

YILDIZ TECHNICAL UNIVERSITY
FACULTY OF CHEMICAL AND METALLURGICAL ENGINEERING
CHEMICAL ENGINEERING DEPARTMENT

MODELLING OF AN ADSORPTION STUDY USING NON-LINEAR REGRESSION AND ARTIFICIAL NEURAL NETWORK

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ETHIC DECLARATION

We declare that all information in this graduation thesis has been obtained in according to academic rules and ethical conduct. We also declare that, as required by these rules and conduct, we have fully cited and referenced all material and results that are not original to this work and we haven't falsified and/or fabricated research data and results of the study.

Yasemin Bingül
Baran Saçkan

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LIST OF ABBREVIATION

ANN: Artificial Neural Networks

IUPAC: International Union of Pure and Applied Chemistry

R-P: Redlich-Peterson

SEM: Scanning electron microscopy

XRD: X-Ray diffractometry

AC: Activated Carbon

RSM: Response surface methodology

LECA: Light expanded clay aggregate

CCF: Central composite face

PUPAIM: R package of Physical and Chemical Adsorption Isotherm Models

LIST OF SYMBOLS

R^2: Correlation coefficient

X^2: Chi-Square

Ce: Concentration of adsorbate at equilibrium

qe: Amount of adsorbed matter per unit mass of adsorbent

β: Nonlinear parameter estimates that will be calculated

ε : Error

d : width of the pore for slit – type pores

d_o: pore diameter for cylindrical pores

K_f : Freundlich constants

n: Freundlich constants

q_m :Maximum adsorption capacity

K_s; Equilibrium constant for heterogeneous solids

ms: Constant related to the Sips isotherm

ÖZET

Adsorpsiyon, kimya endüstrisindeki temel süreçlerden biridir. Adsorban malzeme, istenmeyen veya ayrılmak istenen malzemeyi çözeltiden çıkarmak için çok önemlidir. Adsorpsiyon izotermleri, adsorpsiyon işlemlerinin tanımlanması için gereklidir. Bu çalışmada, deneysel adsorpsiyon verileri, iki parametreli (Freundlich ve Langmuir) ve üç parametreli (Sips ve Redlich-Peterson) adsorpsiyon izoterm modellerinin doğrusal olmayan regresyon analizi kullanılarak değerlendirilmiştir. Deneysel adsorpsiyon verilerinin doğrusal olmayan regresyon analizi MATLAB ve R yazılımı ile gerçekleştirilmiştir. En uygun teorik adsorpsiyon izotermini seçmek için % hata, korelasyon katsayısı (R^2) ve Ki-Kare (X^2) değerleri incelenmiştir.

Çalışmanın ikinci bölümünde, son on yılda tercih edilen yeni tahmin yöntemi olan Yapay Sinir Ağı (ANN) modellemesi de adsorpsiyon verilerine uygulanmıştır..Verileri tahmin etmek için ANN modelleme çalışması incelenmiştir.

Anahtar Kelimeler: Doğrusal Olmayan Regresyon, Yapay Sinir Ağı, MATLAB, R Programlama, Adsorpsiyon İzotermi

ABSTRACT

Adsorption is one of the fundamental processes in the chemical industry. The quality or adsorbent material is crucial to remove unwanted or wanted material from solution. Adsorption isotherms are essential for the description of adsorption processes. In this study, experimental adsorption data were evaluated using nonlinear regression analysis of two-parameter (Freundlich and Langmuir) and three-parameter (Sips and Redlich-Peterson) adsorption isotherm models. Non-linear regression analysis of experimental adsorption data was carried out via MATLAB and R software, respectively. The % Error, correlation coefficient (R^2) and Chi-Square (X^2) values were examined to choose the most fitted theoretical adsorption isotherm.

In the second part of the study, Artificial Neural Network (ANN) modelling, which is the novel prediction method of choice in the last decade, was also applied to the adsorption data. ANN modeling study has been studied to predict data.

Keywords: Non-linear Regression, Artificial Neural Network, MATLAB, R Programming, Adsorption Isotherm.

1. INTRODUCTION

Adsorption is the collection of which might be normally decoded in answer on a suitable interface. The interface can be between liquid-gas liquid-solid or liquid-liquid. Adsorption in wastewater treatment is the process of using substances called adsorbents that have properties that can hold these substances in order to remove certain substances in wastewater.

Adsorption is similar to an equilibrium reaction. When the solution comes into contact with a certain amount of adsorption, the concentration of the substance adsorbed in the solution decreases until it is balanced with those on the surface of the adsorption. After the adsorption balance is established, the concentration of the adsorbed substance in the solution phase remains constant. The amount of adsorption that can be held with an adsorption is a function of the concentration and temperature of the adsorption. At constant temperature, against the solute concentration remaining in solution in equilibrium, the amount of solute adsorbed is graphically obtained by the resulting function called adsorption isotherm. Adsorption isotherms are linearized and their constant is calculated. In nonlinear analysis, computer programs are used.

MATLAB and R programs are two of the well-known programs in the engineering area and these programs are used for various things. But in research it is only considered two things in which these programs can be used. Firstly it investigated these programs by trying to solve nonlinear regressions with the help of data from adsorption experiments and it will observe which adsorption isotherm is more consistent for the dataset.

In recent years these programs have also started to be used in Artificial Neural Network and it is a very interesting development for data analysis science. Because ANN is the element of artificial intelligence meant to simulate the functioning of the human mind. The inputs are what the ANN learns from to provide the desired output. That means if ANN learns the adsorption dataset and forms a pattern about the adsorption dataset it is used. Then it can be obtained in every single combination of different parameter values. So the second part of research is about ANN and teaching the dataset to ANN and receiving some prediction values. In this study it is tried to improve the ANN efficiency by adding some parameters which can be reached from the dataset.

2. ADSORPTION AND MODELLING APPLICATIONS

In Chemical Engineering, adsorption can be explained as the separation process when certain phase components of a liquid are transferred to a solid surface. One or more physical and chemical events are effective in adsorption, and these events occur between two separate phases. During the separation process, the adsorbed phase is called adsorbate, and the adsorption phase is called adsorbent. The most important feature for adsorbent material is the pore, which determines the use of adsorbent. The total number of pores, pore form and pore size; determination of adsorption ability and the dynamic adsorption rate of the material. Popularly, the pores are divided into macro -, meso -, and micro. Consistent with the IUPAC classification, pores are classified as shown in Table 2.1.

Table 2.1 Classification of pores by size (IUPAC, 1985)

Type of Pore	**Diameter of Pore d (nm)**
Macro pores	d>50
Meso pores	$2 \leq d \leq 50$
Micro pores	d<2
Ultra micro pores	d<0.7
Super micro pores	$0.7<d_o<2$

d_o: pore diameter for cylindrical pores, d:width of the pore for slit – type pores

Adsorption molecules enter into macropores, mesopores, and micropores. Micropores usually make up the largest portion of the inner surface and total pore volume. In microporosity, the attractive forces are more potent, and the pores are charged with low relative pressures. For this reason, most of the adsorption of gas adsorbents occurs in this region. The total pore extent and pore size distribution determine the adsorption potential. (Gürten, 2008)

Ion exchange: this is the displacement of ions adsorbed from solution to solid with similarly charged ions of surfactant.

Ion mating: this is the adsorption of surfactant ions to inversely charged positions that are empty.

Acid-base interaction: this is an adsorption that occurs either by hydrogen bonding or by a Lewis acid-base reaction between the adsorption and the adsorption.

Adsorption by polarization of electrons: this is a mechanism that occurs when the substance to cling to the surface contains electron rich aromatic nuclei, when the adsorbent contains strong positive regions. Adsorption occurs as a result of interaction between electron rich aromatic nuclei and positive positions

Adsorption by dispersion forces: occurs through the London-Van der Waals dispersion forces between the adsorbent and adsorbate molecules. As the molecular weight of the adsorbed substance increases, the rate of adsorption also increases.

Hydrophobic bonding: this is a mechanism that occurs as a result of the reciprocal attraction force between hydrophobic groups in the surfactant and the tendency of these groups to escape from the aqueous environment.

2.1. Adsorption Isotherms

Adsorption isotherm is the equilibrium relationship between concentrations in the moving phase and adsorbent phase at a given temperature. For gases, isotherms are expressed as a percentage of moles against partial pressure. For liquids, the concentration is denoted by a unit of mass, such as ppm, while the concentration on the solid surface is expressed as the amount of adsorbed matter per unit mass of the adsorbent (Do, D.D., 1998).

2.1.1. Two-Parameter Adsorption Isotherm Models

Two-parameter isotherm models; Langmuir, Freundlich isotherms can be given as examples.

2.1.1.1. Langmuir Isotherm

The Langmuir isotherm was first developed by Langmuir in 1918 to explain the adherence of the amount of gas adsorbed on the surface to gas pressure. This model was often used to remove heavy metals in aqueous solutions. The adsorption is proportional to the fraction of the adsorbent surface that is open, while the desorption is proportional to the fraction of the

adsorbent surface that is covered. The Langmuir equation can be written in the following linear form:

$$q_e = \frac{Q.b.Ce}{1+b.Ce}, \quad (2.1)$$

where Ce is concentration of adsorbate at equilibrium ($_{mg.g}^{-1}$) (Do, D.D., 1998).

2.1.1.2. Freundlich Isotherm

Freundlich isotherm takes the form of an equation when written in terms of concentrations.

$$q_e = K_f \times C_e^{\frac{1}{n}} \quad ,(2.2)$$

Q_e refers to the amount of adsorbed matter per unit mass of adsorbent known as capacity, the Freundlich constants K_f and n, and the adsorbent concentration at C_e equilibrium.

The Freundlich equation is often used in the adsorption of organic matter in liquid solutions onto activated carbon. It can also be applied in gas phase systems with heterogeneous surfaces where the pressure range is not very wide. Freundlich isotherm does not have properties suitable for Henry's Law Behavior at low pressures and doesn't have a finite limit at very high pressures. For this reason, this isotherm is usually valid in the narrow range of adsorption data(Do, D.D., 1998).

2.1.2. Three-Parameter Adsorption Isotherm Models

Three-parameter isotherm models are Sips, Redlich-Peterson (R-P), Toth, Fritz–Schlunder, Radke–Prausnitz, Khan, Radke–Prausnitz, Kble–Corrigan, Jossens and multilayer physisorption isotherm models.

2.1.2.1. Sips Isotherm

At low concentrations, the Sips isotherm resembles the Freundlich isotherm. The Sips isotherm is not valid in a narrow range of pressure (or concentration), such as Freundlich, and also has a finite limit when the pressure is too high

Sips isotherm takes the form of Equation when written in terms of concentrations and adsorption capacity.

$$q_e = \frac{q_m . K_s . C_e^{ms}}{1 + K_s . C_e^{ms}} \text{,(2.3)}$$

q_m in equality; maximum adsorption capacity ($mol.g^{-1}$), C_e; liquid phase concentration in equilibrium ($mg.L^{-1}$), K_s; refers to the equilibrium constant for heterogeneous solids, and ms refers to a constant related to the Sips isotherm (Do, D.D., 1998).

2.1.2.2. Redlich-Peterson Isotherm

The Redlich-Peterson isotherm is a mixture of the Langmuir and Freundlich isotherms. The numerator is from the Langmuir isotherm and has the advantage of drawing the Henry region at countless dilution . The mechanism of adsorption is a mix and does not comply with perfect monolayer adsorption.

This model is defined by subsequent expression:

$$q_{e=} \frac{K.Ce}{1+a.Ce^{\beta}}, \textit{(2.4)}$$

Here, Ce; liquid phase concentration in equilibrium ($mg.L^{-1}$), K and a express isotherm constants and β; coefficient ranging from 0 to 1.

2.2. Non-linear Regression

Regression analysis is the expression of the relationship between a variable and one or greater variables by the way of a mathematical function. Regression is divided into two according to the type of mathematical function, as linear and nonlinear regression models. Linear models give estimates with normal distribution and minimum variance, while nonlinear regression models usually do that only when the sample size is too great. It is more difficult to attract conclusions than linear models. In addition, normal distribution concept cannot be fully implemented to nonlinear regression models (GAZELOĞLU C. , saraçlı s.,2013)

There are many proposed methods for parameter estimation of nonlinear regression models. Some of them are known as Least Squares, most likelihood (maximum likelihood) and Gaussian Newton methods. Estimate values are reached using iterations in all methods.

Theoretical competence, necessity of methods whose approaches are different. Safety, normality tests were conducted and the validity of their results was accepted.

$$y = f(x, \beta) + \varepsilon,$$

Here; β refers to nonlinear parameter estimates that will be calculated, and ε refers to an error.

With the development of computer technology in the 1980s, the analysis of isotherm models by nonlinear methods made progress. Unlike linearization, the non-linear approach usually entails minimization or maximization of error participation (between experimental data and isotherm estimation), depending on the convergence criterion.

2.3. Artificial Neural Network

Artificial intelligence, a computer, a machine or computer-aided, usually human qualities, solution finding, understanding, meaning extraction, generalization, and learning from past experiences, as well as high in relation to the process logic is defined as the ability to perform tasks in the world of science.

