Journal of Science-FAS-SEUSL (2022) 03(02) 11-19
ISSN:2738-2184

Mathematical treatment using spectrophotometry to determine the unknown concentration of a random solution

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Abstract:
Concentration is one of the primitive aspects in chemistry, which describes the extent of abundance of a solute in a given solution. Determining the concentration of a solution that does not has a chemical formula and with unknown molecular weight is one amongst the difficult topics. In this study, we have analyzed the concentration of such solutions using a comprehensive mathematics along with Beer – Lambert law for the UV spectrophotometer results. Experimental studies were conducted using the standard solutions of Biochar, Coir, Wood bark and Sawdust those prepared by mixing the raw substrates with water at 1:2 ratio. The solutions were prepared using the specimens extracted from same *Coccus nucifera* tree to verify that the prepared concentrations of solutions would be in same range since each of them contains similar type of organic content. The objective of the study has been achieved by proving that the concentration found using this novel approach for each specimens are almost equal since the specimens are from same origin. A comprehensive understanding in finite integrals is compulsory to get proficiency with this method. Furthermore, this approach can be successfully used to find the concentration of any random solutions such as to find the concentration at a cup of morning coffee. The benefits of this novel model has vast scientific scopes in future at resolving several queries related to medical, commercial, scientific and industrial issues related with concentration of solutions.

Keywords: Concentration, Beer – Lambert law, UV spectrophotometer, finite integral

1. Introduction

Concentration is defined as the extent of the mixing of a particular substance with another substance. The concentration has a peak magnitude, beyond which a substance cannot be further dissolved. This is called the saturation phase. In terms of advanced chemistry, concentration can be termed as the abundance of a solute given as the ratio of total volume of the mixture. Studying the concentration is important to describe a chemical reaction, since it quantifies the ability of molecules to collide within the solution. Furthermore, it helps to determine the rate of reactions and the equilibrium features.

The concept of chemical concentrations has been recognized as one of the most difficult areas to learn, to teach and to implement (Novick and Menis, 1976). Past studies have formulated numerous ways to express the concentration in terms of molarity, mole fraction, molality, normality and the formality. Recent studies have also shown an extended utilization of modern technological devices to identify the concentration of solutions. The probability of success in using android smartphones to determine the concentration of the colored $NiSO_4$ solution to overcome the experimental drawbacks in colorimetric instruments have been studied using the data generation and RGB values (Irwansyah et al., 2018). Hence, mathematical computations have been worked out using the principles of mole and stoichiometry through mathematical treatment to find the Concentration of the solutions (Jadhav et al., 2019). There have been

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studies based on the concept of the effective concentration to represent the metal bioavailability in soils. In this method, the effective concentration was measured using Ethylenediaminetetraacetic acid (EDTA) extraction to find the concentration of Copper (Cu) in order to identify the most influential supply modes of soils (Zhang et al., 2001). The common feature in all these past studies was the utilization of a chemically known compound with its either chemical formula or its concentration. Therefore, finding the concentration has been confined to the compounds with known chemical attributes.

The aim of this research is to propose the most comprehensive way to find the concentration of an anonymous solution. The previously mentioned methods and their sub contents cannot be interpreted to identify the concentration of a domestically existing mixtures like milk coffee, drinking water, soft drinks and soil solutions. Because each of the previously mentioned methods are heavily relying on mole content, chemical formula, known percentage of ions and the stoichiometry. Although the concentration of a Coke can be stated in perspective through its constituents of Phosphoric acid (Coke and Diet., 2021), the entire concentration of a Coke bottle cannot be simply stated like the concentration of 200ml, 0.1moldm^{-3} HCl solution bottle. Therefore, it is a necessity of time to device a comprehensive method to find the concentration of a random solution.

The authors have used UV spectrophotometer, and used Beer Lambert law to determine the concentration six soil solutions. Specimen solutions were prepared under known proportions to empirically state that the six specimens are of same concentrations. It has been devised that, if the computed results provide same values for all six specimens then the methodology can be declared acceptable. A successful method to find the concentration of random solutions would contribute for humankind in various fields such as finding the viability to have a food or drink in terms of its impact on human health through finding its concentration and comparing with the acidity of Hydrochloric acid in the human digestive system. Hence several damages due to the intense exposure to domestic chemicals can be mitigated through determining their toxicity based on the concentrations. The primary objective of this study is to propose the mathematical model to model to quantify the concentration of a sample, for which its concentration is not measured previously or unknown. In this study, four heterogeneous solutions with empirically equal concentrations were prepared using organic wastes of Coir, Biochar, Wood bark and Sawdust those extracted from same Coconut tree (*Coccus nucifera*). The solutions were undergone for spectroscopic analysis and ultimately the numerical magnitudes of concentrations were determined using the proposed mathematical ideologies to verify the hypothesis.

