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Numerical Simulation of the Spectroscopic Properties of the Laser Dye for Low Concentrations

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ABSTRACT

In the current study, a mathematical model using the MATLAB program was studied depending on the logistic power peak function to simulate the change in the absorbance with the different values of the concentrations of Rhodamine B. There are five parameters that have been applied to the concentration values of this laser dye that are proposed by the logistic power peak function of the seventh degree. To measure the absorption measurements, a range of concentrations from $4.7x10^{-7}$ to $3.76x10^{-6}$ M was prepared from Rhodamine B and dissolved in deionized water with a peak absorption at 556 nm. A JASCO V-630 spectrophotometer was used to record the spectra of the dye. The intensity is detected using a silicon photodiode (S1337). The results were found that the suggested function approved the relationship between the absorbance and the values of the concentrations with a significant accuracy depending on the high values of the correlation coefficients between the approximated original data which were determined more than 99.2%. The advantages of this function represent by providing parameters, which are used to describe the mathematical processes with high-resolution property profiles.

KEYWORDS: Laser dye, low concentrations, molecular physics.

الخلاصة

في الدراسة الحالية، تم دراسة نموذج رياضي باستخدام برنامج الماتلاب بالاعتماد على دالة Logistic power peak function لمحاكاة العلاقة بين قيم الامتصاص مع مدى من التراكيز المنخفضة للصبغة الليزرية رودامين B. تم استخدام خمسة عوامل رئيسية بالاعتماد على الدالة اعلاه وبالرتبة السابعة وتطبيقها على قيم تراكيز هذه الصبغة الليزرية. لتحديد القياسات العملية لاطياف الامتصاص، تم تحضير مدى من التراكيز المولارية من 4.7×10^{-7} والى 3.76×10^{-6} من صبغة الرودامين B المذابة بالماء اللايوني وتم تسجيل اعلى قمة له في 556nm وايضا تم الاعتماد على جهاز JASCO V-630 spectrophotometer لتحديد هذا الاطياف والكشف عنها بواسطة silicon photodiode (S1337). من خلال النتائج التي تم الحصول عليها في الدراسة الحالية ، تم تسجيل ملائمة تطبيق الدالة المقترحة على طبيعة العلاقة بين قيم الامتصاص والتراكيز المحضرة عمليا وبنسبة عالية من الدقة وذلك بالاعتماد على قيم معامل التصحيح بين القيم الاصلية المقربة والتي قد وصلت الى **99.2%**. ولهذا فان دالة Logistic power peak function لها فائدة كبيرة في الحسابات النظرية وذلك من خلال تجهيزها للعوامل المطلوبة وبدقة عالية جدا.

INTRODUCTION

Theoretical study in geometry plays an important role in many practical applications, especially in physics, as it works on proposing simulation and mathematical functions of systems in practice [1-3]. When the atoms interact with different forms of energy leads to three emissions, phenomena, fluorescence, and absorption, and they deal with the spectroscopy area which interests in the study of the energy exchange between matter and electromagnetic radiation [4, 5]. Regarding the absorption spectroscopy, has been developed and it has a big role in a wide range of analytical techniques [6], as a result, it is considered an important technique to determine the spectroscopic properties of the chemical compounds depending on the concentration and this leads to determine the kinetics of reactions such as the stopped-flow technique to measure the biological reactions [7]. The most configuration of a spectrophotometer represents by the single beam arrangements which depend on the light beam passing through a sample cell to the detector. To determine the spectroscopic properties of the material depending on the absorption measurements of the samples, the laser dye is considered the best choice for studying these characteristics due to their strong absorption in the visible region of the spectrum [8]. Rhodamine B is

a hydrophilic xanthene dye. It is considered an important dye due to its advantages such as broad fluorescence in the visible region of the electromagnetic spectrum, high absorption coefficient, high quantum yields high photostability [9-12]. As a result, it has many applications in different fields of technology and science especially with low concentrations factor because it leads to reduce the cost, energy and waste [13,14].