The superior properties of the human brain have compelled scientists to work on it, and a mathematical modelling has been attempted to be extracted, inspired through the neurophysiological structure of the brain. Diverse artificial neural network models were evolved with the idea that its physical components ought to be modeled effectively, that allows to absolutely model all the behaviors of the brain. In this manner, a different branch of science has emerged from the algorithmic calculation method of latest and current computer systems referred to as Artificial Neural Networks. In a general sense, ANN may be defined as a system designed to model the way the brain performs a function. ANN consists of connecting artificial nerve cells with each other in various way diverse approaches and is typically organized in layers. It is able to appear with electronic circuits as hardware or as software program on computers. In keeping with the brain's approach of processing data, ANN is a parallel distributed processor with the capability to store and generalize facts after a learning procedure (Ataseven, 2013).

It is similar to the human brain in two ways:

1.Information is obtained by the network through the learning process.

2. It uses interneuron coupling forces, known as synaptic weights, to store information

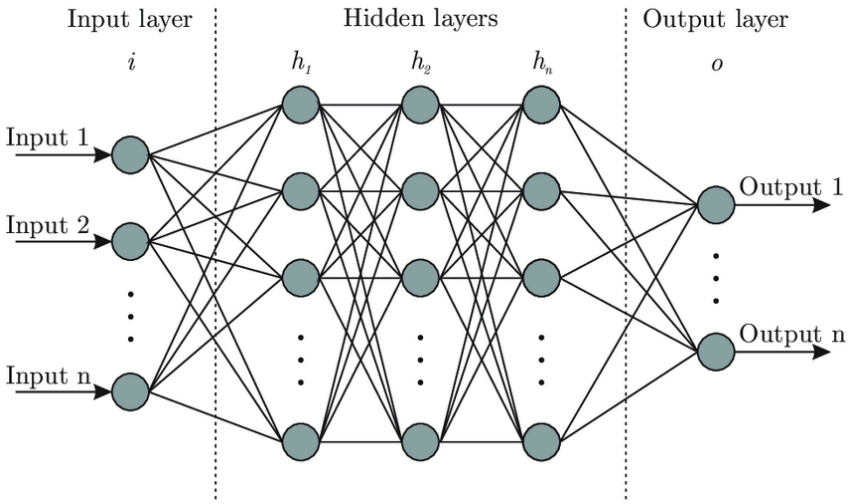


Figure 2.1 Hidden Layers on ANN(2019,Lavanya)

Artificial neural networks are data-based systems created by connecting artificial nerve cells in layers and target to use the human brain's capacity to examine and make very fast selections below exclusive situations to solve complicated issues the usage simplified models (Ataseven, 2013).

Although the structure of an artificial neural network and the variety of nerve cells range, any well-known rule for the formation of an artificial neural network reference Artificial neural networks with fewer hidden layers than the range of hidden layers required are inadequate to solve complicated problems, while artificial neural networks with too many hidden layers face undesirable instability. The trouble encountered after figuring out the variety of hidden layers is that each discovered in determining how many neurons will be involved in the layer. There is no problem for the input layer; this number is the number of entries in the device it is equal to the number. In an identical way, the output layer can also be decided by means of the favored variety of outputs. The principal problem is figuring out wide variety of neurons in hidden layers. The conventional matrix algorithm says that matrix dimensions must be identical to both number of inputs or number of outputs. Unluckily, there are no mathematical tests as to how many neurons can be most efficiently observed in the hidden layer. Trial and error methods should be applied and decided (Ataseven, 2013)

3. LITERATURE RESEARCH

In this study, literature research was conducted with four articles, two of non-linear regression and two of artificial neural networks.

In the non-linear Regression Analysis for the Adsorption Kinetics and Equilibrium Isotherm of Phenacetin onto Activated Carbons study, nonlinear kinetic and equilibrium adsorption isotherm models were applied to the adsorption of phenacetin on Activated Carbon obtained from white sawdust and pumpkin peels. In contrast, linear and nonlinear adsorption isotherm models with two parameters shows that variations of nonlinear adsorption isotherm equations to linear forms indirectly alter their error structures. While the graphs show that equilibrium adsorption isotherm models are suitable for studying phenacetin adsorption, they show that one of the key variables does not take into account the existence of a systematic error in kinetic models or kinetic data collection. Confirms that the precursor mixture is one of the new ways to prepare activated carbon (Sadeu Ngakou,2019)

In the second article research, response surface methodology (RSM) and ANN were used in modeling study by Cu^{2+} adsorption optimization use of light expanded clay aggregate (LECA). An approach is advanced for the assessment of the heavy metallic adsorption process. LECA was used as a green and low-cost adsorbent to eliminate $Cu^{2+}$from aqueous solution in the discrete device. The effect of operational parameters inclusive of preliminary pH, temperature, initial Cu^{2+} concentration and sorbent dosage had been studied in the usage of the CCF design. The same design was also used to obtain a training kit for the ANN. A comparison between the model outcomes and experimental information gave an excessive correlation coefficient (R^2 ANN 0:962, R^2 RSM 0:941) and showed that the two models have been capable of predicting Cu^{2+} elimination by LECA. Langmuir and Freundlich adsorption isotherm models had been carried out to equilibrium information at different temperatures. The outcomes found out that the Freundlich adsorption isotherm fit better than the Langmuir adsorption isotherm(Shojaeimehr, 2013).

Thermodynamic studies have proved that Cu2+ elimination the use of LECA is a spontaneous, endothermic random and compatible process with physical adsorption mechanism. The good performance of copper elimination makes LECA an abundant and cheaply available adsorbent in nature for the treatment of copper-contaminated wastewater. As a result, LECA can be an alternative to high-priced adsorbents.

In the third article, an artificial neural network model is proposed for the estimation of adsorption and photocatalysis performance of TiO_2 photocatalysts. The network become trained using experimental information obtained at different pH with different TiO_2 doses and initial dye concentration. Different algorithms and transfer functions had been tested for hidden layers to discover the most appropriate and reliable network. The optimal number of neurons in the hidden layer turned into found with trial and error. Those neural network models efficiently estimate the method's adsorption efficiency (%dye removal), adsorption ability (loading), and photocatalytic performance.

The study of the ANN model for adsorption and photocatalysis shows that finding a reliable network model is a vital task. The developed ANN model should be properly checked before being applied to any actual automatic water treatment process. There must be a good alignment between the simulated results and the experimental results; otherwise it will be difficult to achieve the desired water quality. This study shows that not all algorithms and transfer functions are suitable for this process (Dutta, 2013).

In the last article, the goal is to gain an excessive capacity and stable adsorbent that can separate uranium ions from acidic solutions to safely dispose of uranium waste released at different pH and concentrations at each stage of the Nuclear Fuel Cycle process. Parameters includes pH, contact time, concentration, temperature and solid-liquid ratio that are effective in Uranium uptake of AC/PAN composites were studied. Isotherms of Freundlich, Langmuir, Temkin and DR (Dubinin-Radushkevich) were investigated to characterize the adsorption process. Linear and nonlinear regression analysis became applied to the process and it was observed that the experimental and theoretical values were in an agreement(Aslani, Amik, 2021).

4. MATERIALS AND METHODS

In this study, experimental adsorption data was fitted to two parameters (Freundlich, Langmuir) and three parameters (Sips, R-P) theoretical adsorption models by using non-linear regression methods. The adsorption data were taken from Cr(VI) adsorption onto peach stone based steam activated carbon (Duranoglu, 2008). In order to carry nonlinear regression, R and MATLAB programs were used. In addition, experimental adsorption data was also evaluated by using Artificial Neural Network (ANN) with the MATLAB program.

4.1. Non-Linear Regression Analysis of Adsorption Data

The experimental adsorption data (obtained at 295K) used in non-linear regression modelling and ANN study were given in Table 4.1 and 4.2, respectively. All adsorption data were taken from a previous study (Duranoğlu, 2008). Adsorption data given Table 4.1 were obtained at 295K and 30 ppm initial Cr(VI) concentration with different AC amount.

Table 4.1 Experimental adsorption data for Nonlinear Regression Study (Duranoğlu, 2008)

pH2		**pH4**		**pH6**	
Ce (mg/L)	qe (mg/g)	Ce (mg/L)	qe (mg/g)	Ce (mg/L)	qe (mg/g)
25.2000	143.6364	26.5500	103.8542	28.8730	49.5893
16.6900	130.0877	22.4980	100.4111	26.7800	47.7451
11.3640	129.2051	14.5750	97.4713	23.6750	47.4702
4.5980	119.1239	11.8580	95.5194	21.3850	45.8259
1.7370	110.3074	8.3800	90.4492	13.7150	43.1130
0.3230	89.1343	3.2110	80.0113	8.4280	38.7033
0.1000	77.3892	1.6530	72.1787	3.9630	32.1195
0.0080	49.8608	0.1130	51.0097	1.4080	25.2860

0.0020	38.8153	0.0400	37.8546	

Table 4.2 Experimental adsorption data for ANN Study (Duranoğlu, 2008)

qe(mg/g)	AC (mg)	pH	T (K)	Ce(mg/L)	qe(mg/g)	AC (mg)	pH	T (K)	Ce(mg/L)
143.64	2.2	2	295	25.2	125.76	2.8	3	295	24.41
130.09	5.7	2	295	16.69	115.16	5.1	3	295	19.71
129.21	7.8	2	295	11.36	108.18	7.9	3	295	14.36
119.12	11.3	2	295	4.6	103.42	10.3	3	295	10.15
110.31	13.5	2	295	1.74	105.17	13.9	3	295	2.22
89.1343	17.5	2	295	0.32	86.89	17.7	3	295	0.7
77.3892	20.3	2	295	0.1	72.67	21.5	3	295	0.21
49.8608	31.6	2	295	0.01	52.9	29.7	3	295	0.04
38.8153	40.6	2	2950	0.002	38.94	40.3	3	295	0.07
qe(mg/g)	**AC (mg)**	**pH**	**T (K)**	**Ce(mg/L)**	**qe(mg/g)**	**AC (mg)**	**pH**	**T (K)**	**Ce(mg/L)**
103.85	2.4	4	295	26.55	49.59	2.8	6	295	28.87
100.41	4.5	4	295	22.5	47.75	5.1	6	295	26.78
97.4713	8.7	4	295	14.58	47.47	8.4	6	295	23.68
95.5194	10.3	4	295	11.86	45.83	11.2	6	295	21.39
90.4492	12.8	4	295	8.38	43.11	20.8	6	295	13.72
80.0113	17.7	4	295	3.21	38.7	30	6	295	8.43
72.1787	20.7	4	295	1.65	32.12	43.1	6	295	3.96
51.0097	30.8	4	295	0.11	25.29	59.8	6	295	1.41
37.8546	41.6	4	295	0.04					
qe	**AC (mg)**	**pH**	**T (K)**	**Ce(mg/L)**	**qe**	**AC (mg)**	**pH**	**T (K)**	**Ce(mg/L)**
102.04	4.9	2	305	18.65	126.2	5	2	318	16.03
101.76	7.8	2	305	12.78	113.08	7.8	2	318	11.01
92.24	10.5	2	305	9.28	107.74	10.4	2	318	6.24
84.45	15.4	2	305	2.64	91.3	15	2	318	1.26
70.99	19.8	2	305	0.54	71.07	20.1	2	318	0.08
48.92	29.2	2	305	0.08	46.35	30.9	2	318	0.01

4.1.1 Non-Linear Regression Analysis of Adsorption Data Using the MATLAB Program

MATLAB is a programming and numeric computing platform used by millions of engineers and scientists to analyze data, develop algorithms, and create models. Also MATLAB gives

permission to write code specific to the working area. But also in MATLAB there is a section which includes apps. These apps are interactive applications written to perform technical computing tasks. Apps are included in many MATLAB products. In that section there are two different types of apps, one of them is developed by MATLAB and the other one is developed by the community. In this study Curve Fitting Toolbox Application developed by MATLAB was used.

In order to define the dataset to MATLAB. Primary data should be written on the editor screen in MATLAB under the ‘load census’ command. As shown in Figure 4.1

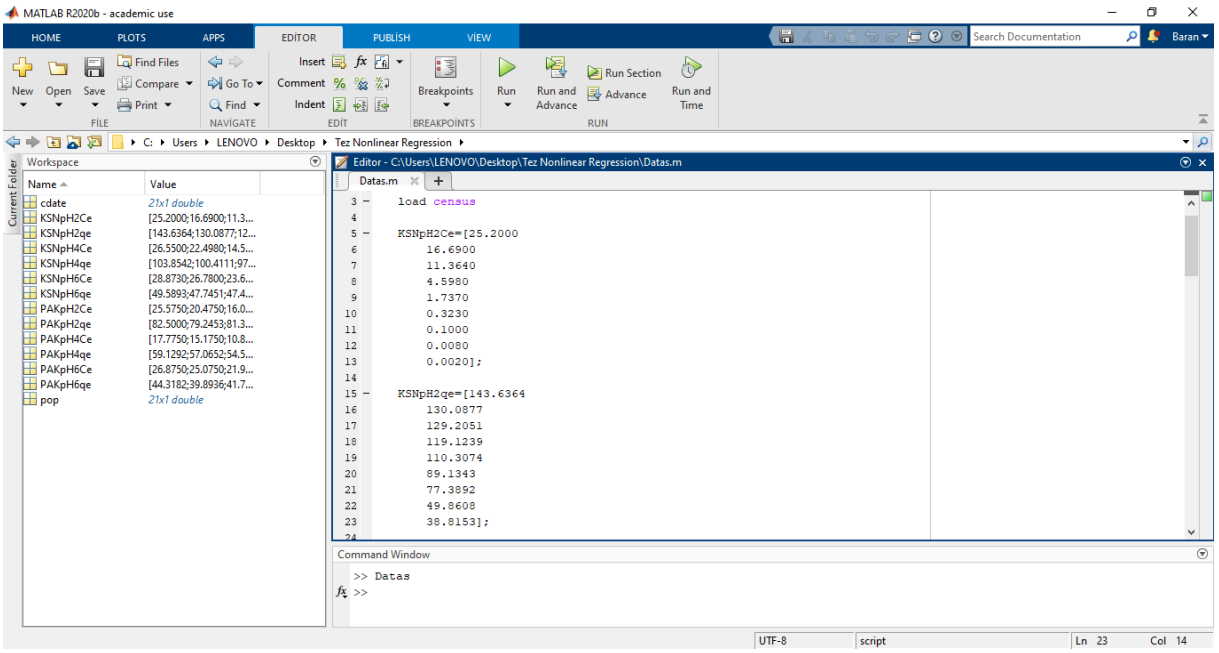


Figure 4.1 Defining the data from MATLAB

After running this editor screen the data is on the MATLAB platform and ready to use in the Curve Fitting Toolbox Application. After that Curve Fitting Toolbox should be opened from the Apps title, as shown in Figure 4.2.