2. Theory

1. Principle of UV – Visible spectroscopy

Spectroscopy is formed due to the interaction of matter with light. The purpose of authors to intend with the UV – Visible (Ultraviolet and visible) absorption spectroscopy is to calculate the attenuated quantity of light beam after it reflects or passes through the selected specimens. UV – Visible spectroscopy is complied with the absorption of ultraviolet light or visible light by chemicals. This absorption would result the formation of spectra, which is distinct. Spectrum is produced due to excitation and de-excitation of matter caused by its absorption of light. In this experimental scenario, electrons present in the chemical compound undergo for excitation from ground state. Furthermore, the amount of ultraviolet radiation can be stated as the difference in ground state energy and the excited state energy

2. UV – Visible spectroscopy and Beer – Lambert law

According to the Beer – Lambert law, the intensity rate of the beam decreases along the solution thickness is directly proportional with the concentration of the absorbing compound in the particular solution, and also directly proportional with the intensity of incident monochromatic radiation, during the incident of monochromatic light rays with a solution. From this law, it is understandable that the absorption of the radiation can be sophisticated with greater number of absorbing compounds capable to absorb light in specified wavelength.

The equation derived from the Beer – Lambert law is as follows:

$$A = \mathcal{E}.L.C$$

A = Absorbance
$\mathcal{E}$ = Molar absorptivity,
L = Length of the light path
C = Concentration
From the Beer – Lambert law,
Absorbance $A = \log (I_0/I)$ ⟶ **Eq. 1**
$I = I_0 e^{-\varepsilon L}$ (Linear attenuation equation)
$I_0 / I = e^{\varepsilon L}$
$\therefore \varepsilon L = \ln (I_0/I) = 2.303 \log (I_0/I)$ ⟶ **Eq. 2**
By substituting Equation (1) in Equation (2),
$\varepsilon = [2.303 \log (I_0/I)] / L$

$$\mathcal{E} = \frac{2.303A}{L}$$

L = Cuvette width
I_0 = influent UV intensity
I = effluent UV intensity

3. Methodology

The specimens were prepared by using the six candidates for growing mediums namely Bio char, Coir, Saw dust and Wood bark. The complete list of constituents for all the six specimens were unknown and such that the analytical finding of the concentration was seemingly impossible using the existing methods. Specimen solutions were prepared in 1:2 (v/v) ratio according to ASTM E70 standards. It was empirically stated usually that if same pH range of solutions (soils, suspensions and pigments) were prepared using identical solvents under 1-part solute: 2-part solvent, it would be approximately same concentrations. The reference blank used here is pure distilled water. The thicknesses of specimens were assumed to equal to the Length Cuvette which was 1cm for all the cases. Since all the specimens were extracted from the same coconut tree (*Coccus nucifera*), the concentrations should almost be identical. pH values of the specimens were determined to be as follows:

Table 1: pH of the test specimen solutions

Heterogeneous solution	**Trial 01**	**Trial 02**	**Trial 03**	**Mean**	**Rank**
Wood bark	7.57	7.61	7.55	7.577	2
Saw dust	7.19	7.21	7.28	7.227	6
Coir	7.39	7.39	7.37	7.383	4
Biochar	8.03	7.99	7.95	7.990	1