Daway *et al.* (2014) [15] investigated the use of the lognormal function to determine the negative chromatic dispersion curves in a highly dispersive dual-concentric core pure silica photonic crystal fiber (PCF). This investigation depends on a simulation process for the experimental results which were recorded by the plane wave expansion (PWE) method. The use of the lognormal function was matched well with the experimental results, and this study proved that can evaluate PCF performance using a theoretical model by measuring negative dispersion and dispersion bandwidth with more accuracy. In 2020, Al-Arab *et al*. [16] established a theoretical model to estimate some photo-physical processes in fluorescein dye which was mixed with titanium dioxide nanoparticles depending on the experimental measurements of fluorescence spectra measurements. The model was based on curve fitting using the Logistic Power Peak function. The obtained results stated that this model had matched the experimental shapes. In another hand, Myers *et al* (2020) [17] used Parametric and non-parametric (Pearson Type IV (PIV) and the logistic power peak (LPP) functions) to evaluate continuous soil profile characteristics. In this work, the authors submitted the use of asymmetric peak functions to model complex and anisotropic soil depth profiles. The advantages of this function represent by providing parameters, to describe pedogenic processes, as well as, demonstrating the application of these functions to record high-resolution soil property depth profiles. Moreover, Al-Arab *et al*., (2021) [18] estimated the theoretical models of photophysical processes using the absorption and fluorescence spectral of Fluorescein dye-doped by Ag nanoparticles in distilled water. This model depends on the curve fitting using Logistic Power Peak (LPP) function and they have excellent matching shapes with the experimental shapes.

MATERIALS AND METHODS

To determine the absorption measurements, a range of concentrations from from $4.7x10^{-7}$ to $3.76x10^{-6}$M was prepared from 0.15g of Rhodamine B(Sigma, Aldrich, UK), and dissolved in 100 mL deionized water with a peak absorption at 556 nm. After that, the concentrations were prepared by taking 100, 200, 300, 400, 500, 600, 700, 800, and 900 mL from the stock solution respectively, and then dissolved in 100 mL of deionized water. To record the spectra, A JASCO V-630 spectrophotometer was used (see Figure 1). It is used to record the absorption spectrum of Rhodamine B in a wavelength range from 400 to 600nm. The light source is represented by the A deuterium and Halogen lamps. The principal work depends on the light that is entered into the grating to reduce the wavelength range of the light. After that, the light is divided into two beams, the first beam passes through the reference cell, and the other beam passes through the sample cell. The intensity is detected using a silicon photodiode (S1337) (JASCO spectrometer sheet).

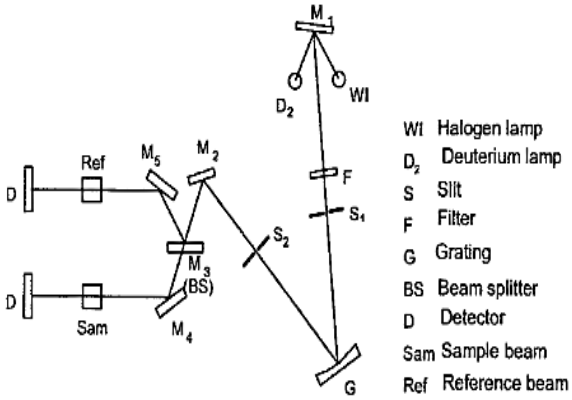

Figure 1. The working principle of the JASCO spectrometer.

RESULTS AND DISCUSSIONS

In this study, it was directed to find mathematical criteria to study the relationship between wavelength and absorbance depending on the various parameters of the concentrations of Rhodamine B in order to find a mathematical model to unify all parameters.

The best model that simulates this relationship has been proposed based on the logistic power peak function, which was chosen because it is considered the best approximation of the data and with the least error, the study was conducted

to find out the degree of correlation between actual and approximate data based on this function that is given by:

$$y = a + \frac{b(1+n)^{\frac{-e+1}{e}} n(e+1)^{\frac{e+1}{e}}}{n} = exp\left(\frac{x + dln(e) - c}{d}\right)$$

Where y denotes the absorbance, x denotes wavelength in (nm) and a,b,c,d, and e represent the parameters of our function (Table 1). These coefficients are considered the functions of the concentration of the solution (Figure 2) and they belong to the relationship which is drawn in a theoretical form for experimental data for seven parameters (Figure 3). In this function, there are five parameters as in Table 1 obtained when the error was as small as possible between the approximate and actual data in that function.

Table 1. Values of parameters a, b, c, d, and e for the logistic power peak function at different concentrations.

