889 |
| 0.0339 | 10 | 0.00339 |
| 0.0217 | 11 | 0.001972727 |
| 0.0143 | 12 | 0.001191667 |

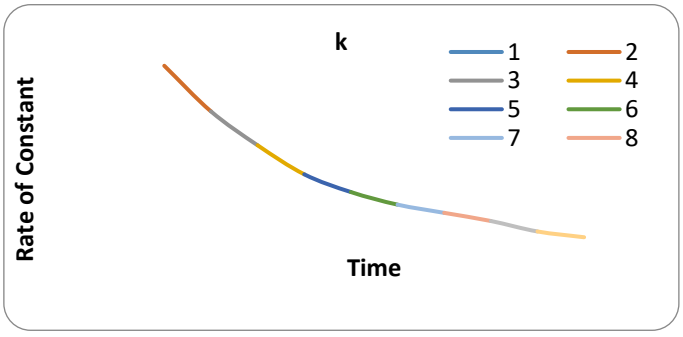


**Figure 4.** The correlation time and constant rate.

**Table 3.** The results of experimental data for (ln K) and (1/T).

| [A]t (mM) | time (s) | k | 1/T | ln k |
|---|---|---|---|---|
| 0.0731 | 3 | 0.024366667 | 0.333333 | 1.098612 |
| 0.0728 | 4 | 0.0182 | 0.25 | 1.386294 |
| 0.0681 | 5 | 0.01362 | 0.2 | 1.609438 |
| 0.0582 | 6 | 0.0097 | 0.166667 | 1.791759 |
| 0.0511 | 7 | 0.0073 | 0.142857 | 1.94591 |
| 0.0448 | 8 | 0.0056 | 0.125 | 2.079442 |
| 0.0404 | 9 | 0.004488889 | 0.111111 | 2.197225 |
| 0.0339 | 10 | 0.00339 | 0.1 | 2.302585 |
| 0.0217 | 11 | 0.001972727 | 0.090909 | 2.397895 |
| 0.0143 | 12 | 0.001191667 | 0.083333 | 2.484907 |

***Note:*** *Time : T & Rate Constant : k*

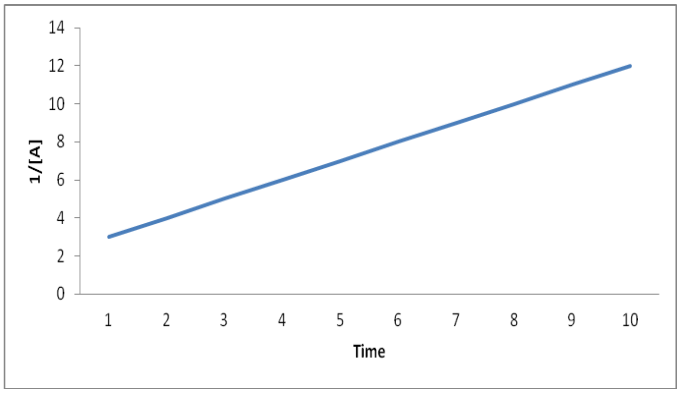


**Figure 5.** Reaction process plot of time versus ln 1/[A].

The plot of the log of concentration versus time yields a straight line with a slope of k. Since this plot is linear, therefore the reaction is 1$^{st}$ order.

The method for evaluating the collision needs a strategy to allow such a collision as a function of minimum activation energy and accepted collision probability level to generate energy. The estimation of collision probabilities in chemical reaction models is crucial for understanding reaction kinetics and mechanisms. Recent studies have increasingly focused on refining these estimations using advanced computational techniques and statistical methods. For instance, in their 2022 study, Zhang et al. employed Monte Carlo simulations to assess collision dynamics in gas-phase reactions. Their findings highlighted the significance of molecular orientation and energy distribution in collision outcomes, suggesting that traditional models may underestimate collision probabilities when these factors are not adequately considered[6].

Moreover, advancements in machine learning have begun to play a pivotal role in enhancing the accuracy of collision probability estimations. Smith and Lee[7] introduced a novel framework that integrates neural networks with quantum mechanical calculations to predict the likelihood of chemical collisions. Their approach demonstrated improved predictive capabilities over conventional methods, particularly for complex reactions involving multiple species. The integration of machine learning techniques not only accelerates computational processes but also allows for the inclusion of a broader range of variables that influence collision frequencies[7].