Table 2: EC of the test specimen solutions

Heterogeneous solution	**EC**
Saw dust (60:40)	1153.48

Coir (60:40)	860.962
Wood bark (60:40)	975.484
Bio char (60:40)	1184.31

4. Results and discussion

1. Coir

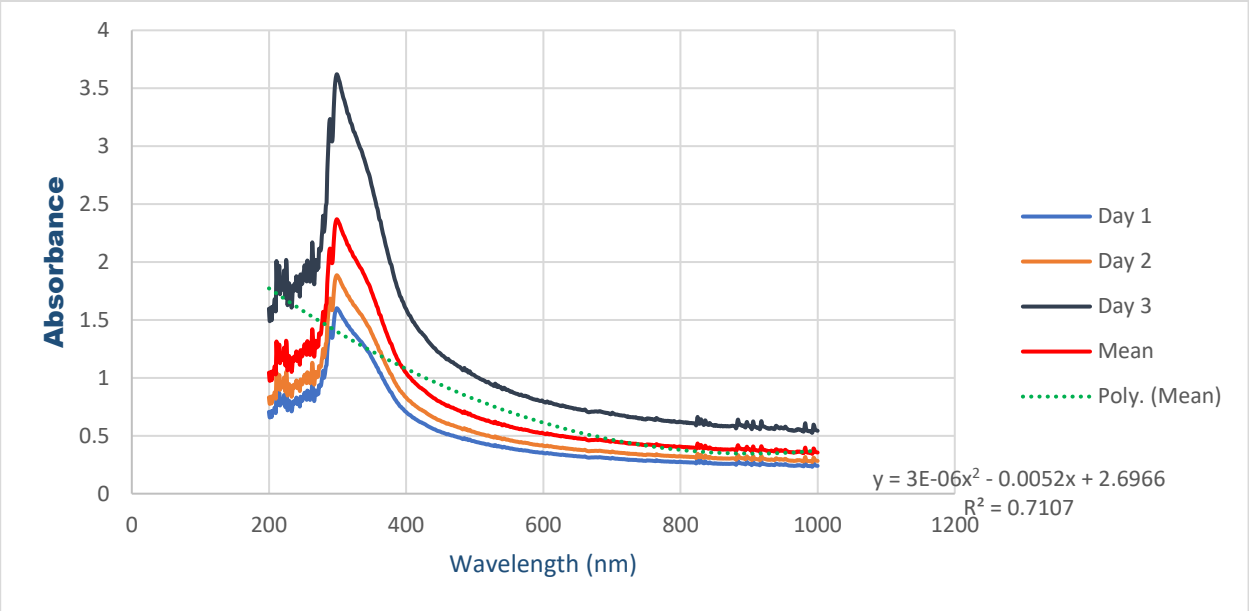

Figure 1: Absorbance curve of Coir solution

Equation of mean line $y = 3x\ 10^{-6}x^2 - 0.0052x + 2.6966$

Peak Area by using Gauss' Integrals (Weimer.,2002)

$$A_P = 0.5 \times \int_{200x\ 10^{-9}}^{1000x\ 10^{-9}} (3x\ 10^{-6}x^2 - 0.0052x + 2.6966)dx$$

$A_P = 1.079 \times 10^{-6}$

Corresponding wavelength from $y_{(x= 1.079x10^{-6})}$ = 634nm

For this wavelength Corresponding Peak Absorbance from Figure 1 $A_{b1} = 0.490$

$$\varepsilon = \frac{2.303A}{L} = \frac{2.303 \times 0.490}{1} = 1.128\ M^{-1}cm^{-1}$$

By Beer Lambert equation, $A = \varepsilon.L.C$

$$\therefore \quad C_{coir} = \frac{A}{\varepsilon L} = \frac{0.490}{1.128\ M^{-1}cm^{(-1)} \times 1cm} = 0.4344M$$