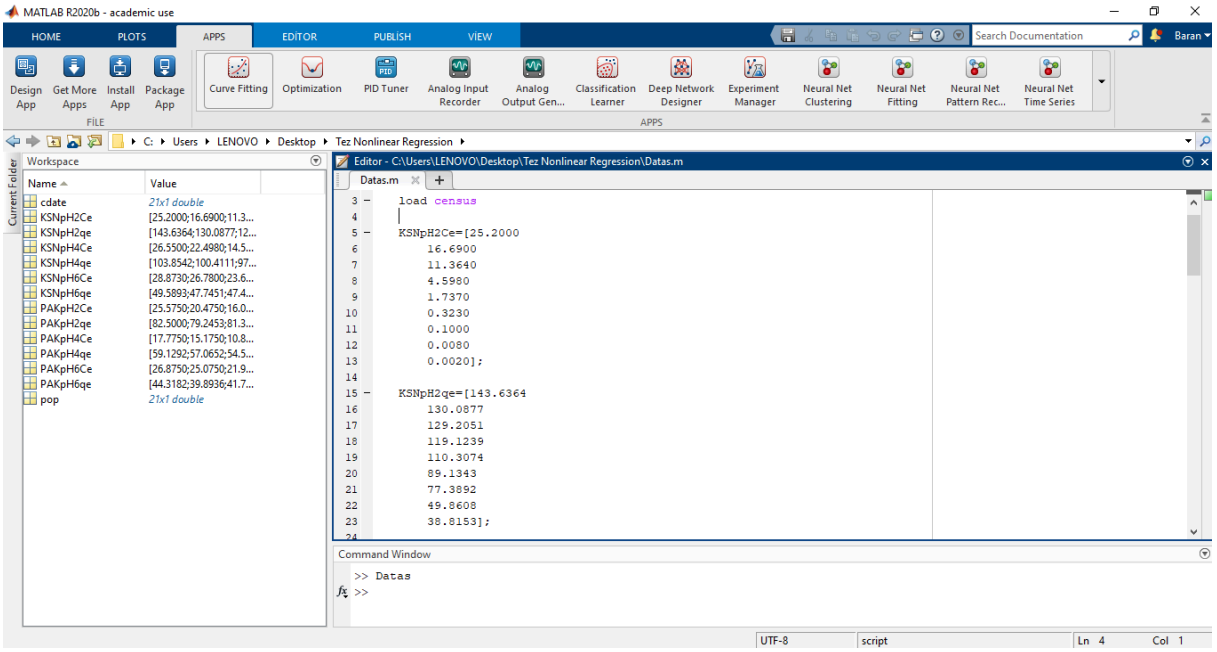


Figure 4.2 Curve Fitting Toolbox in MATLAB

When the application screen is open the first thing is give work a name. Then the application permits you to choose X and Y values. In that case X and Y values chosen as pH2 Ce for X and pH2 qe for Y value. As shown in Figure 4.3 and Figure 4.4

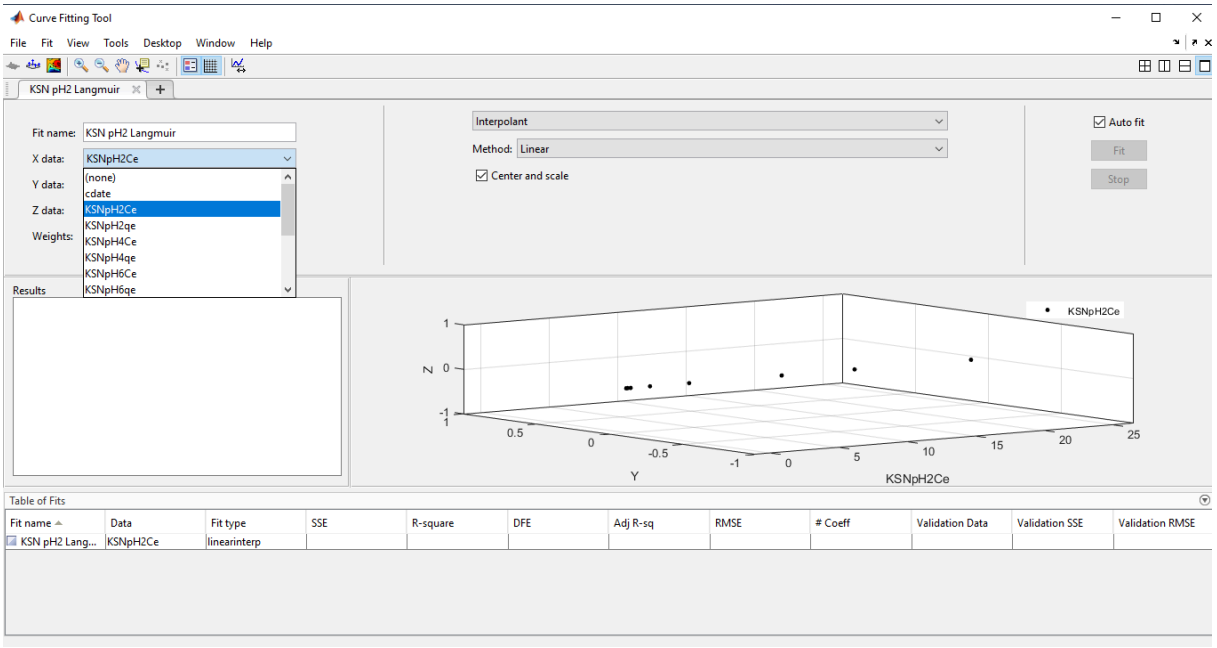


Figure 4.3 Defining dependent and independent variables

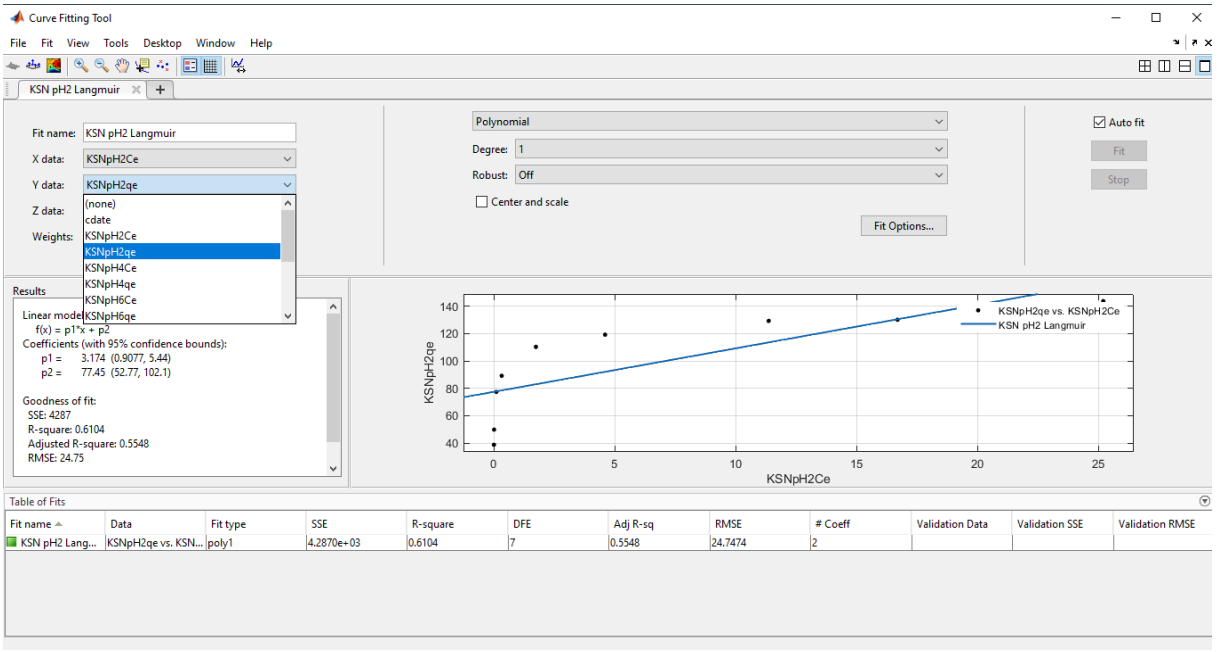


Figure 4.4 Defining Adsorption Isotherm Equation in MATLAB

Afterwards time is defined as the adsorption isotherm which will be applied to that application. In order to perform on adsorption isotherms, choosing Custom Equation will be the right choice.

Later on define the equation, in that case defining Langmuir Equation is taken as an example. As shown in Figure 4.6

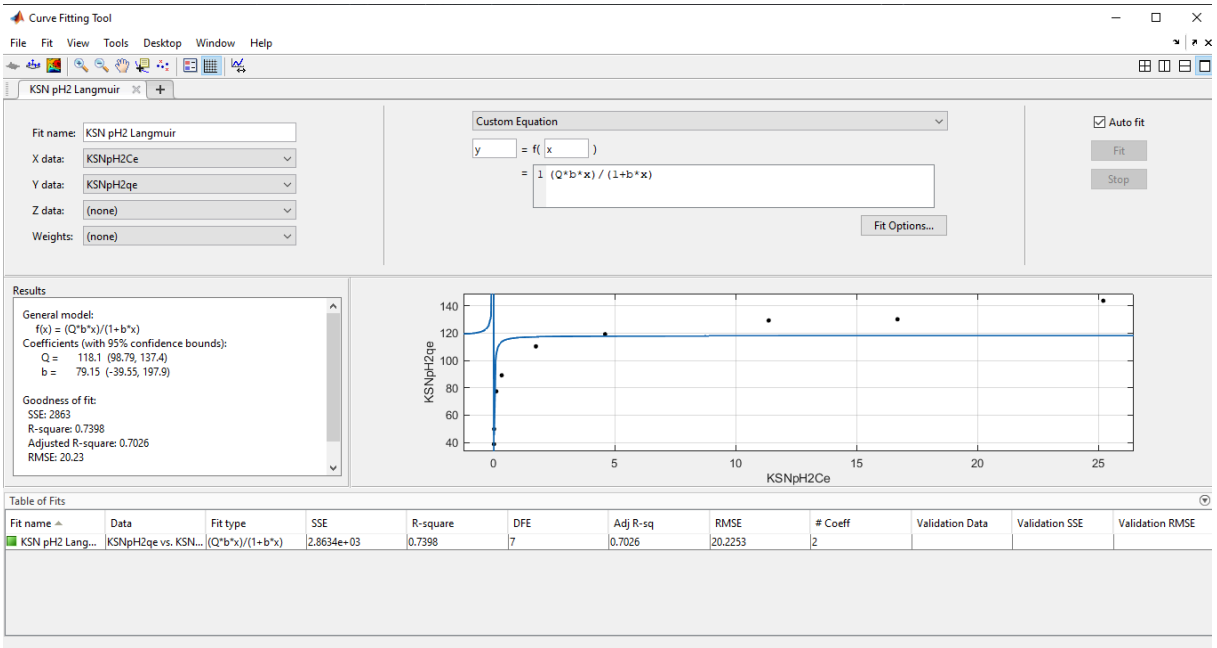


Figure 4.6 Defining Adsorption Isotherm Equation in MATLAB

The regression is done with the last step. Left side box titled results shows that unknown variables and R-square values.

There is a way to change some of the fitting options by pressing the Fit Options button as shown in Figure 4.7 (It may be changed robust, algorithm, minimum change in variables for finite-difference gradients, maximum change in variables for finite-difference gradients, maximum number of function evaluations, maximum iterations, termination tolerance for the function value, termination tolerance for x, lower and upper bounds of unknown variables.)

