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Application of Soft Computing for Evaluation of Bismuth Adsorption onto Coconut Skin in Kinetic Aspects

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Abstract

Bismuth has been on sale since ancient times but was sometimes confused with lead, until 1753 when it was distinguished from lead. The origin of the word bismuth is not clear. It may be derived from the Arabic word "biasemutum" (similar to kohlrabi) or the German words Weisse Masse and Wismuth meaning white mass, which became the Latin, word Bisemutum in the 16th century. Isolation and measurement of small amounts of bismuth are of particular importance in two ways, including environmental hazards and industrial applications. This study investigates the synthetic parameters of the process of adsorption of bismuth by coconut skin. In the first step, the order of the bismuth adsorption synthetic reaction was obtained based on nonlinear regression analysis, and then the reaction constant-coefficient was calculated using a combination of MATLAB and GA Simulink environment. The results and calculations showed that the relevant reaction which is quadratic and the constant coefficient of bismuth adsorption reaction is equal to 0.0076 L\mg.h.

Keywords: Bismuth • Coconut skin • Adsorption synthetic • Nonlinear regression • Simulink • Genetic algorithm

Introduction

Bismuth is a weak, trivalent, white crystalline, heavy and brittle metal with a slight pink tinge and is chemically similar to arsenic and antimony. Bismuth is the most magnetic of all metals and has less thermal conductivity than all elements except mercury. Bismuth compounds are used in cosmetic, pigment and medicinal manufacturing [1]. Bismuth has unusually low toxicity compared to other heavy metals, and bismuth alloys have been used as substitutes for lead since lead toxicity was identified in humans. However, it should be noted that bismuth itself can lead to many acute and chronic epidemiological effects. Therefore, different adsorbents and methods are used to remove or pre-concentrate bismuth from water and wastewater sources. Madrakian et al. [2] used a fast, accurate and sensitive method based on spectrophotometry to measure bismuth ions. In this method, bismuth ion is adsorbed on the activated carbon surface after reacting with thiourea and bromide ion in an acidic environment. After concentrating the complex, it is absorbed by a solution of bromide ion in dimethylformamide solvent and measured at 375 nm. The results showed that the calibration curve for measuring bismuth ion is in the range of $1x10^{-7}$-$1.5x10^{-7}$ mol/L and its detection limit is $8x10^{-10}$ mol/L. Also, the effect of other disturbing ions on the bismuth ion absorbance was studied and finally this method was used to measure very small amounts of bismuth in aqueous samples. Afkhami et al. [3] also used cloud point extraction and spectrophotometric measurements to measure small amounts of bismuth. In this method, after mixing the bismuth ion with the mixing agent of red bermogallol, it was extracted in 114X ion-ion micelles surfactant medium. By optimizing various parameters that affect the extraction efficiency, it was found that the calibration curve of bismuth measurement is linear in the range of 4.6-120 µg/L and the detection limit of its measurement is 2 micrograms per liter. Also, the disturbance effect of other ions was investigated and finally, this method was used to pre-concentrate and measure bismuth in urine samples. Zanavaras et al. [4] used a flow injection method with a spectrophotometric detection system to measure small amounts of bismuth ions. In this method, methylene blue has been used as a mixing agent with bismuth, and after the formation of the methylene blue-bismuth complex; the color intensity was measured at a wavelength of 548 nm. Parameters affecting extraction efficiency were studied and it was found that under optimal conditions the calibration curve of bismuth measurement is linear in the range of 0-75 mg/L. Finally, this method was used to measure bismuth in drug samples and to evaluate the accuracy of the method; the results were compared with results obtained from the flame atomic absorption device. Rastegarzadeh et al. [5] used a liquid-liquid extraction method based on scattering and ultraviolet-visible spectrophotometric measurement system to pre-concentrate small amounts of bismuth. In this method, after the complexion of bismuth with iodide ion, the ionic complex of bismuth-iodide is formed; this becomes non-ionic after reaction with methyl triactylammonium chloride and is extracted in carbon tetrachloride solvent. By optimizing different parameters affecting extraction efficiency, it was found that the calibration curve of bismuth measurement is linear in the range of 5-4 micrograms per liter and has a detection limit of 1.6 micrograms per liter. Finally, this method was used to measure bismuth ions in tablets and blood serum samples. Due to its high selectivity and the availability of a flame atomic absorption device, this technique is widely used to measure bismuth. In 2015, Chamsaz et al. [6] used a liquid-liquid dispersion microextraction method based on ion-pair formation and a graphite furnace atomic absorption measurement system to pre-concentrate very small amounts of bismuth. In this method, thiocyanate ion was used to form an anionic complex with bismuth, and after reaction with the cationic surfactant steel pyridinium chloride, the complex was ionized and extracted in carbon tetrachloride extracting solvent. Various parameters affecting the extraction efficiency were studied and in optimal conditions, it was found that the calibration curve of bismuth measurement is in the range of 0.8-3 micrograms per liter. Finally, this method was used to measure very small amounts of bismuth in aqueous and serum samples. Shemirani et al. [7] used the cloud point extraction method to pre-concentrate small amounts of bismuth. In this method, after mixing with di-tizone ligand, bismuth ion is extracted in Michelle Triton 114 X-medium. Also 20 µl is injected and measured into the graphite furnace atomic absorption device after dilution by tetrahydrofuran solvent. When parameters affecting the extraction efficiency were optimized, results showed that the calibration curve of bismuth measurement is linear in the range of 0.4-0.6 µg/L and the standard deviation of bismuth measurement is less than 5%. Finally, this method was used to pre-concentrate and measure small amounts of bismuth in aqueous and biological samples (blood and hair serum). Tekman et al. [8] used solid phase extraction method and atomic