2. Sawdust

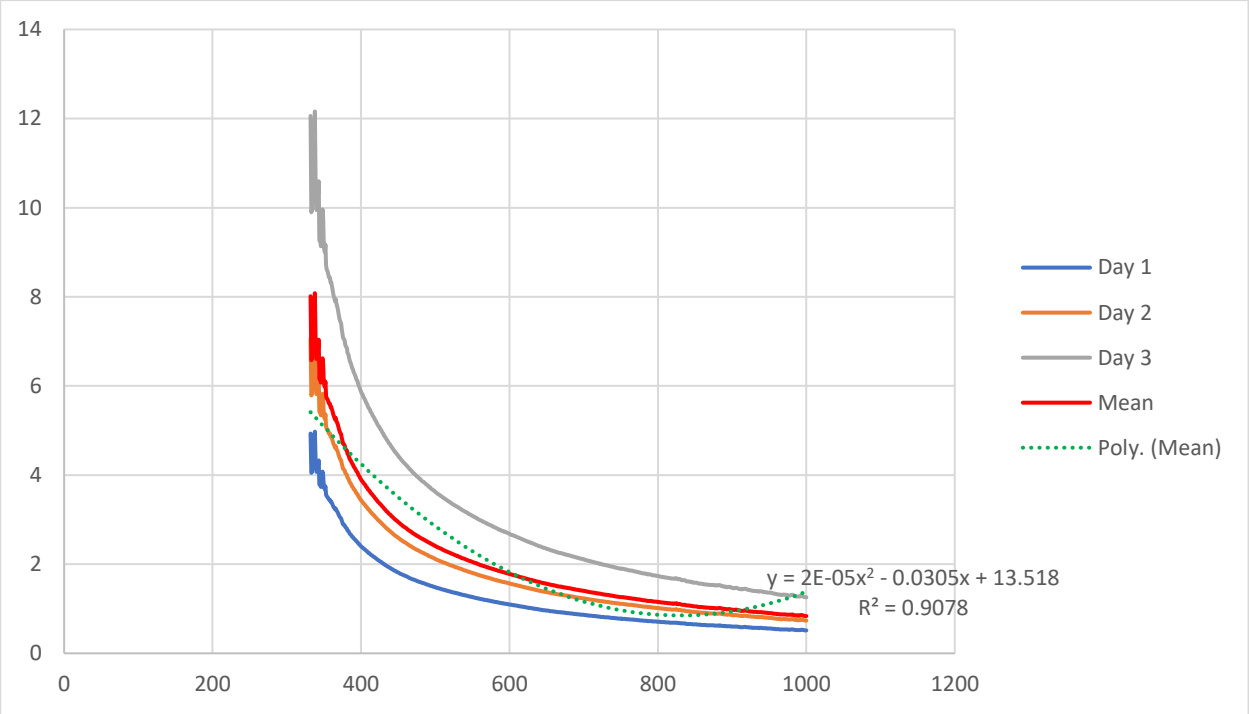

Figure 2: Absorbance curve of Sawdust solution

Equation of mean line $y = 2x\ 10^{-5}x^2 - 0.0305x + 13.518$

Peak Area by using Gauss' Integrals

$$A_P = 0.5 \times \int_{332x\ 10^{-9}}^{1000x\ 10^{-9}} (2x\ 10^{(-5)}\ x^2 - 0.0305x + 13.518)dx$$

$A_P = 4.515 \times 10^{-6}$

Corresponding wavelength from $y_{(x= 4.515x10^{-6})}$ = 629nm

For this wavelength Corresponding Peak Absorbance from Figure 1 $A_{b2} = 1.5$

$$\text{Ɛ} = \frac{2.303A}{L} = \frac{2.303 \times 1.5}{1} = 3.455\ M^{-1}cm^{-1}$$

By Beer Lambert equation, $A = \text{Ɛ}.L.C$

$$\therefore \quad C_{\text{Saw dust}} = \frac{A}{\text{Ɛ}L} = \frac{1.5}{3.455\ M^{-1}cm^{(-1)} \times 1cm} = 0.4342M$$