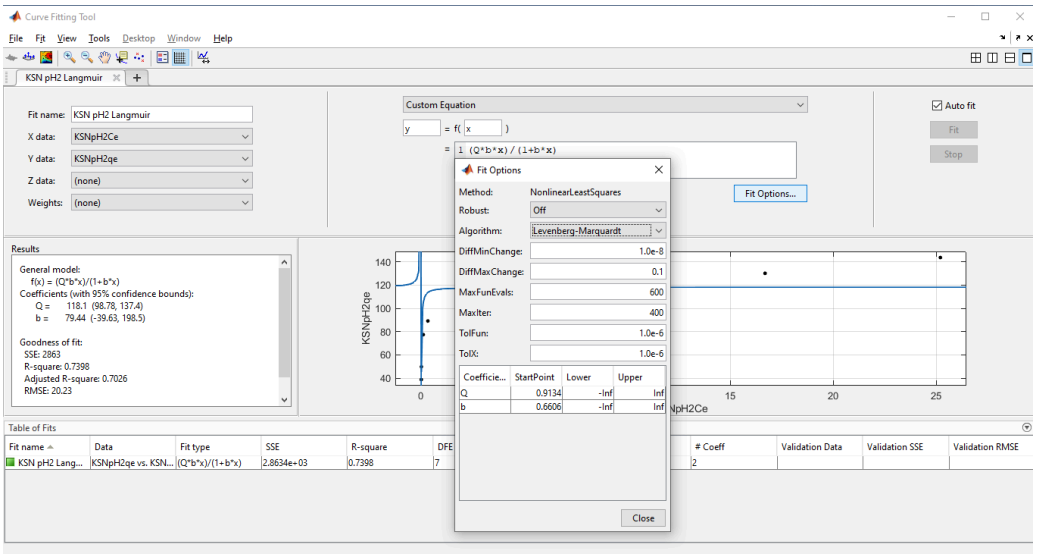


Figure 4.7 Fitting in MATLAB

When the regression is done and, to obtain the code which was used, there is a generate code button under the file section in this application as shown in Figure 4.8.

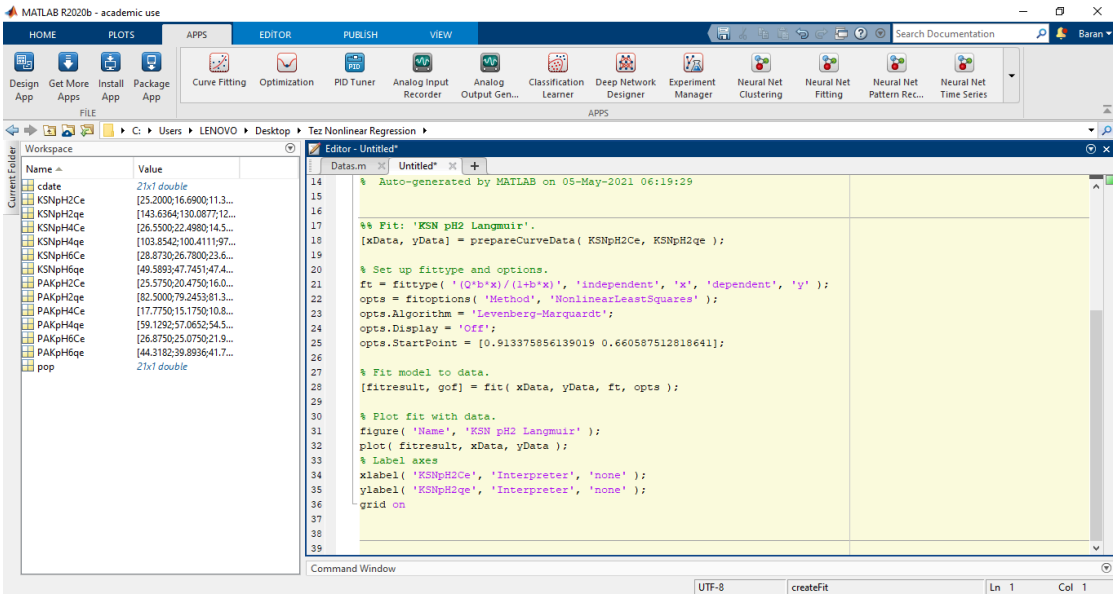


Figure 4.8 Codes on Editor Screen in MATLAB

4.1.2. Non-Linear Regression Analysis of Adsorption Data Using the R Programming

R is a language and environment for statistical computing and graphics. R provides a wide variety of statistical (linear and nonlinear modelling, classical statistical tests, time-series analysis, classification, clustering) and graphical techniques, and is especially extensible [1]. It is an environment inside which statistical strategies are implemented. R may be extended with packages. In this thesis, 'PUPAIM' adsorption isotherm package was used. Isotherm equations offer physical adsorption of gases and vapor and gives the most critical characteristics of industrial adsorbents that consist of pore volume, pore size or energy distribution (Ayawei,2017).

This is shown in Figure 4.10 and how to encode in the R program by using a ph2 experimental dataset for each adsorption isotherm method. Firstly, the dataset is defined in the r program as ph2set.

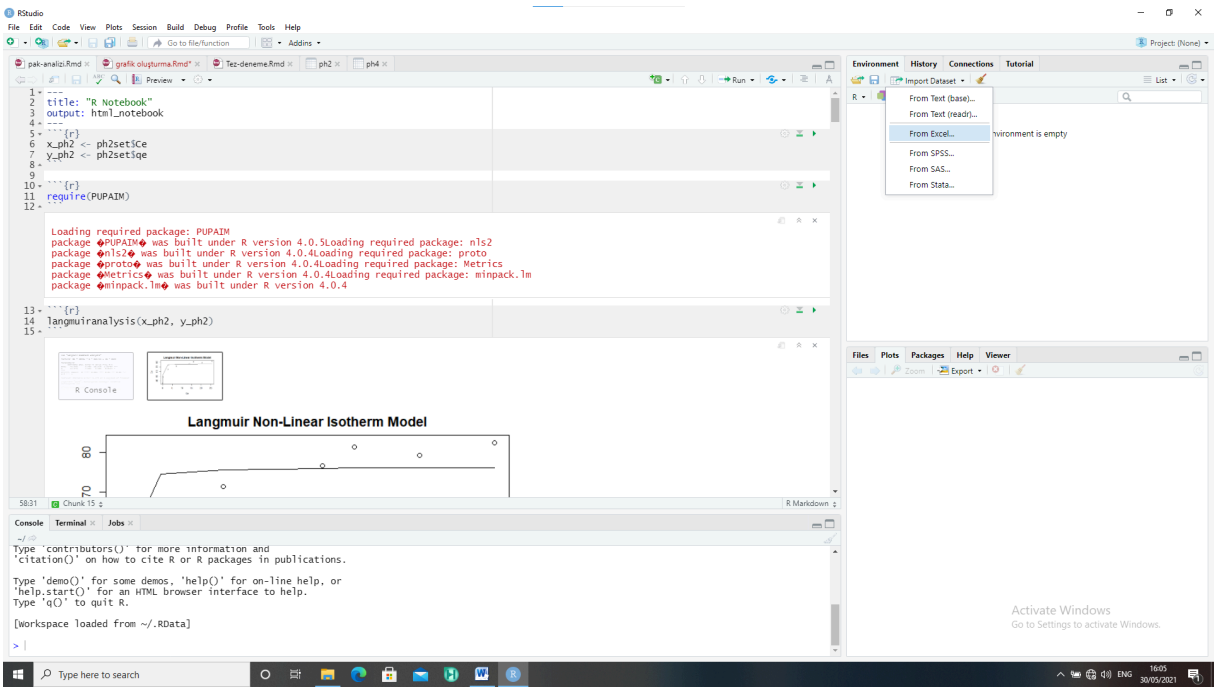


Figure 4.9 Encoding in the R program by using ph2 experimental dataset for each adsorption isotherm method

The dependent variable (q_e) is separated as y_ph2 from the defined ph2set. The independent variable (C_e) is separated as x_ph2 from the defined ph2set, this operation is shown in the Figure 4.11.

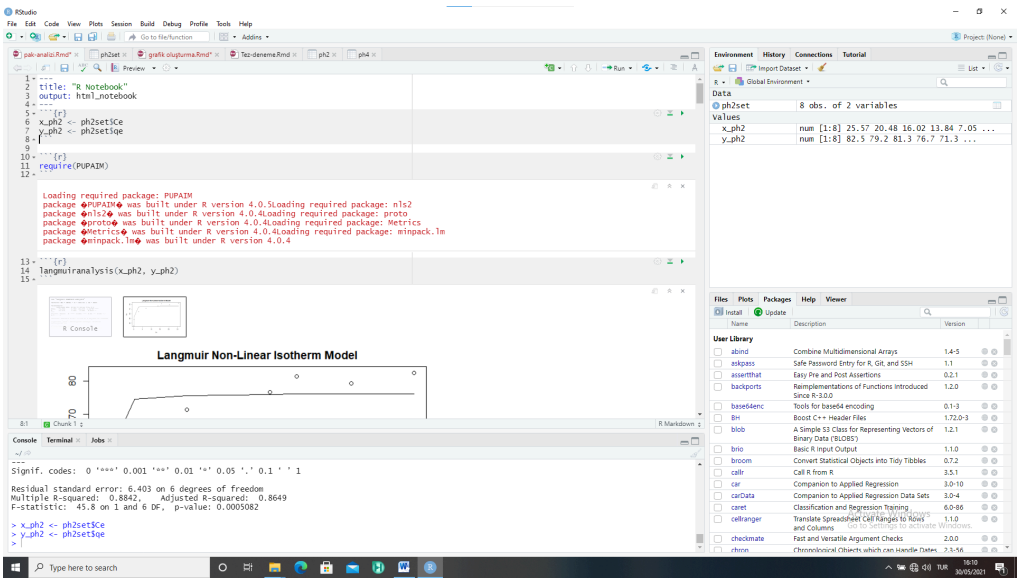


Figure 4.10 Definition of dependent and independent variables in R

This can be checked that the values are defined from the R Environment tab. R package 'PUPAIM' is downloaded and turned active to be used in this study. Writing of the download code is shown in the figure 4.12

```
install.packages("PUPAIM")
require(PUPAIM)
library(PUPAIM)
```

```
Loading required package: PUPAIM
package 'PUPAIM' was built under R version 4.0.5Loading required package: nls2
package 'nls2' was built under R version 4.0.4Loading required package: proto
package 'proto' was built under R version 4.0.4Loading required package: Metrics
package 'Metrics' was built under R version 4.0.4Loading required package: minpack.lm
package 'minpack.lm' was built under R version 4.0.4
```

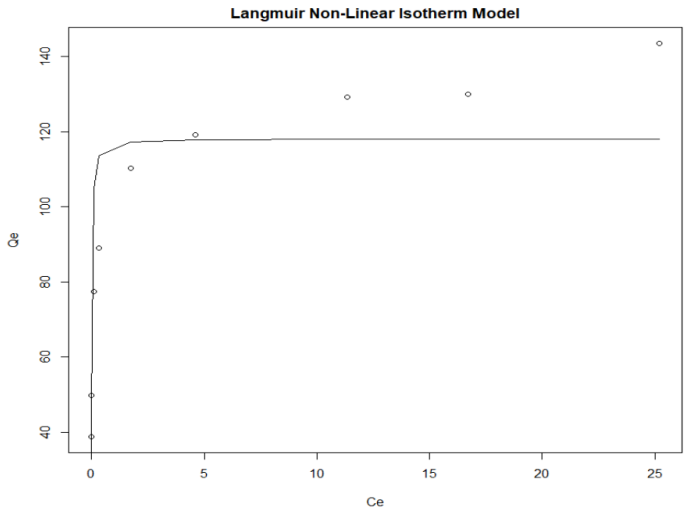
Figure 4.11 Downloading Codes of 'Pupaim' R package

R package 'PUPAIM' Codes are written that respectively run all adsorption isotherm models. This operation gives the graph of the resulting model, dot represents experimental data and line shows the values it estimates from the Langmuir adsorption isotherm equation. The console R shows which equation it uses, the optimal values of Q and b, the values r predicts. This operation is shown in the Figure 4.13

Codes:

```{r}
langmuiranalysis(x_ph2, y_ph2)
```

Graphical Model:



Console:

```
[1] "Langmuir Isotherm Analysis"

Formula: Qe ~ (Qmax * b * Ce)/(1 + (b * Ce))

Parameters:
     Estimate Std. Error t value Pr(>|t|)
Qmax  118.096      8.167  14.459  1.8e-06 ***
b      79.293     50.275   1.577    0.159
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*'
0.05 '.' 0.1 ' ' 1

Residual standard error: 20.23 on 7 degrees
of freedom

Algorithm "port", convergence message:
relative convergence (4)

$`Predicted Values`
[1] 118.03721 118.00711 117.96537 117.77326
117.24503 113.65854 104.87064  45.83730
16.16497
```

Figure 4.12 Demonstration of the results obtained from R

4.2. Artificial Neural Network Studies of Adsorption Data

In this study, a neural net fitting application of MATLAB was used. The Neural Net Fitting application opens the working panel. Input and target data are loaded separately to be used in the model.