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absorption measurement system of graphite furnace in order to pre-concentrate and measure small amounts of bismuth, lead and nickel. In this method, a syringe containing silica gel modified with 3-aminopropyl trimethoxysilane was used as the adsorbent. After adsorption, the ions were adsorbed by a decomposition column with HCl 2 mol/L solution and injected into a graphite furnace atomic absorption device for measurement. Shakerian et al. [9] used solid phase extraction method and hydride production measurement method for pre-concentration and measurement of small amounts of bismuth. In this method 2-mercaptobenzothiaz placed on the surface of alumina coated with sodium dodecyl sulfate, which traps bismuth ions, used as the decomposition column. The bismuth ions are then adsorbed by a 2 mol/L hydrochloric acid solution containing thiourea and transferred to the reduction cell to form hydride and reduced by the addition of sodium borohydride. By optimizing different parameters, it was determined that the calibration curve of bismuth measurement is linear in the range of 40-1250 ng/L and the standard deviation is 2.3%. Finally, this method was used to measure small amounts of bismuth in different water samples.

In a fundamental study, Chaudhari [10] also removed bismuth from water sources using coconut shells. It also evaluated the chemical kinetics at different times. This study aims; (i) first, using nonlinear regression relations determine the bismuth adsorption reaction order (based on Chaudhari research) and then (ii) calculate the bismuth adsorption reaction constant using a combination of MATLAB software simulation environment and fixed genetic algorithm.

Materials and Methods

Bismuth Adsorption Using Coconut Shell

As mentioned earlier; Chaudhari provided a method to remove bismuth ion (Bi+3) using the coconut shell. Curves regarding the capacity and reaction kinetics of bismuth adsorption by coconut shell are shown in (Figures 1, 2).

Calculating the Order of Adsorption Reaction

To calculate the order of the chemical reaction, regression analysis of changes in the remained bismuth concentration over time was used as described in (Table 1).

Determination of Bismuth Adsorption Kinetic Coefficient Using a Combination of Simulink and Genetic Algorithm

There are several methods for analyzing a differential equation; In this study, the simulation of ODE 45 method in MATLAB 2013b Simulink environment and optimization of the total squared error have been implemented using a genetic algorithm (GA) (Figure 3) [11].