3. Wood bark

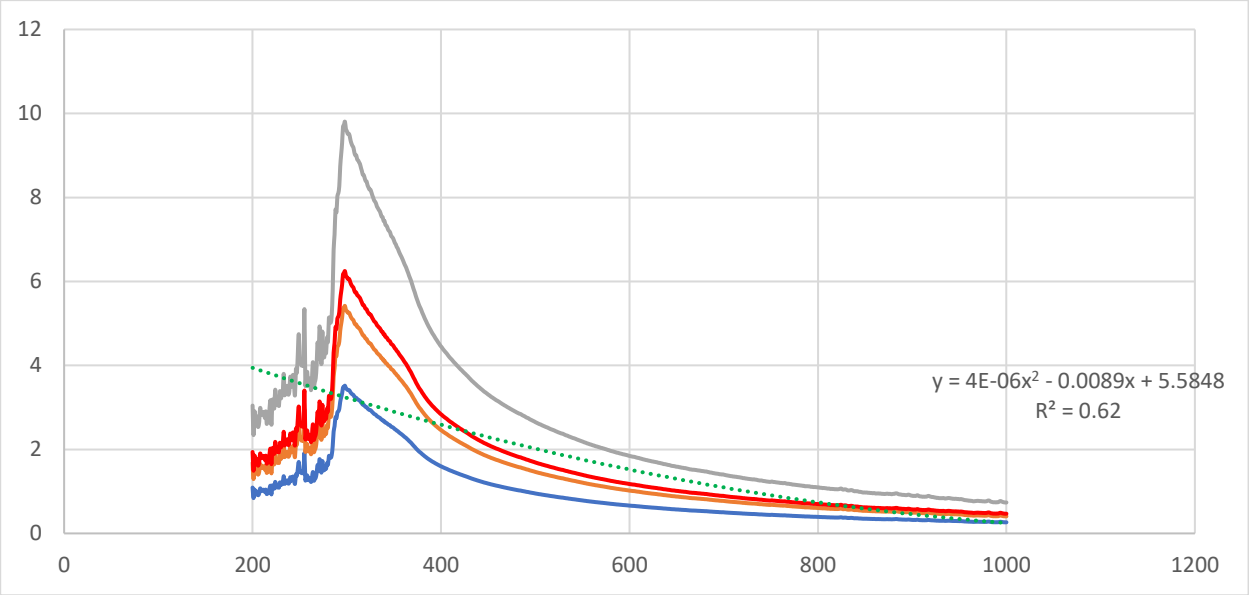

Figure 3: Absorbance curve of Wood bark solution

Equation of mean line $y = 4x\ 10^{-6}x^2 - 0.0089x + 5.5848$

Peak Area A_P by using Gauss' Integrals

$$A_P = 0.5 \times \int_{200x\ 10^{-9}}^{1000x\ 10^{-9}} (4x\ 10^{-6}x^2 - 0.0089x + 5.5848)dx$$

$A_P = 2.234 \times 10^{-6}$

Corresponding wavelength from $y_{(x= 2.234x10^{-6})}$ = 600nm

For this wavelength Corresponding Peak Absorbance from Figure 1 A_{b3}= 1.176

$$\text{Ɛ} = \frac{2.303A}{L} = \frac{2.303 \times 1.176}{1} = 2.708\ M^{-1}cm^{-1}$$

By Beer Lambert equation, $A = \text{Ɛ}.L.C$

$$\therefore \quad C_{\text{Wood bark}} = \frac{A}{\text{Ɛ}L} = \frac{1.176}{2.708\ M^{-1}cm^{(-1)} \times 1cm} = 0.4343M$$