Parameters	4.70E-07	9.39E-07	1.41E-06	1.88E-06	2.35E-06	2.82E-06	3.29E-06	3.76E-06
a	0.001634	0.001634	0.003112	0.003466	0.003931	0.004711	0.00532	0.005826
b	0.052549	0.052549	0.162288	0.210433	0.264673	0.312591	0.366703	0.423397
c	554.8796	554.8796	554.8581	554.8717	554.8473	554.8437	554.8456	554.8648
d	-5.70126	-5.70126	-5.76301	-5.78221	-5.78775	-5.79458	-5.78533	-5.79287
e	4.456058	4.456058	4.396098	4.383709	4.386577	4.388898	4.391133	4.392019

Figure 2 illustrated the Relation between each parameter (a,b,c,d, and e logistic power peak function) and the values of concentrations by using a seventh-degree polynomial Table 2 illustrated the value of these coefficients, from these figures we can see all of them have a correlation coefficient of 1, which is an exact match between the approximate and the original value.

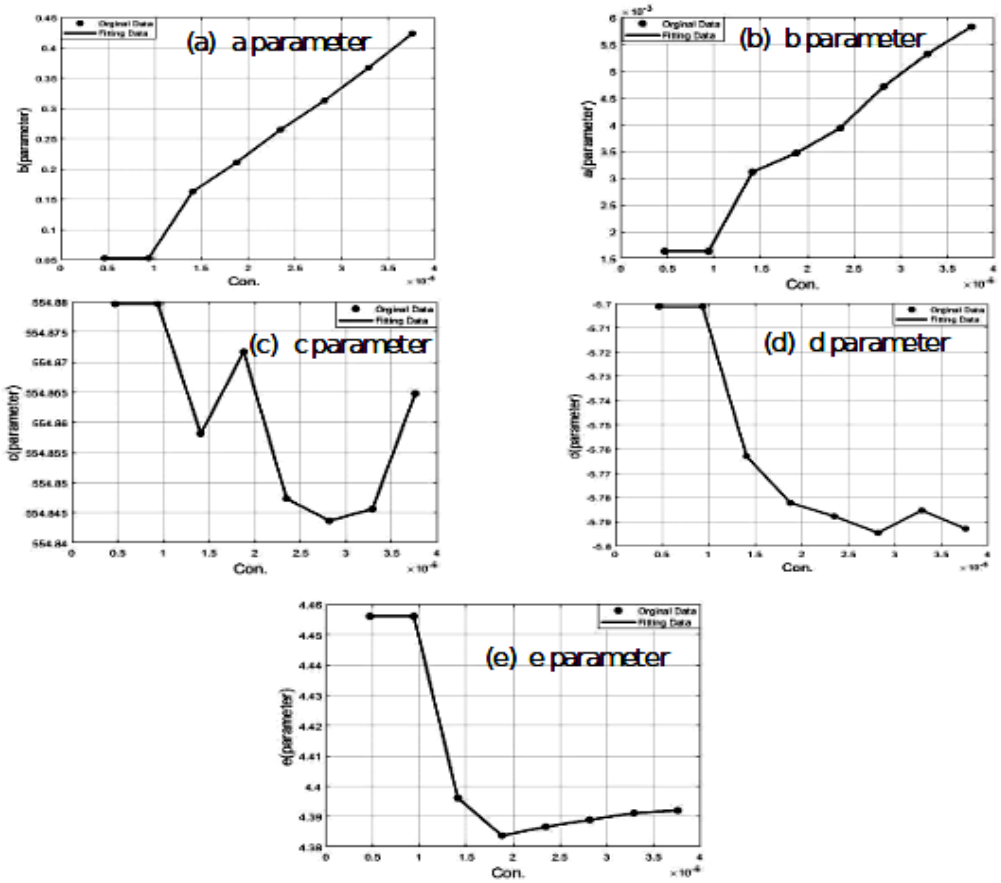

Figure 2. The original data and the approximated data for each parameter in the simulation function by using a seventh-degree polynomial.

Figure 3 represents a comparison between the original data and the approximated data based on the function (logistic power peak function) at different concentration values through this figure, we notice the extent of the good representation and the high conformity of the proposed approximation function, this behavior was reflected in the values of the correlation coefficients that approached more than (99.2%), according to the table for each chart in Table 3.

Table 2. The relationship between the values of absorbance at different values of concentrations.