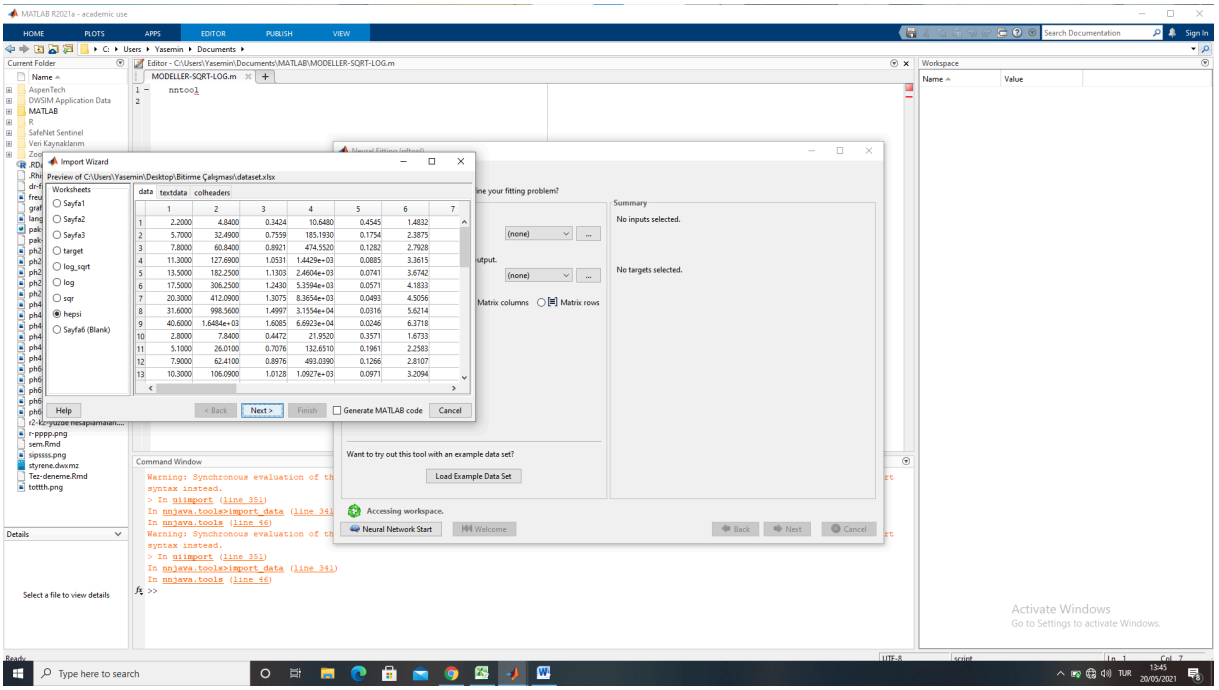


Figure 4.13 Loading of input and target data in Matlab

The code "nntool" runs on the editor page. This panel is the area where the data to be modeled is loaded as in Figure 4.15

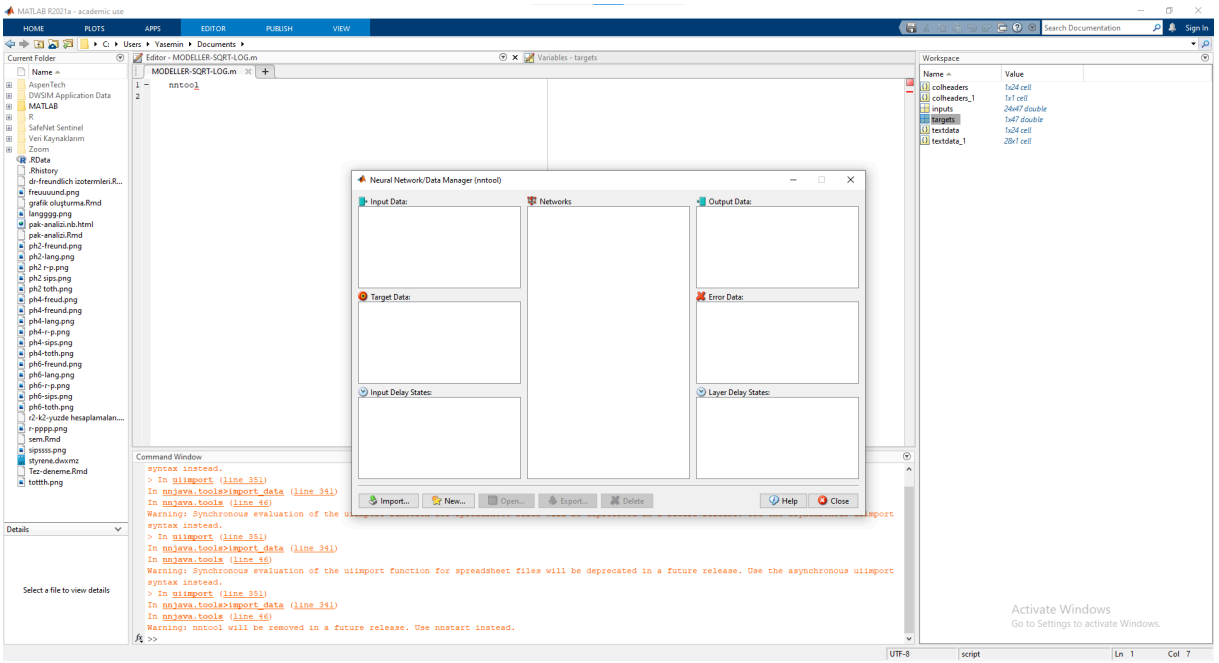


Figure 4.14 Editor page of "nntool"

Input and target data are added to the work panel. Network type feed-forward backpropagation, training function trainlm, performance function MSE, number of neurons 18 are selected and network1 model is created. This phase of the study is shown in Figure 4.16

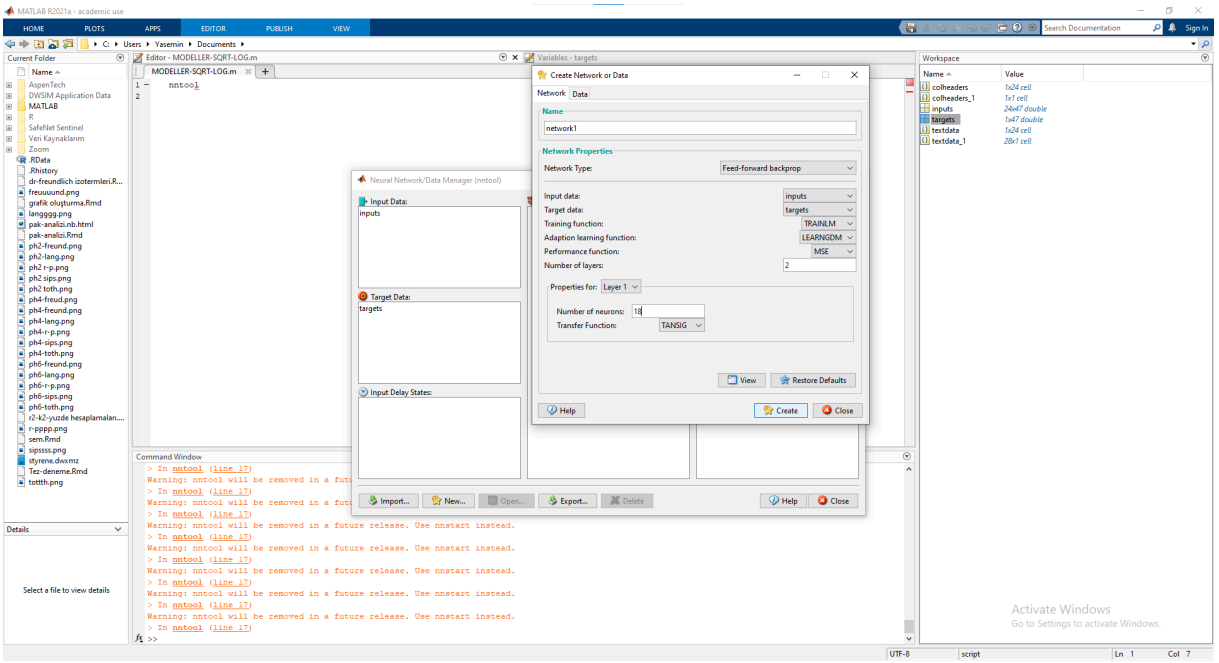


Figure 4.15 ANN modeling panel

It is switched to the train tab, input and target data are selected, network train is selected. The Panel is shown in Figure 4.17.

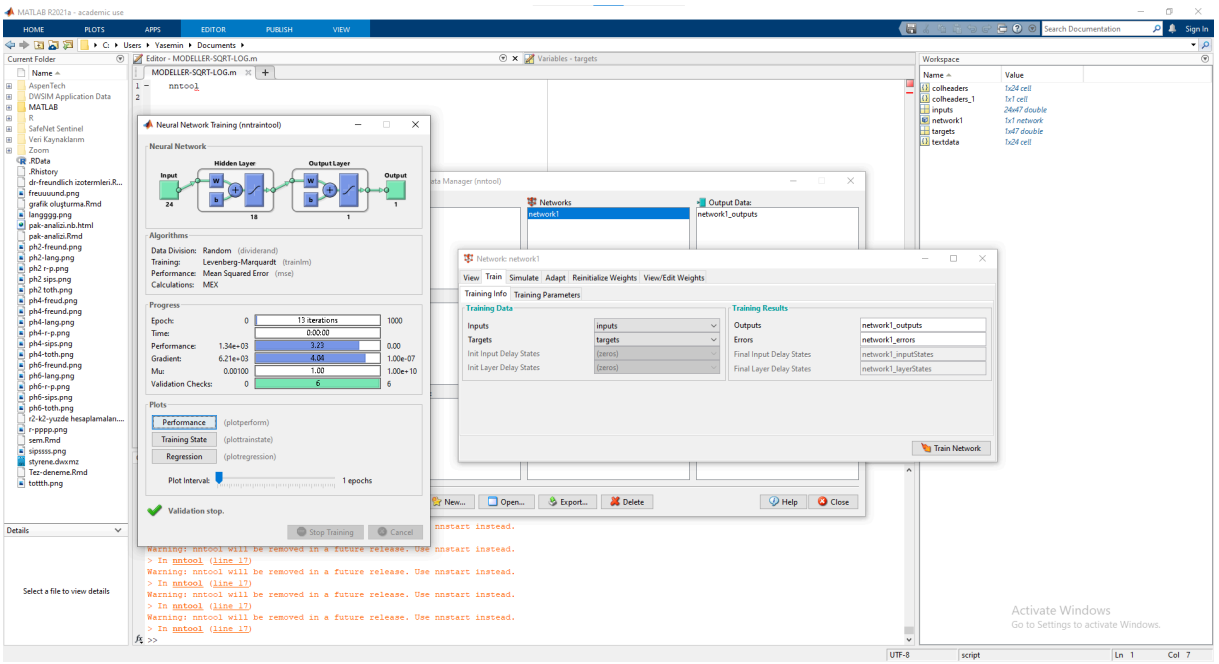


Figure 4.16 Train panel of the model formed

Compatibility of training, validation and test sets are observed from the charts. It is shown in Figure 4.18

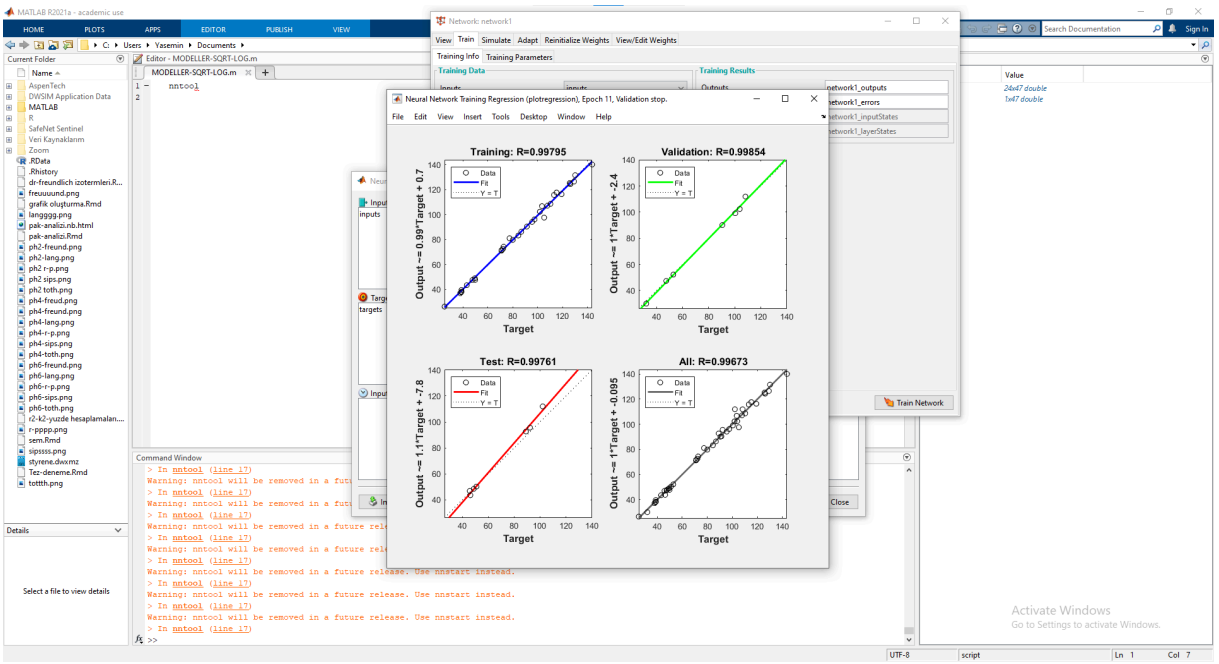


Figure 4.17 Graphical panel

The output and error values of the modeled sets are recorded. In order to estimate the experimental inputs given in the model, random data is deleted from target data and all stages are repeated.

5. RESULTS AND DISCUSSION

5.1. Results for nonlinear regression analysis of adsorption data in MATLAB

All of the obtained results for every pH value and adsorption isotherms in MATLAB are shown in Table 5.1.