4. Bio char

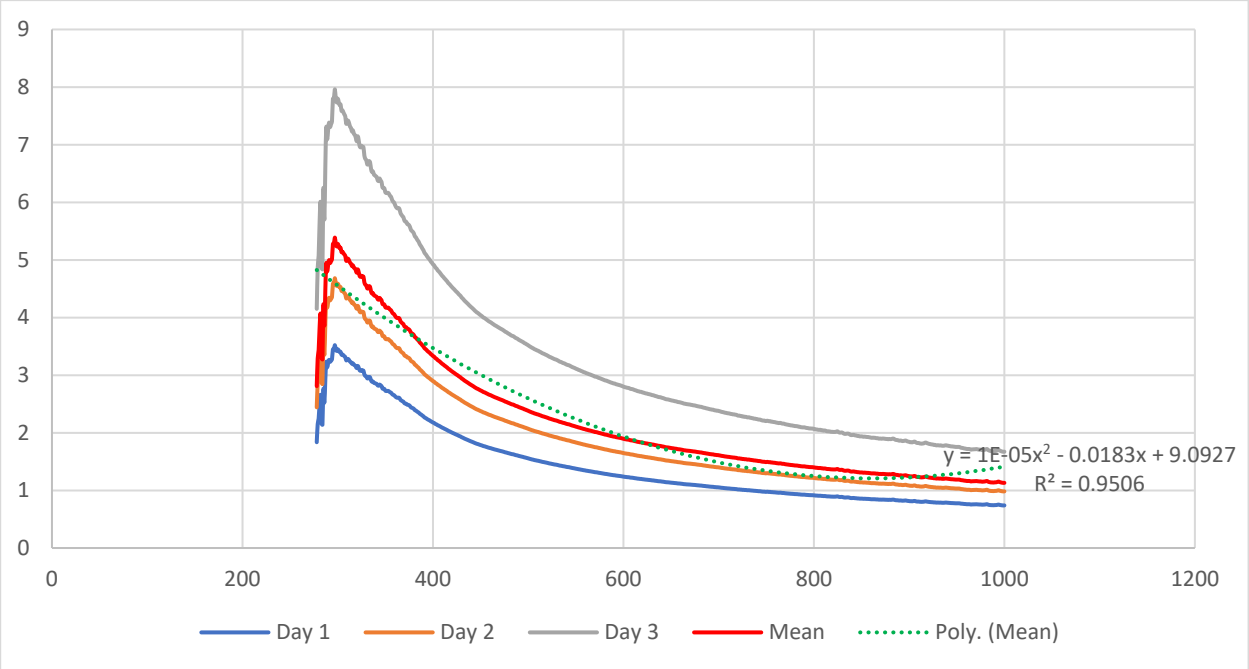

Figure 4: Absorbance curve of Bio char solution

Equation of mean line $y = 1x\ 10^{-5}x^2 - 0.0183x + 9.0927$

Peak Area by using Gauss' Integrals

$$A_P = 0.5 \times \int_{278x\ 10^{-9}}^{1000x\ 10^{-9}} (1x\ 10^{-5}x^2 - 0.0183x + 9.0927)dx$$

$A_P = 6.565 \times 10^{-6}$

Corresponding wavelength from $y_{(x= 6.565x10^{-6})}$ = 639nm

For this wavelength Corresponding Peak Absorbance from Figure 1 $A_{b4} = 1.771$

$$\varepsilon = \frac{2.303A}{L} = \frac{2.303 \times 1.771}{1} = 4.079\ M^{-1}cm^{-1}$$

By Beer Lambert equation, $A = \varepsilon.L.C$

$$\therefore \quad C_{Bio\ Char} = \frac{A}{\varepsilon L} = \frac{1.771}{4.079\ M^{-1}cm^{(-1)} \times 1cm} = 0.4342M$$

When all the results are approximated for 3 decimal places,

$C_{Coir} = C_{Saw\ dust} = C_{Wood\ bark} = C_{Biochar} = 0.434M$

The experimental readings were recorded at three days to get the most rationalized magnitudes for Absorbance data since the proceedings were based on mean values. Furthermore, this approach would have mitigated the influence of various discrepancies occurred at the experiment scenarios. During the preliminary works, it was assumed that the concentrations of all solutions might be identical. Because, all the specimens are entitled with majority of soil aggregates. Since the worldwide pH range of soils exist from 5.0 to 9.0 (Alkali or Alkaline | Dirt Diggers Digest, 2021) the pH magnitudes were separately measured to find whether the specimens would exhibit acidic or alkaline properties. The pH results in this experiment have shown that all specimens have pH values greater than 7.0 therefore the specimens are considered alkaline and buffered at these higher pH values.

Distilled water was selected to be the blank in UV spectrometer tests. Distilled water does not

contain any ions. Therefore, it was strongly evident that ions participating in chemical reactions and ionic exchanges are entirely from the main source of specimens. The solutions were prepared under extreme conditions for 24 hours in order to prepare clean specimens. It has facilitated the spectrometer readings with clean wavelengths based on their ionization intensity. Since there were no any previous thermal conductivity studies conducted in this aspect, the authors were unable to compare the results with any preceding studies. Several reasons can be given for scarcity of research on concentration of random solutions where its number of moles or chemical formula are unknown. The concentrations found for all specimens in this experiment are same, thus satisfies the hypothesis. Furthermore, this method of mathematical approach with UV – Visible spectrophotometer could be effectively used to find the concentration of any available solutions.

5. Conclusion

This laboratory experiment illustrates a simple way to determine the concentration of any solutions available in commercial and industrial sites using the spectrophotometer and Beer – Lambert law. The successful implementation of this test indicates that the spectrophotometer could be used for determining the concentration of an unknown sample using standard preparation of solution. The data analysis of this experiment is straightforward, quick and simple. The experiment setup could be utilized to get best results for the concentration of solutions domestically found at home: coffee, soft drinks and pharmaceuticals. Overall results of experiments have shown that there would be potential for using this test to find the viability of using compounds with complying with human safety.

6. Acknowledgements

My special thanks go to my ever-loving parents for spending on my studies and for giving me space and support to complete this research project. I would like to express my gratitude for the following personals:

1. Dr. AMM. Majeed Dean, Faculty of Bio Systems Engineering, SEUSL
2. Dr. SM. Junaideen, Dean, Faculty of Engineering, SEUSL
3. Dr. Janaka Perera, Department of Civil Engineering, SLIIT

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