The first issue is to analyze the probability of collision that allows estimating the impact of strategy on the molecule lifetime and improving it if needed. This approach only considers encounter events related to collision events. It applied to improving the probability of collision. To compute the probability of collision, describing the problem within the framework of probability theory is needed. Describing the uncertainties of the spatial and temporal of molecules by knowing the probability density functions (pdf), then the probability of collision can be determined by assuming that the gas molecules move linearly with random directions.

In addition to computational innovations, experimental techniques have also evolved to provide better insights into collision probabilities. Recent work by Kim et al.[8] utilized laser-induced fluorescence to measure reaction rates in real-time, allowing for direct observation of collision events. Their results indicated that environmental factors, such as temperature and pressure, significantly affect collision probabilities, thereby emphasizing the need for models that incorporate these variables. This experimental validation supports the theoretical advancements and underscores the importance of a multidisciplinary approach in accurately estimating collision probabilities in chemical reaction models[8].

The methodology addresses the capabilities of the strategy as a function of the orbital data accuracy. This analysis is done in a statistical approach by the current uncertainties of experimental data.

Simulation modelling has been used for illustration and analyzing. For example, a numerical method deployed to analyze the movement of fluids, mass transfer, heat transfer, and chemical reactions[13]. A comprehensive and complete statistical analysis of the accuracy of the data sets is provided by the application of MINITAB, with their detailed analysis of the collision performance as a function of distance, size, and accuracy of data, velocity, and geometry. Modification of existing literature reviews proposed and implemented[10].

Another issue is to address the impact derived from the collision. By applying the proposed mathematical equation for estimating the probability of collision among particles, an analysis of an adequate strategy regarding the increase of collision with a low number of particles is achieved.

There were several assumptions:

1. Then position uncertainty can be described by Normal distribution
2. The particles move at constant velocities
3. The changes of velocities  neglected
4. The spatial scale during the collision is constant
5. Statistical Evaluation of Collision Probability

To estimate the appropriate strategy of particle collision to reach the minimum energy, consider the mean number of events to be encountered along with the chemical reaction. This estimation helps to define the suitable strategy for improving the likelihood of collision to an acceptable level and size the fuel or energy consumed. The study applied MINITAB software to analyze the ability of experimental data and estimate data uncertainty[10].

The drawback of the study is on this statistical analysis not on the collision computation theory, however, the uncertainties associated with the particles.

A. Most parameters in the collision computation

The molecule's collision probability is evaluated. However, the biggest obstacle to this approach is to get the data for the computation of the collision probability and the uncertainty associated with the two particles at the time of the collision and the minimum required energy to proceed the reaction forward. The minimum required energy needs to be evaluated to ensure an appropriate and enough energy along the chemical reaction

gained. The probability of collision is defined as the likelihood of hitting a point in the desired area[4]. Once a possible encounter between two or more particles is described, it is required to evaluate the associated energy of collision by considering:1) Particle's collision, 2) Orientation of particles, and 3) Enough energy to make this reaction occur

B. Collision probability

The collision probability at an instance in time can be calculated by multiplying the probability density by the volume of the region.

The probability density, f(x) obtained through (8),(9) :

$$Pc = V * f(x) \tag{8}$$

$$f(x)= 1 /\sigma\sqrt{2\pi} \exp [-(r-L)^2/2\sigma^2 ] \tag{9}$$

where, r is the radius and L is the mean

$$k = 1/ (2\pi)^{3/2} Q^{1/2} \tag{10}$$

Q is a covariance

The Probability of collision (P) can be determined by following equation;

$$P = 3/4\pi R^3 f(x) \tag{11}$$

where $V= 3/4\pi R^3$, the estimation of the collision probability is not easy to figure especially if the movement of the molecules is randomly in the circle shape. Therefore, the orientation of particles (Spatial scale) increases the likelihood of a collision occurring.

C. Geometric probability

The geometric probability is defined as the measurement of the feasible region over the total sample space. The size of the particle is a major factor in the collision phenomena; a large object has a more significant collision probability than a small object [3,4]. According to Johnson, the geometric features of a collision between space objects, **Figure 7**, occurred near the intersection of their orbit's planes. Therefore, the difference in orbital altitude and arrival time when they pass by the intersection of their orbit planes can be used to evaluate dangerous encounters. (the geometry of the objects determines the collision depending on the orientation of two objects at the time of the event)[3,4].