Table 5.1 Constants of Adsorption Isotherm models obtained from nonlinear regression analysis via MATLAB

		ph2	**ph4**	**ph6**
Freundlich	K_f	97.17	66.45	24.05
	N	8.268	7.126	4627
	R^2	0.9826	0.9909	0.9943
	%Error	5.2774	2.8234	1.286
	$X^2 Error$	0.3109	0.0860	0.0092
Langmuir	Q	118.1	92.99	50.13
	B	79.17	12.22	0.5563
	R^2	0.7398	0.845	0.9387
	%Error	23.4847	10.0805	5.0248
	$X^2 Error$	4.1310	0.9924	0.1193
Sips (Langmuir-Freundlich)	q_m	202.2	190.3	98.12
	K_s	1.029	0.5586	0.3054
	Ms	0.2336	0.2307	0.3519
	R^2	0.9954	0.9959	0.997
	%Error	1.5993	1.8821	0.9384

	$X^2 Error$	0.0438	0.0377	0.0043
Redlich Peterson	K	62300	5096	141.7
	A	620.3	72.65	5.2430
	β	0.8943	0.8802	0.8188
	R^2	0.9937	0.9975	0.9966
	%Error	2.7299	1.3291	1.0209
	$X^2 Error$	0.0913	0.0171	0.0050

$$R^2 = \frac{\Sigma[(q_m - q_{e,mean})^2]}{\Sigma(q_m - q_{e,mean})^2 + (q_m - q_e)^2}, \quad (4.1)$$

$$\chi^2 = \frac{\sum_1^N \left[\frac{(q_e - q_m)^2}{q_m}\right]}{N}, \quad (4.2)$$

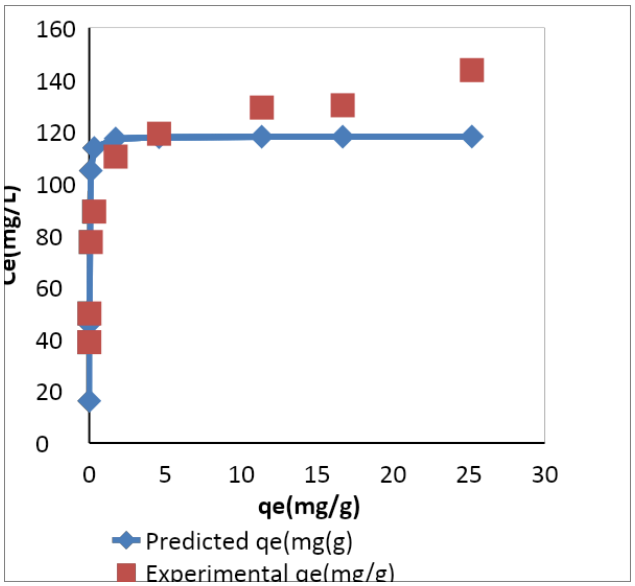
$$\%\ Error = \frac{\sum_1^N \left[\frac{(q_e - q_m)}{q_e}.100\right]}{N}, \quad (4.3)$$

Here, q_e, $q_{e,mean}$ and q_m are respectively experimental equilibrium adsorption capacity($mg.g^{-1}$), the average of experimental adsorption capacities($mg.g^{-1}$) and theoretical equilibrium adsorption capacity($mg.g^{-1}$) values, and N refers to the total number of experimental data.

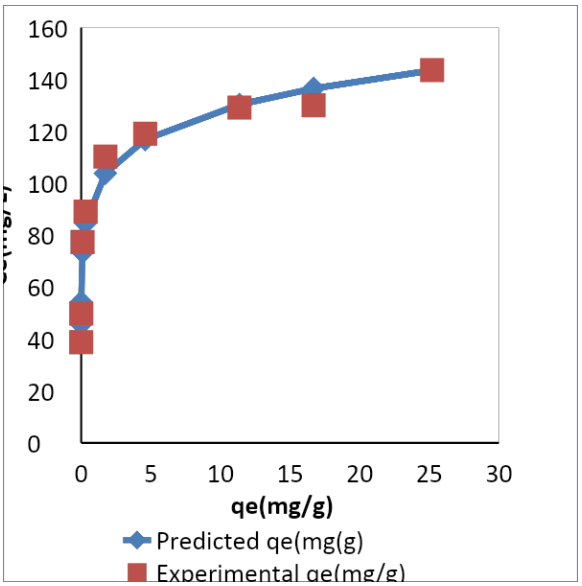
Table 5.1 shows the constants of each adsorption isotherm, when two parameter adsorption isotherms are compared, % error values of the Freundlich (ph2:5.28, ph4:2.82, ph6:1.28) is lower than Langmuir's (ph2:27.29, ph4:10.08, ph6:5.02) for each pH. When three-parameter adsorption isotherms are compared, the % error of Sips (ph2:1.59, ph4:1.89, ph6:0.95) is lower than the % error of R-P (ph2:2.72, ph4:1.33, ph6:1.02) for each pH values.

Langmuir, Freundlich, Sips and Redlich-Peterson adsorption isotherms with experimental data obtained at pH2 are shown in Figure 5.1.

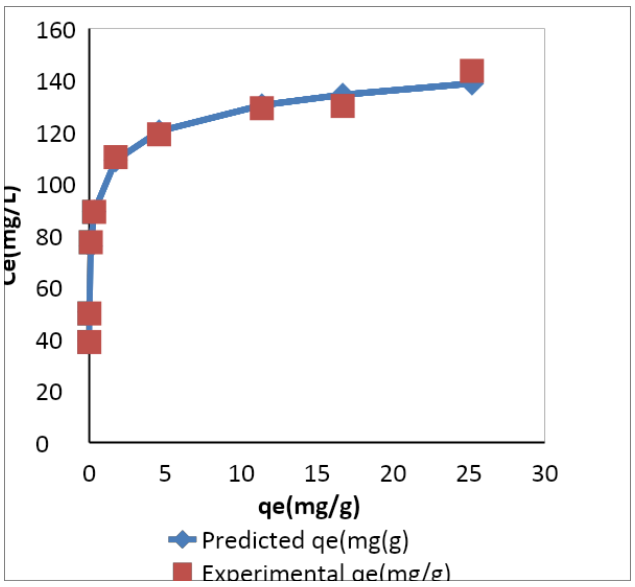
Langmuir



Freundlich



Sips



R-P

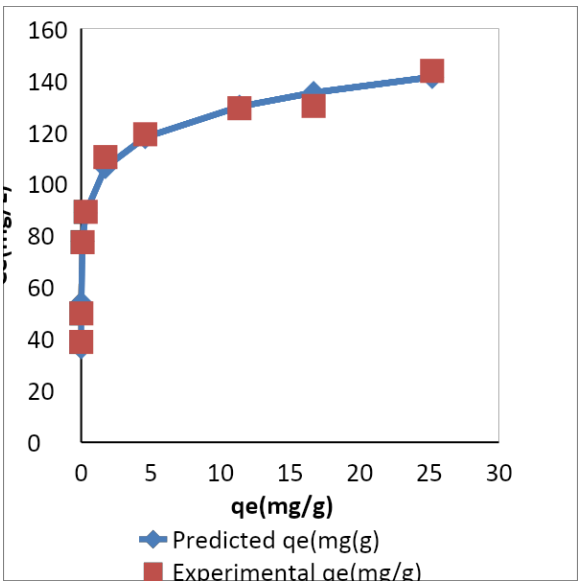


Figure 5.1 Theoretical and experimental adsorption isotherms for pH2 dataset obtained via MATLAB

As can be seen from Figure 5.1, The predicted values of Freundlich and Sips Adsorption Isotherms are closer to the experimental values for pH2. When Chi-Square and R^2 are encountered, the most optimal model is the Sips isotherm for pH2.

Langmuir, Freundlich, Sips and Redlich-Peterson adsorption isotherms with experimental data obtained at pH4 are shown in Figure 5.2.

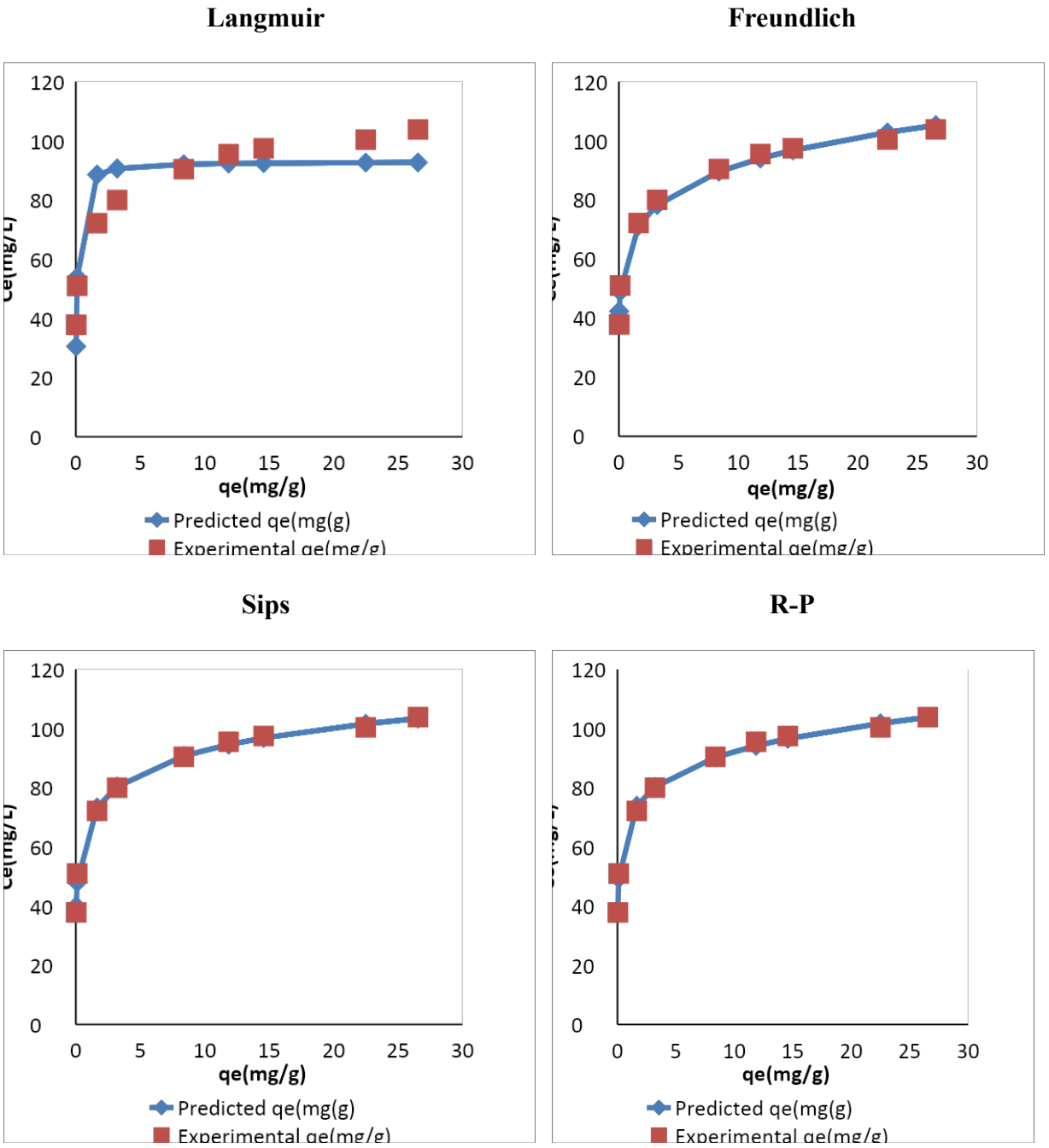


Figure 5.2 Theoretical and experimental adsorption isotherms for pH4 dataset obtained via MATLAB

As can be seen from Figure 5.2, The predicted values of Freundlich, Sips and R-P Adsorption Isotherms are closer to the experimental values for pH4. In this case, it can compared R^2 values of adsorption isotherms. R^2 of R-P as 0.9975 highest and Chi-square of R-P as 0.0171 lowest. R-P is the most suitable model for pH4.