In the next step, the initial values for the synthetic coefficients of each reaction are considered and the difference between these values and the coefficients calculated from the real measurements is optimized by the genetic algorithm using the cost function of the total squared error.

Genetic algorithm ⟶ min $(Ro\text{-}Rd)^2$

Initial population = 50

Number of iteration = 50

Mutation rate = 0.2

Crossover probability = 0.8

Results and Discussion

At the beginning of the analyzes in this section, the data depicted in Figure (2) were separated by Extraction (x-y) software, and the initial calculations of the zero, first, and second reaction order was performed, the results of which are summarized in (Table 2). Also, diagrams related to the distribution of residual concentration over time in reactions with orders of zero, first, and second are shown in (Figures 4-6) respectively.

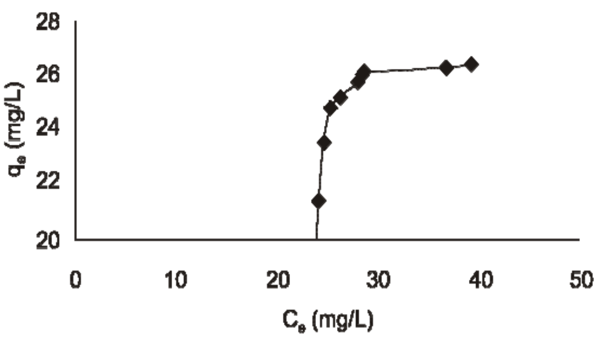

Figure 1. Absorption capacity curve relative to the equilibrium concentration of bismuth by coconut shell.

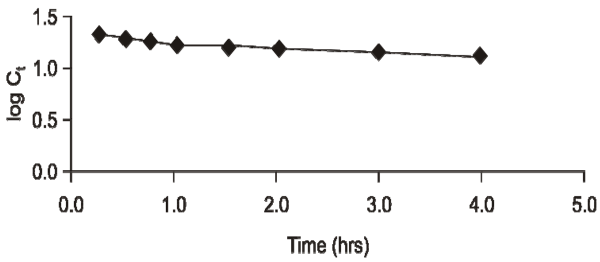

Figure 2. Bismuth kinetic curve by coconut shell absorber.

Table 1: Nonlinear regression analysis of kinetic changes in bismuth ion concentration to determine the order of adsorption reaction.

Details	Statistical analysis steps
Regression analyzes and R2 coefficient for (c – t) graph are studied in this section.	Zero-order control
Regression analyzes and R2 coefficient for (Ln(c) –t) graph are studied in this section.	First-order control
Regression analyzes and R2 coefficient for (Ln(c) –t) graph are studied in this section.	Second-order control
Reaction order is determined based on the maximum amount of R2 and minimum amount of SE	Reaction order determination