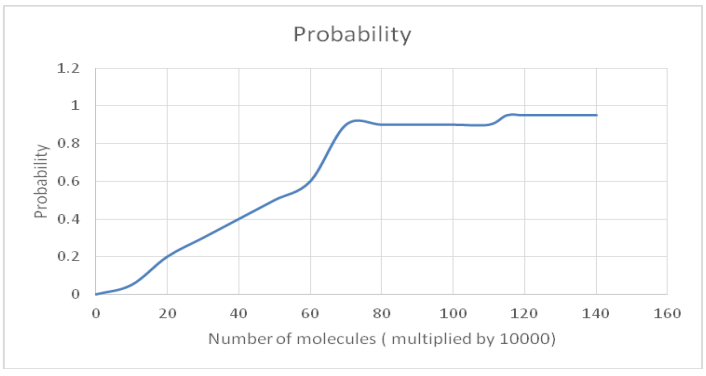


**Figure 6.** The geometric probability curve.

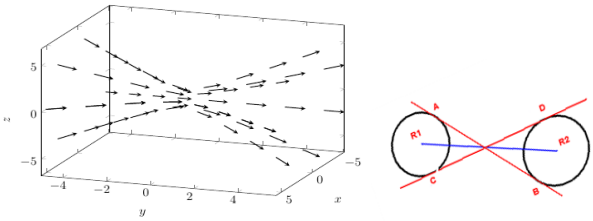


**Figure 7.** The probability of particles collision in random space.

It can be calculated by the velocities of motion in the cross-section. Assume the objects arrive at the same time, and then the normal distribution probability was used to evaluate the uncertainty in the relative radical position.

D. Linear probability model:

The probability that might cause a collision among two particles linearly mathematically equals to Measure of collision region and length of molecule divided by total space. The minimum energy required to progress a reaction is known a activation energy. To compare this energy to kinetic energy provided by collision of molecules is a primary factor affecting the rate of reaction. If the velocity of the flow is known along the tube, then the concentration at different positions and times can be detected by the following (12).

$$ds/dt = [1/2(RT/m)]^{1/2} \quad (12)$$

where, ds/dt is the velocity, m is mass in gram,T is the temperature in K, and R is constant . This gives a relationship between the activation energy $E_a$ and the velocity of the particles V. The best solution would be to use (13) as follows:

$$\ln k = \ln A - 2(E_a / mv^2) \quad (13)$$

By plotting ln k versus $1/v^2$, that gives a slope of $E_a/m$. The mathematical model describes the effect of the particles' speed on the probability of collision. However, the mass of the particles also plays an important role in the collision probability since a bigger size of particle is more likely to collide than a smaller size. For a reaction to take place, the reactants need to travel at a certain speed when they collide. The equation shows that the activation energy of a reaction might decrease when more molecules travel. It is important to mention that the rate will increase by more travelling molecules and less activation energy. Solving the energy of activation can be calculated by the following relationship (14):