Polynomial coefficients	a	b	C	d	e
a7	-1.7E+38	-2.2E+40	3.02E+40	1.04E+39	5.39E+39
a6	2.88E+33	3.47E+35	-4.6E+35	-3E+34	-9.1E+34
a5	-2E+28	-2.2E+30	2.84E+30	2.9E+29	6.38E+29
a4	7.57E+22	7.65E+24	-9.2E+24	-1.3E+24	-2.4E+24
a3	-1.6E+17	-1.5E+19	1.69E+19	3.3E+18	5.1E+18
a2	1.85E+11	1.63E+13	-1.7E+13	-4.3E+12	-6.1E+12
a1	-105971	-8944374	8808874	2712255	3551538
ao	0.023834	1.877486	553.1755	-6.29968	3.701384

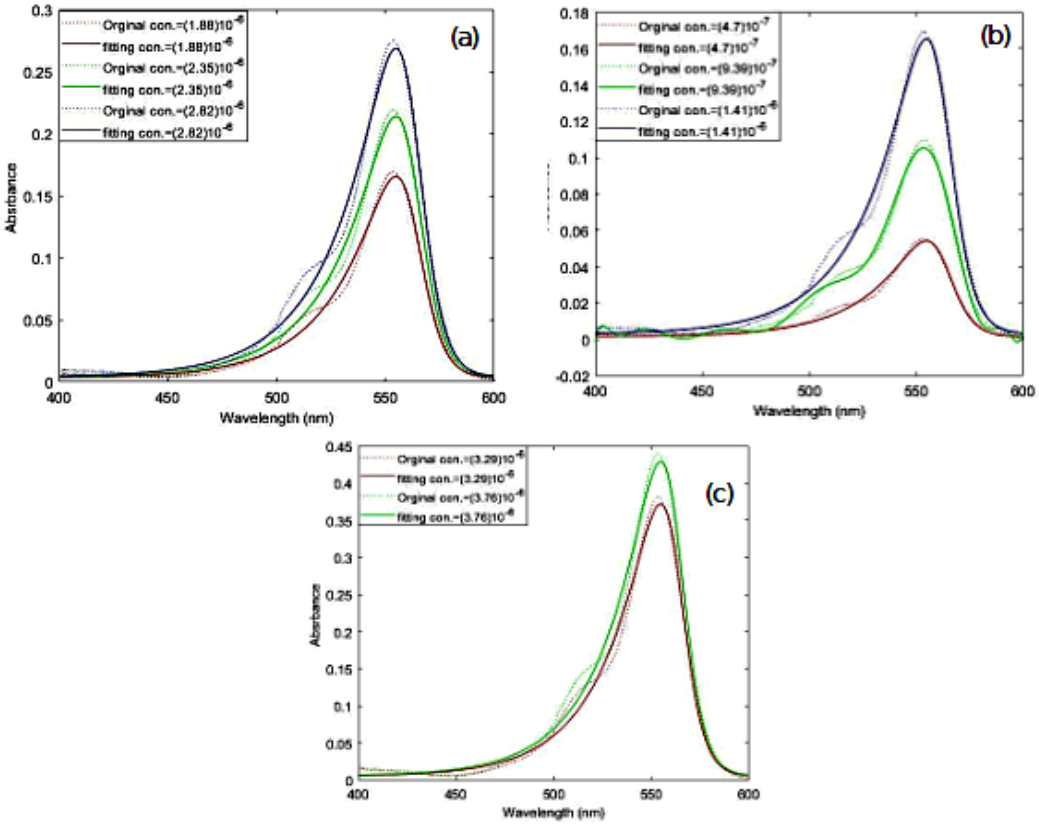

Figure 3. The relationship between the values of absorbance at different values of concentrations at (a) (1.88, 2.35 & 2.82) ×10-6, (b) (4.7,9.39 & 14.1) ×10-7 and (3.29 & 3.76) ×10-6 for the original and fitting data.

Table 3. Correlation coefficients between the approximate and the original data at each concentration value.

Concentration (M)	Pearson Correlation coefficient
$4.7x10^{-7}$	0.993
$9.39x10^{-7}$	0.992
$14.1x10^{-7}$	0.993
$18.8x10^{-7}$	0.992
$23.5x10^{-7}$	0.992
$28.2x10^{-7}$	0.993
$32.9x10^{-7}$	0.992
$37.6x10^{-7}$	0.993

CONCLUSIONS

In this study, a mathematical model was proposed that simulates the relationship between absorbance and concentrations at different values of concentration. A function (logistic power peak function) has been proposed to simulate this relationship, which contains five parameters that have been linked to the concentration values by proposing a function of the seventh degree. By analyzing the results, it was found that the proposed

function succeeded in representing this relationship with very high accuracy, which means that the value is close to one, as the correlation coefficients between the approximated original data were higher than 99.2%.

Disclosure and conflict of interest: The authors declare that they have no conflicts of interest.

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