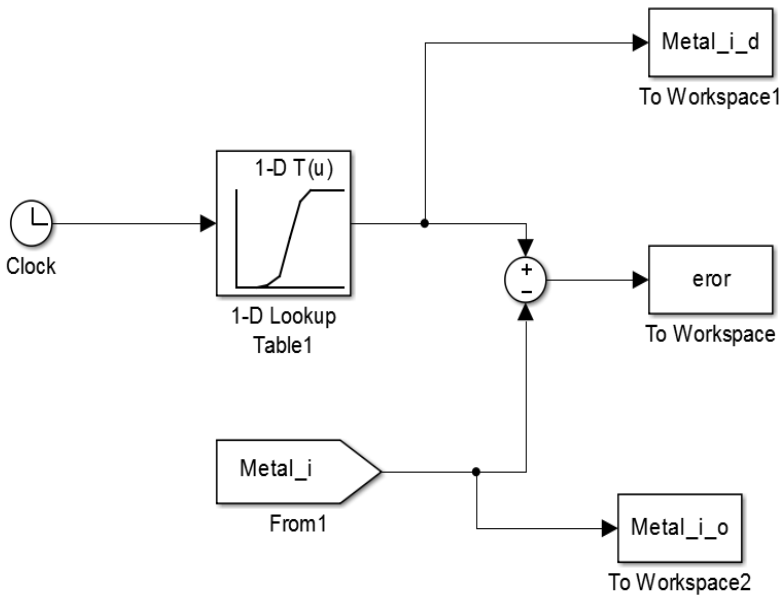

Figure 3. Differential equation analysis process using a combination of ODE45 method and genetic algorithm.

Table 2: Preliminary calculations of the reaction order of bismuth adsorption by coconut skin.

Time (hr)	Ct	ln [Ct]	1/Ct
0.27048	21.0899	3.04879	0.04742
0.53323	18.9574	2.94219	0.05275
0.7728	18.166	2.89955	0.05505
1.03555	16.3291	2.79295	0.06124

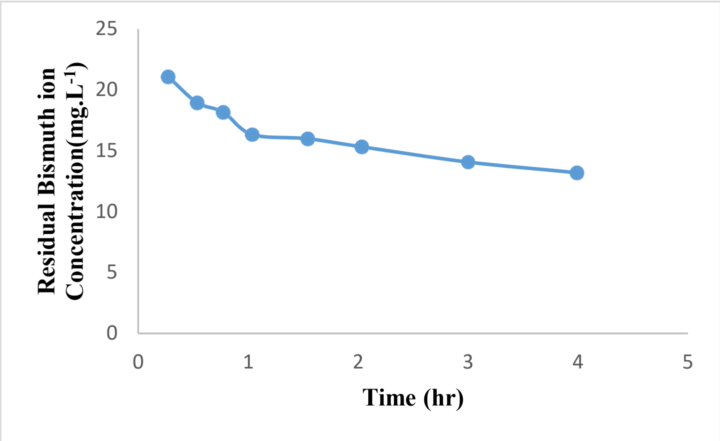

Figure 4. Distribution of kinetic changes in residual bismuth concentration in the zero order adsorption reaction.

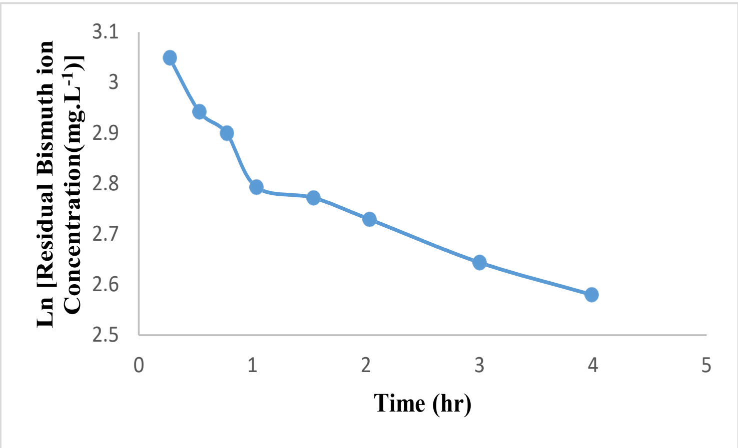

Figure 5. Distribution of kinetic changes in residual bismuth concentration in the first order adsorption reaction.

In the following, regression analyzes have been performed in the ToolPak Analysis environment of Excel2013 software and the results for grades zero, first and second are described in (Table 3).

As shown in the table above; the quadratic reaction produces the highest values of the regression coefficient (R-Square) and correlation. On the other hand, the error values resulting from data fitting (Standard Error) in the quadratic reaction create better conditions than the other two cases. It should be noted that the P-value of the second-order adsorption reaction is less than 0.001 and fulfills the appropriate conditions in terms of analysis of variance. The comparison of the predicted values of the models (zero, first, and second-order) with the real values is shown in (Figures 7-9).