$$E_a = ½ (\ln k_2/k_1 (m [v_1v_2/v_2 - v_1])) \quad (14)$$

## 3.Result

A. The analysis of model

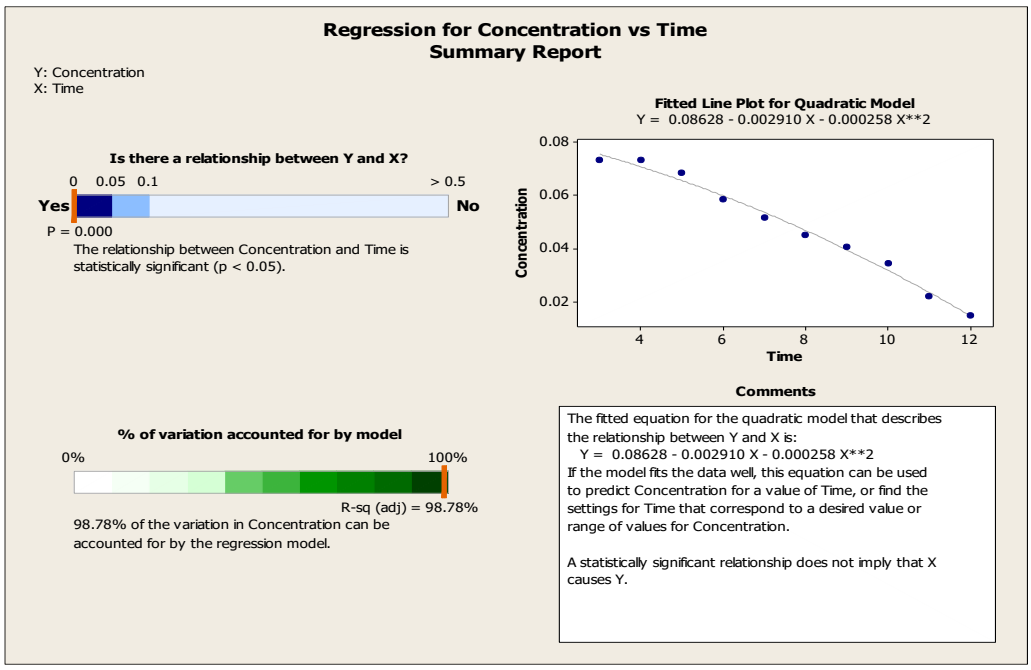


**Figure 8.** Experimental design analysis summary.

The model demonstrates the best-fitted line for all points. The fitted equation for the quadratic model used to predict concentration for a value of time or find the settings for the time that corresponds to a desired value or range of values for concentration. Assuming the total probability of the reaction is in agreement with Arrhenius equation (4).

Therefore, the probability of the reactant leads to product (rate constant)

$$dC/dt = kC \tag{15}$$

The exponential term ($e^{Ea/RT}$) represents the fraction of collision with enough energy for a reaction. It describes the effect of activation energy on reaction rate

Total Rate = total change / total time. The Equation of interest (16)

$$dC/C\ dt = A \exp(-E_a/RT) \tag{16}$$

$$\ln C_0/C = [A \exp(-E_a / RT)]\ t \tag{17}$$

Equation (17), [ln $C_0$/C] versus time yields a slope of the total molecule fraction . ($E_a$/RT, the rate of change can be defined by calculating the slope).

A geometric probability equation was applied to evaluate the likelihood of collision between two particles at a constant velocity.

Assume constant rate is the probability of collision (P) which is defined as the desired area divided by total area.

$$P(X=n) = (1-p)^{n} - P \tag{18}$$

where, X is the Variance, E is expected value

$$X= [1-P/P^2] \tag{19}$$

$$E(x) = 1/P \tag{20}$$

The likelihood of success of a particle attack as (21):

$$k = A\ [(1 - (E_a/RT))^{n-1}\ (E_a/RT)] \tag{21}$$

$$X= [1 - (E_a/RT)], \text{ then, } E(x) = 1/ (E_a/RT) \quad (22)$$

Therefore, the constant rate determined and compared with each other as (23):

$$k_2 = k_1 \text{ Exp } (-Ea_1/RT) / \text{Exp } (Ea_2/RT) \quad (23)$$

where $k_2 > k_1$ and $T_1 = T_2$, resulting in less activation energy ($Ea_2 < Ea_1$), **Figure 10**.