Langmuir, Freundlich, Sips and Redlich-Peterson adsorption isotherms with experimental data obtained at pH6 are shown in Figure 5.3

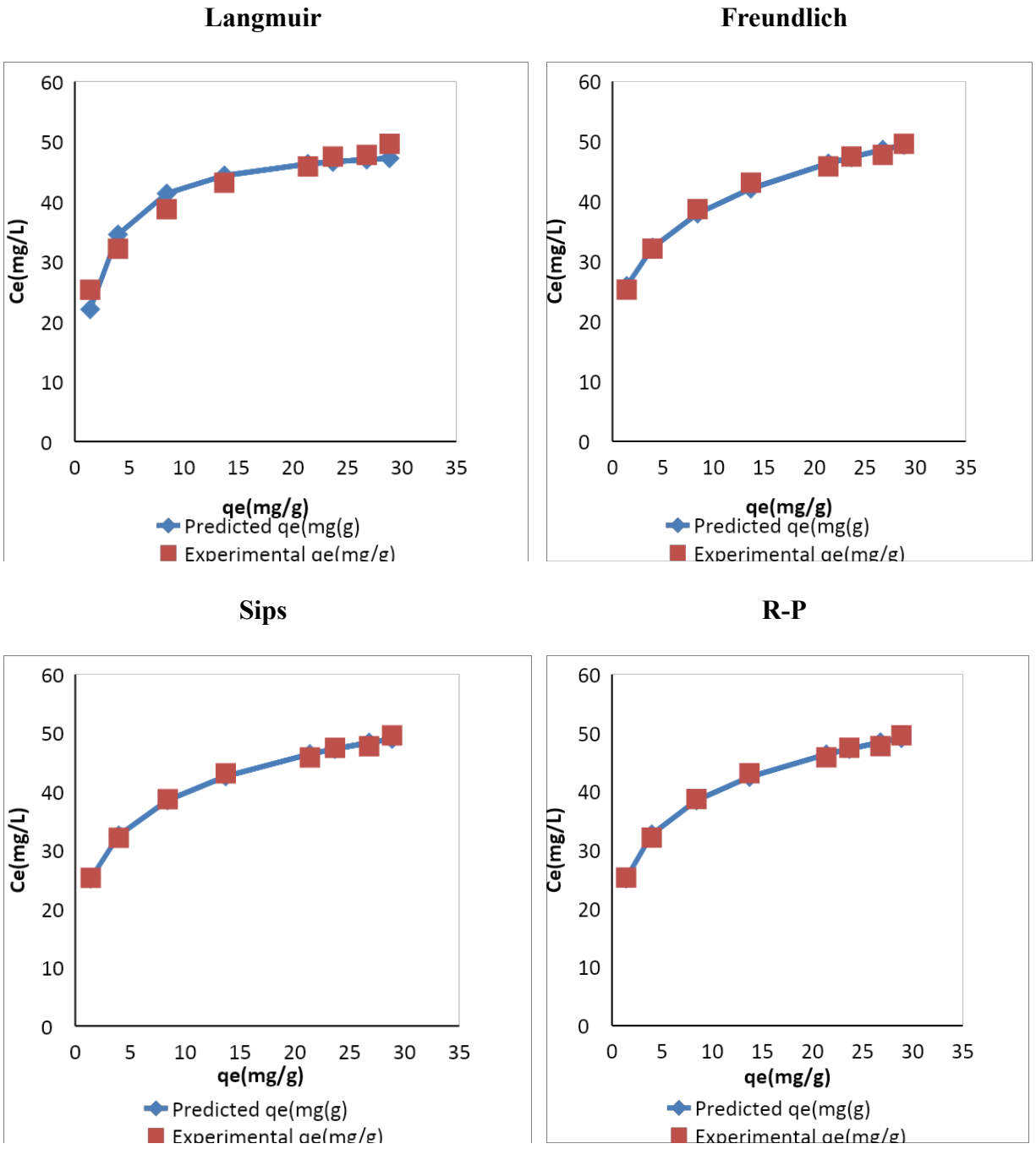


Figure 5.3 Theoretical and experimental adsorption isotherms for pH4 dataset obtained via MATLAB

As can be seen from Figure 5.3, The predicted values of Freundlich, Sips and R-P Adsorption Isotherms are closer to the experimental values for pH6. In this case, it can compared R^2 values of adsorption isotherms. When Chi-Square and R^2 are encountered, the most optimal model is the sips isotherm for pH6.

5.2. Results for Adsorption Isotherms in R Program

All the obtained data from the Table 4.1and non-linear regression of Adsorption Isotherms in R for pH2, pH4, pH6 dataset is shown in Table 5.2

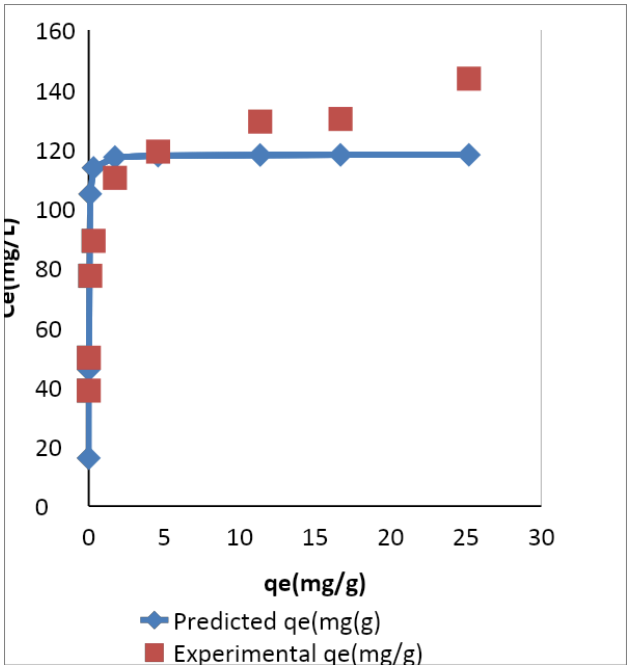
Table 5.2 Constants of Adsorption Isotherm models obtained from nonlinear regression analysis via R Programming

		ph2	ph4	ph6
Freundlich	K_f	97.1713	66.4741	24.0486
	N	8.2678	7.1350	4.6719
	R^2	0.9819	0.9907	0.9942
	%Error	5.5872	2.9169	1.3323
	$X^2 Error$	0.3110	0.0862	0.0093
Langmuir	Q	118.0960	92.9880	50.1279
	B	79.2930	12.2240	0.5564
	R^2	0.8028	0.8595	0.9449
	%Error	19.1866	9.9877	4.8813
	$X^2 Error$	4.1291	0.1194	0.1194
Sips (Langmuir-Freundlich)	q_m	202.1522	190.2323	98.1220
	K_s	1.0290	0.5587	0.3054
	Ms	0.2336	0.2307	0.3505

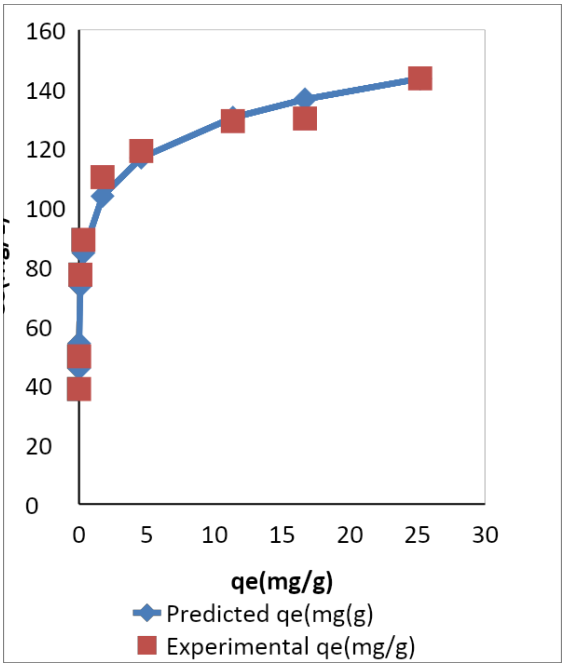
	R^2	0.9954	0.9959	0.9970
	%Error	1.5883	1.8915	0.9450
	$X^2 Error$	0.0438	0.0378	0.0044
Redlich-Peterson	K	62,300	5095	141.6579
	A	620.3	72.64	5.2427
	β	0.8943	0.8802	0.8188
	R^2	0.9937	0.9975	0.9992
	%Error	2.7585	1.3126	1.0366
	$X^2 Error$	0.0914	0.0170	0.0052

Table 5.2 shows the constants of each adsorption isotherm, when two parameter adsorption isotherms are compared, the Freundlich(ph2:5.59, ph4:2.91, ph6:1.33) % error is lower than Langmuir's(ph2:19.19, ph4:9.98, ph6:4.88) % error for each pH; when three-parameter adsorption isotherms are compared, the % error of Sips(ph2:1.59, ph4:1.89, ph6:0.95) is lower than the % error of R-P(ph2:2.76, ph4:1.31, ph6:1.03) for each pH values.

Langmuir



Freundlich



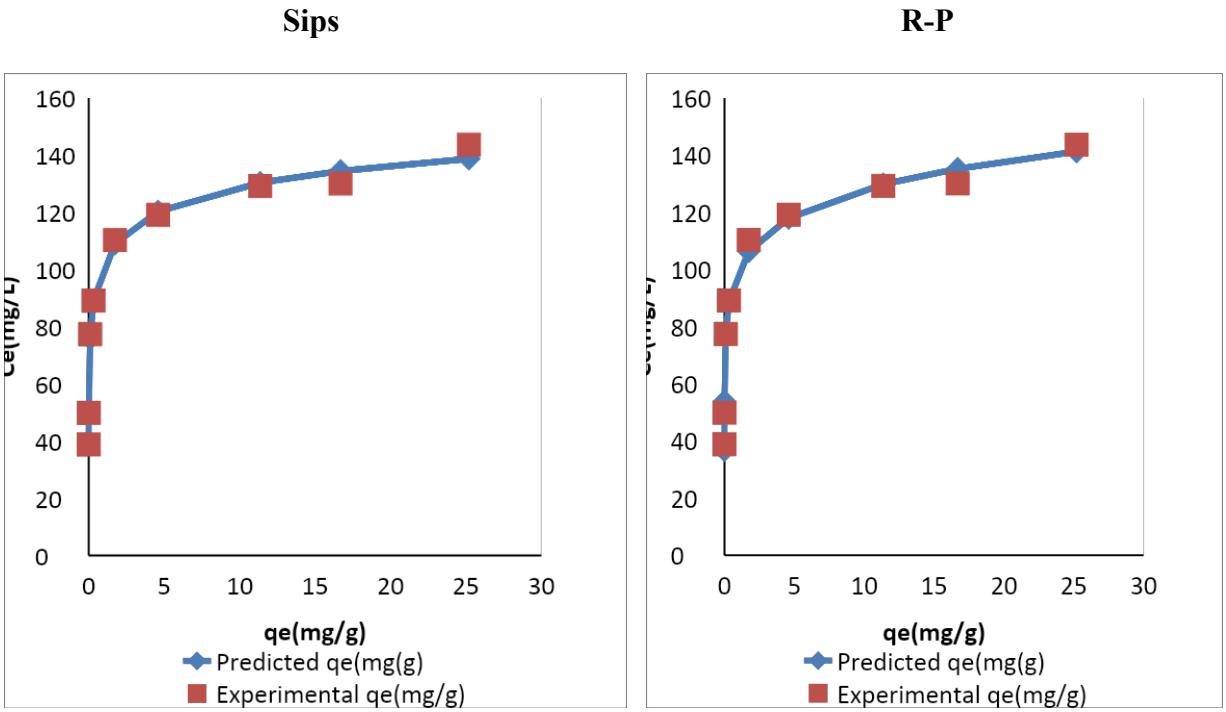
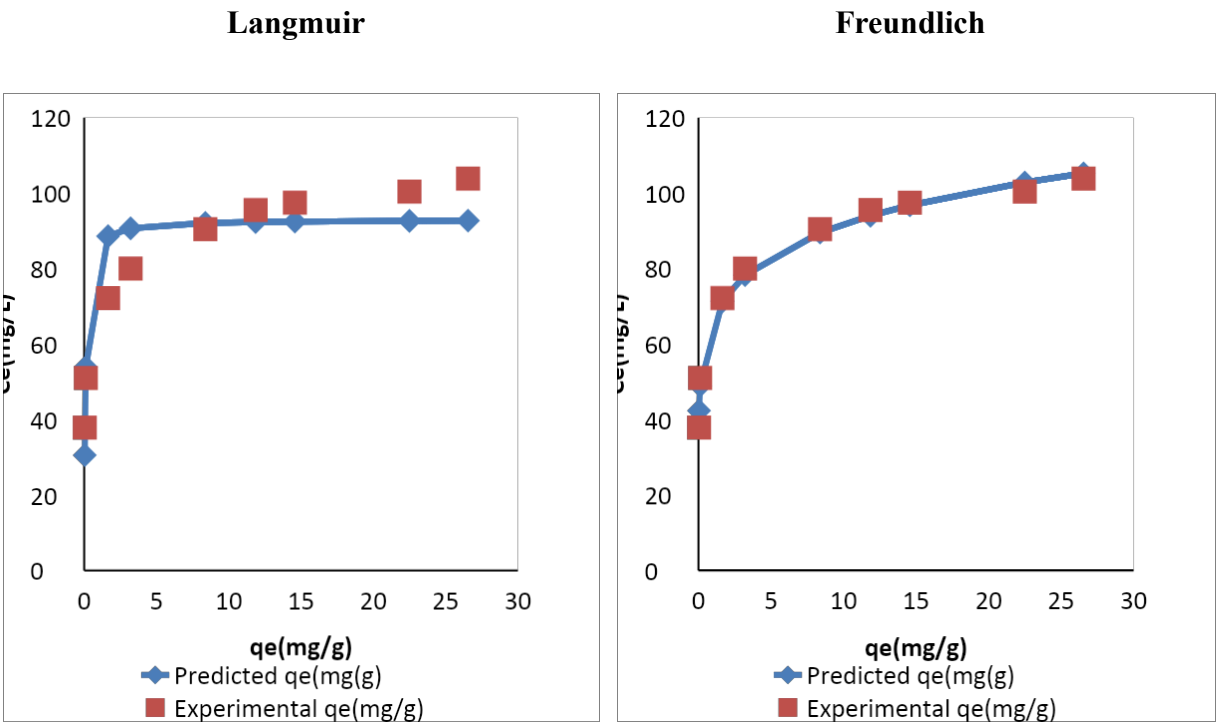


Figure 5.4 Theoretical and experimental adsorption isotherms for pH2 dataset obtained via R

As can be seen from Figure 5.4, The predicted values of Freundlich and Sips Adsorption Isotherms are closer to the experimental values for pH2. When Chi-Square and R^2 are encountered, the most optimal model is the Sips isotherm for pH2.