Considering the three above figures, it can be concluded that the data in the quadratic regression function have the highest convergence with the real data obtained from the experiment and the quadratic model can be considered as the basis for the order of reaction of bismuth adsorption by coconut skin.

Results of the kinetic coefficient evaluation of the bismuth adsorption reaction showed a value of 0.0076 L/mg.h, while in the linearization of the measured data for second order reactions this coefficient was estimated to be equal to 0.007 L\mg.h. As a result, an error of 8% can be considered for the linearization method. The results of the convergence of the objective function in the GA are depicted in (Figure 10).

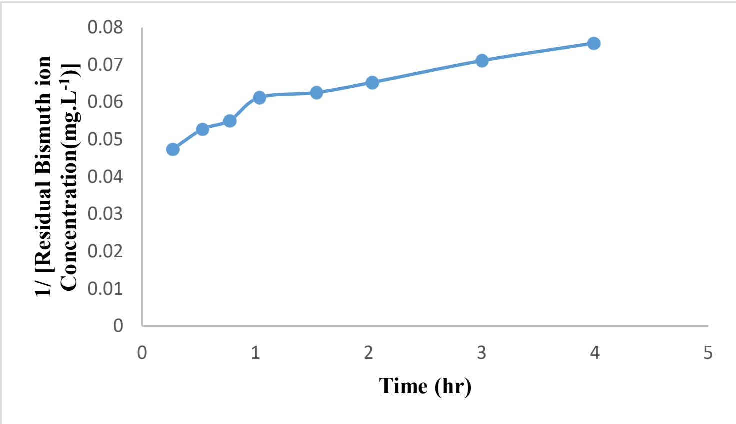

Figure 6. Distribution of kinetic changes in residual bismuth concentration in the second order adsorption reaction.

Table 3: Results of nonlinear regression analysis for adsorption reactions of zero, first and second orders.

Reaction Order	Correlation Coefficient	R - Square	Standard Error	F - Value	P - Value
n = 0	0.7173	0.5146	12.52	7.42	0.0344
n = 1	0.775	0.6	1.89	10.54	0.01753
n = 2	0.87	0.79	0.031	53.71	0.0007

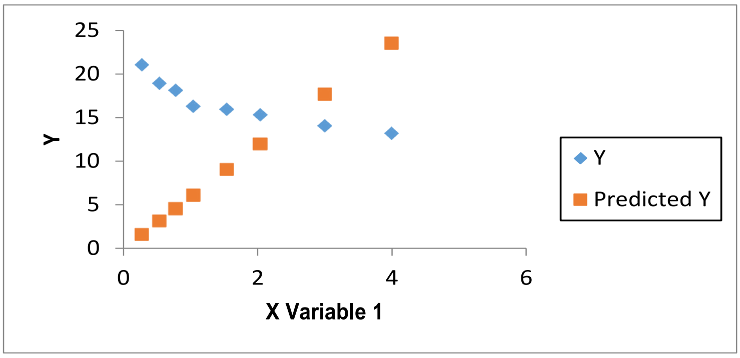

Figure 7. Comparison of regression prediction data and real values in zero order reaction.

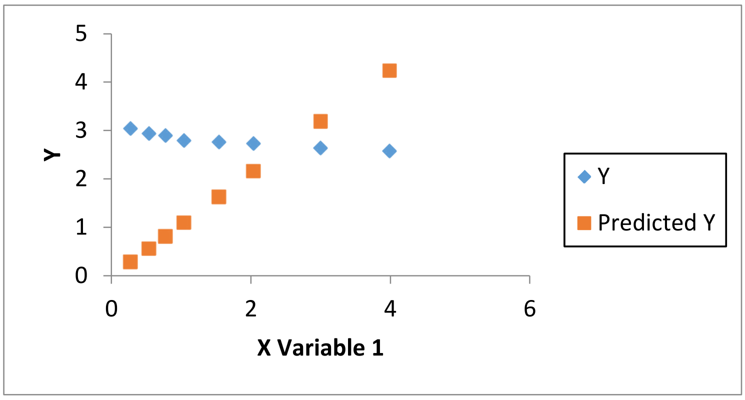

Figure 8. Comparison of regression prediction data and real values in first order reaction.