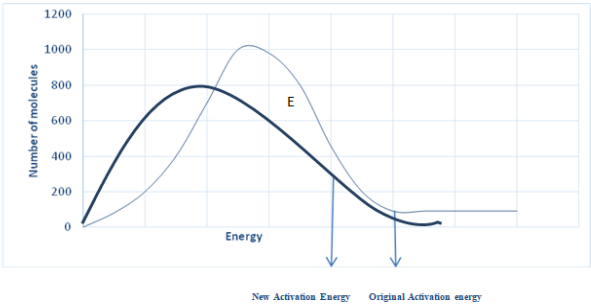


**Figure 9.** The activation energy versus the number of molecules.

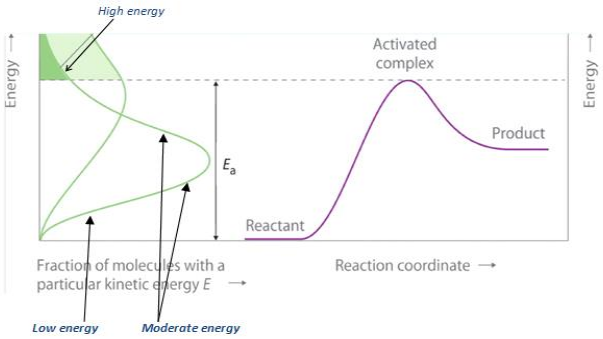


**Figure 10.** The activation energy to the reaction.

The proposed equation described the probability of a particle hitting a point of another particle in the desired area. There are three factors to achieve depending on the spatial scale (orientation of collision), secondly, enough energy to activate the process reaction, and finally, a collision must occur otherwise reaction will not complete. Enough activation energy $E_a$ is the essential element to make a collision between two objects, Ea /RT term represents the probability of collision with enough energy, it has to be as low as possible. However, one minus the fraction of molecules that have energy equal to or greater than activation energy, [1 - ($E_a$./RT)], is the likelihood of there is no collision will occur. The proposed equation describes the collision probability by finding the activated energy level with minimum power. The plotting describes the required energy versus some molecules by reducing the activation energy. Furthermore, the given equation allows us to calculate the mean and variance and control the shape of the curve to improve the probability of particles collision that leads to improve the reactions and decrease the energy consumption of the entire process. Reducing the activation energy will increase the number of particles that have enough energy to react leading to an increase in the probability of the reaction. only those molecules in the shaded zones have higher energy that can overcome the barrier energy Ea and therefore the reaction will occur more rapidly.

B. The probability model of the collision

Mean and variance determine by applying the normal distribution which was the best-fitted model obtained through (24),

$$f(x)= 1 /\sigma\sqrt{2\pi} \exp [-(r-L)^2/2\sigma_2] \quad (24)$$

where, L is the mean that will formulate the equation into (25)

$$f(x)= 1 /\sigma\sqrt{2\pi} \exp [-(a\cos\theta - L)^2/2\sigma_2] \quad (25)$$

$a = 4/\sqrt{2\pi}\,\sigma$

Suppose two particles A and B have been analyzed as follows

X = Time of particle A and Y = Time of particle B

The probability of these two particles to move differently will be:

$P(D<0) = P[a\cos\theta\ D-((a\cos\theta 1- a\cos\theta 2) / \sqrt{\sigma_1^2 + \sigma_2^2}) < ((a\cos\theta 2- a\cos\theta 1) / \sqrt{\sigma_1^2 + \sigma_2^2}) ]$ where,

D = X – Y, the difference in time of particles A and B, this equation is applicable when particle A is faster than B. To determine this probability, the distribution of D is essential.

$X \sim N (a\cos\theta, \sigma 1^2)$ and $Y \sim N (a\cos\theta, \sigma 1^2)$. Thus,

$X-Y \sim N ((a\cos\theta 1- a\cos\theta 2, \sigma_1^2 + \sigma_2^2)$

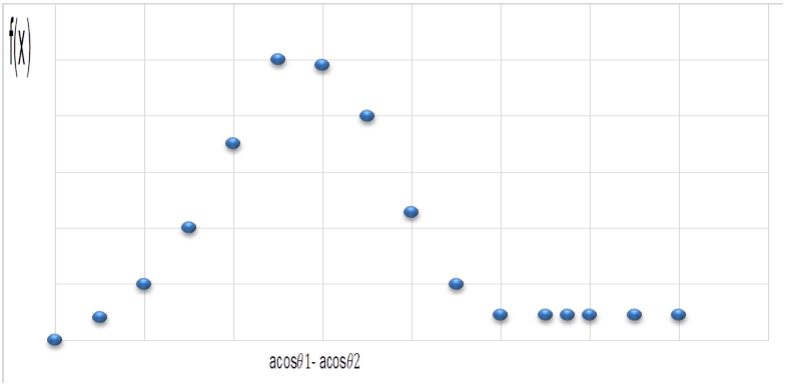


**Figure 11.** The collision probability of two particles normally distributed.

The curve, **Figure 11**, follows the normal distribution model with the parameters of mean and variance of [$a\cos\theta 1- a\cos\theta 2$]. This graph shows the probability of any two particles moving at a different speed. It is more likely that particle A would have collided first increasing the probability of collision. Many researchers have demonstrated that higher travelling speed leads to higher collision probability (4). Furthermore, improving the collision probability of the two or more particles can improve the probability of the reaction and improve the yield with less energy consumption.

## 4. Conclusion

The paper covers important aspects and presents the following points;

- Correlation between the kinetic energy and reaction rate.
- Also, probability of collisions has been analyzed.
- The best-fitted model obtained.
- An expression of the value of the frequency caused by the probability of the particles within the collision zone achieved.

In addition, the correlation of probability of the reactant and fraction of collision plays a significant role in determining how quickly a reaction occurs. It also illustrates the effect of activation energy on the rate of reaction obtained. As concentration of reactants increase, the probability of particle collisions rises, thereby typically increasing rate of reaction. The results showed that the number of collisions per unit area versus the reaction described obstacles as an energy barrier that must be overcome for the reaction to occur. An equation proposed to improve the probability of particles collision impacts on the reaction process.

## Conflict of interest

The authors declare no conflict of interest.

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