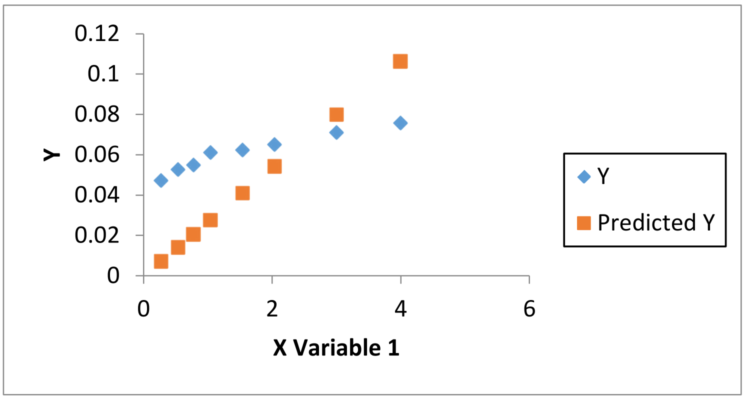

Figure 9. Comparison of regression prediction data and real values in second order reaction.

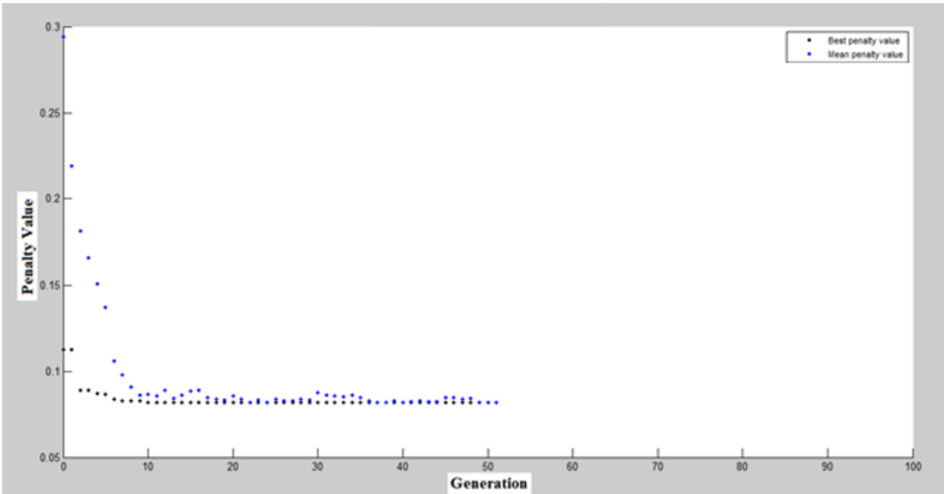

Figure 10. Convergence of the objective function of the genetic algorithm to calculate the values of the constant coefficients of the kinetic reaction.

Conclusion

Bismuth with the Bi symbol in the periodic table has an atomic number of 83 and a mass of 98/208. Its density is equal to 10.05 grams per cubic centimeter and the melting and boiling temperatures are 271 and 1564 degrees Celsius, respectively. Bismuth is a weak, trivalent, white crystalline, heavy and brittle metal with a slight pink tinge that is chemically similar to arsenic and antimony. This mineral has significant epidemiological effects on humans which make the point of being treated and removed from the water or any other sources which are consuming by human beings necessary. This study investigated the kinetics of bismuth removal by coconut shell based on the Chaudhari research. The results showed that the process of adsorption of bismuth by coconut shell is of second order. Also, a constant reaction coefficient of 0.0076 was determined after soft calculations in the combination of MATLAB and GA Simulink environment. Meanwhile, an 8% error was observed in the linearization calculation of the constant reaction coefficient.

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