Langmuir, Freundlich, Sips and Redlich-Peterson adsorption isotherms with experimental data obtained at pH4 are shown in Figure 5.4



Sips **R-P**

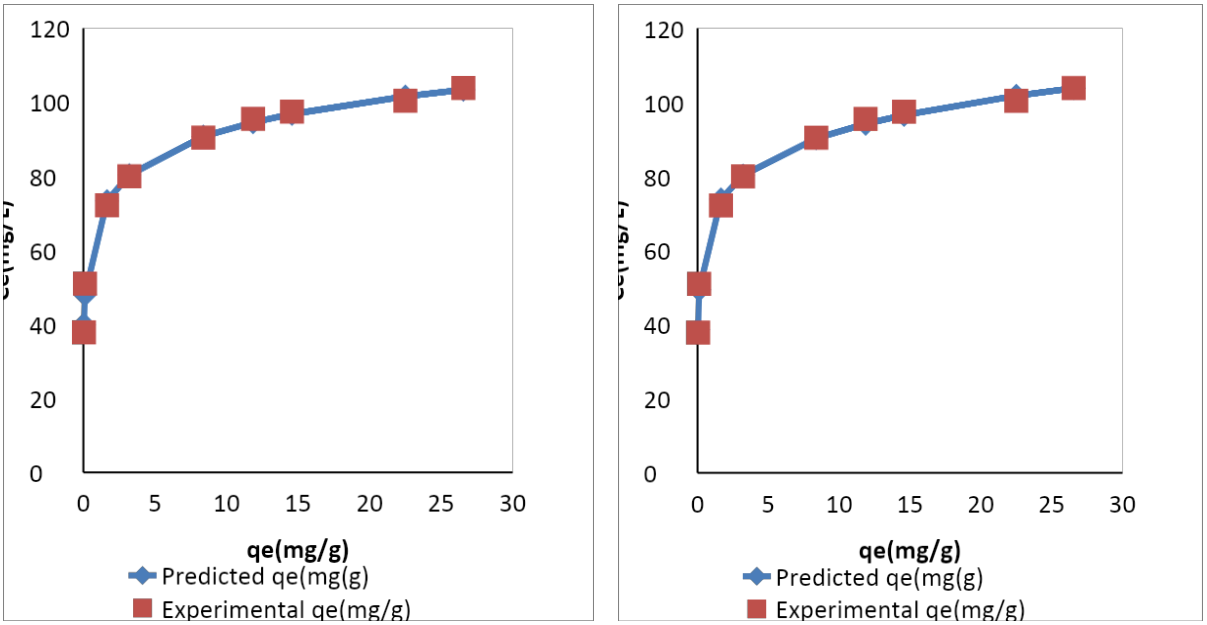


Figure 5.5 Theoretical and experimental adsorption isotherms for pH4 dataset obtained via R

As can be seen from Figure 5.5, The predicted values of Freundlich, Sips and R-P Adsorption Isotherms are closer to the experimental values for pH4. In this case, it can compared R^2 values of adsorption isotherms. R^2 of R-P as 0.9959 highest and Chi-square of R-P as 0.0170 lowest. R-P is the most suitable model for pH4.

Langmuir, Freundlich, Sips and Redlich-Peterson adsorption isotherms with experimental data obtained at pH6 are shown in Figure 5.6

Langmuir **Freundlich**

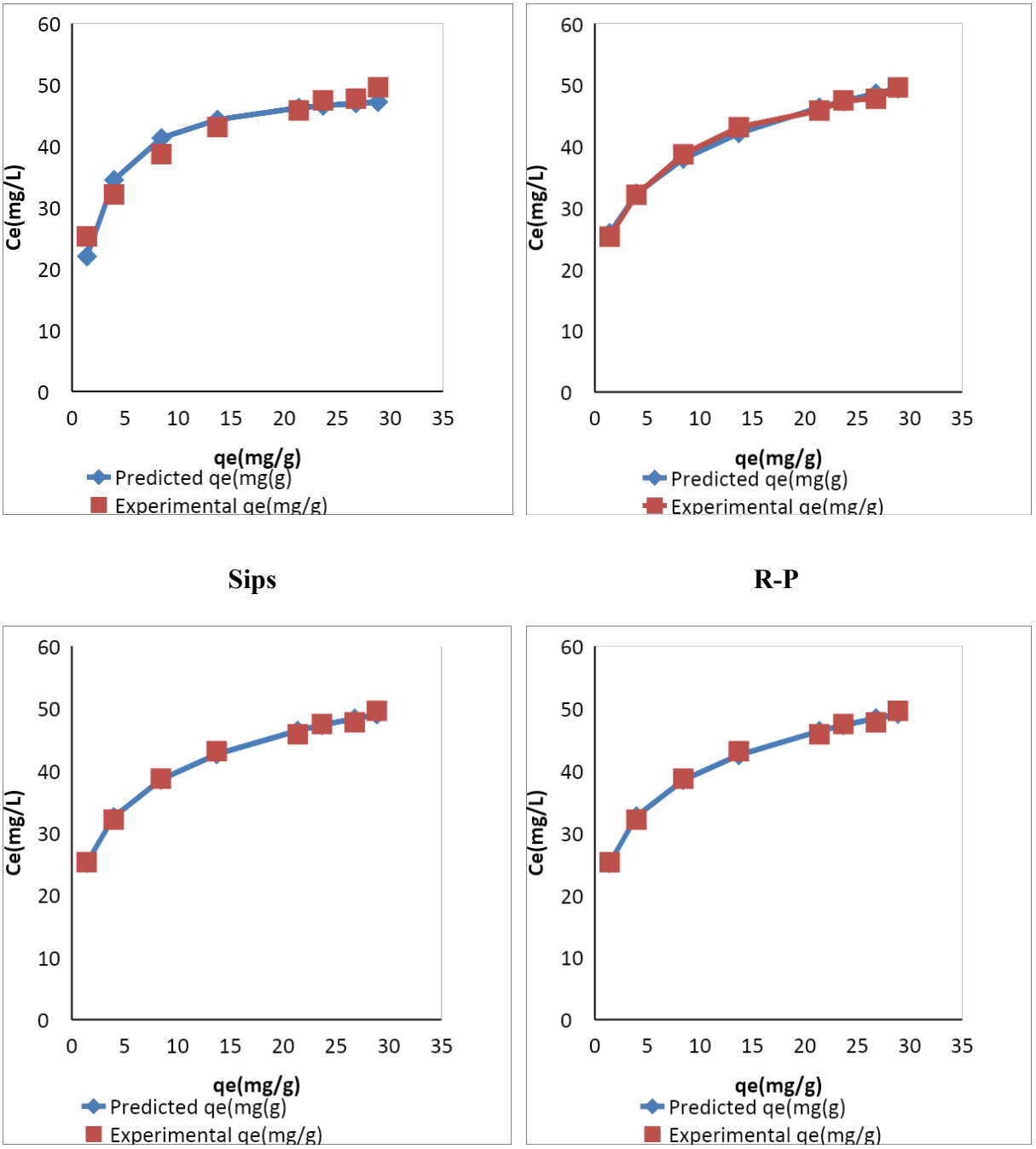


Figure 5.6 Theoretical and experimental adsorption isotherms for pH6 dataset obtained via R

As can be seen from Figure 5.6, The predicted values of Freundlich, Sips and R-P Adsorption Isotherms are closer to the experimental values for pH4. In this case, it can compared R^2 values of adsorption isotherms. When Chi-Square and R^2 are encountered, the most optimal model is the Sips isotherm for pH6.

As a summary table all results, which are obtained by the application of Non-Linear regression are seen in Table 5.3.

Table 5.3 Summary Table for Non-Linear Regression Result

		Matlab	R	Matlab	R	Matlab	R
		pH2	pH2	pH4	pH4	pH6	pH6
Freundlich	Kf	97.170	97.171	66.45	66.474	24.050	24.049
	n	8.268	8.268	7.126	7.135	4.627	4.6719
	R^2	0.9826	0.9819	0.9909	0.9907	0.9943	0.9942
	% Error	5.277	5.587	2.823	2.917	1.286	1.332
	X^2	0.3109	0.3110	0.0860	0.0862	0.009	0.0093
Langmuir	Q	118.1	118.096	92.99	92.988	50.13	50.128
	b	79.17	79.293	12.220	12.224	0.5563	0.5564
	R^2	0.7398	0.8028	0.845	0.8595	0.9387	0.9449
	% Error	23.484	19.187	10.081	9.988	5.025	4.881
	X^2	4.131	4.129	0.9924	0.1194	0.1193	0.1194
Sips(Freundlich-Langmuir)	qm	202.2	202.152	190.3	190.232	98.12	98.122
	Ks	1.029	1.029	0.5586	0.5587	0.3054	0.3054
	ms	0.2336	0.2336	0.2307	0.2307	0.3519	0.3505
	R^2	0.9954	0.9954	0.9959	0.9959	0.997	0.9970
	% Error	1.599	1.599	1.882	1.892	0.9384	0.9450
	X^2	0.0438	0.0438	0.0377	0.0378	0.0043	0.0044
Redlich-Peterson	K	62.300	62.300	5096	5095	141.7	141.658
	a	620.3	620.3	72.65	72.64	5.243	5.243
	B	0.8943	0.8943	0.8802	0.8802	0.8188	0.8188
	R^2	0.9937	0.9937	0.9975	0.9975	0.9966	0.9992
	% Error	2.730	2.758	1.329	1.313	1.021	1.037
	X^2	0.0913	0.0914	0.0171	0.0170	0.0050	0.0052

From Table 5.3, MATLAB and R studies can be examined comparatively. As can be seen that there is no significant difference within the results obtained from MATLAB and R.

5.3 Results for ANN Modelling of Adsorption Data

As described earlier, the structure of the model is invisible because the ANN model creates a model with hidden layers; the estimated values change every time the program and model are run; therefore, R^2, chi-square and % error values change after each run. At the same time, their inputs (such as temperature, pH, activated carbon amount, initial concentration) were previously experimentally determined, but for those whose results were unknown, similar data were randomly extracted from the results of experimental data to conduct prediction studies.

Three different cases were examined, as future model calculations were intended to increase the accuracy of the values to be estimated.

- With raw Data: pH, amount of activated carbon, temperature, ppm, concentration was used as input data on base.
- With modified Data: logarithm, square, square root cube and inverse of inputs were added to the raw data in order to increase the diversity of raw data.

There are three different trials with Raw data and Modified data and one on the average of 20 times repeating with raw data and modified data. %Error, R^2 and Chi-Square values can be seen in Table 5.4 for all different cases.

Table 5.4 Artificial Neural Network Study Summary

	Trials	With Raw Data	With Modified Data	Average of 20 Runs with Raw Data	Average of 20 Runs with Modified Data
% Error	Trial 1	4.5600	2.9755	2.2106	2.7281
	Trial2	1.9946	4.3300		
	Trial3	0.7101	4.1937		
R^2	Trial1	0.9587	0.9882	0.9942	0.9934
	Trial2	0.9944	0.9731		
	Trial3	0.9944	0.9693		
Chi-Square	Trial1	0.5373	0.1700	0.0645	0.0753
	Trail2	0.0672	0.4704		
	Trail3	0.1224	0.4105		

With Raw Data Modelling, R^2 ranged from 0.95 to 0.99; Chi-square ranged from 0.12243 to 0.53725; % Error ranged from 0.7101 to 4.55995. Modified data have also been tried to see if their duplication of the number of data in models affects the modeling but it remained in the range of the previously mentioned range.

In this case of uncertainty, the idea occurred to model raw data many more times and use their averages. In the study of the third model, these results are estimated 0.9942 as R^2 ,

0.0645 as Chi-square and 2.2106 as % error. In the study of the fourth model, these results are estimated 0.9934 as R^2 , 0.0753 as Chi-square and 2.7281 as % error.

Experimental qe is shown in the column one and predicted values from ANN with Raw data, Modified data and Average values of 20 times repeating and %Error values of this predictions are shown in the Table 5.5

Table 5.5 Predicted Values for different cases

Experimental qe	Raw Data						Average of 20 times Repeating on Raw Data	
	Trial 1		Trial 2		Trial 3			
	qe Predicted	Error %	qe Predicted	Error %	qe Predicted	Error %	qe Predicted	Error %
110.3074	117.7072	6.7083	105.9715	3.9307	110.1519	0.1410	107.6660	2.3947
86.8930	87.8756	1.1308	88.9176	2.3299	89.3422	2.8186	72.9584	0.3913
72.1787	70.2302	2.6996	72.1815	0.0039	71.6382	0.7488	72.2470	0.0947
43.1130	42.4421	1.5561	47.0383	9.1047	31.4359	27.0849	42.6860	0.9904
92.2380	72.5736	21.3192	96.6633	4.7977	94.3539	2.2940	100.4890	8.9450
107.7400	106.2163	1.4142	106.9611	0.7229	104.3675	3.1302	104.4480	3.0557

Table 5.6 Predicted Values From ANN with Modified Data and Average Values Of 20 Times Repeating of Modified Data

Experimental qe	Modified Data	Average of 20 times Repeating Modified Data

	Trial 1		Trial 2		Trial 3			
	qe Predicted	Error %	qe Predicted	Error %	qe Predicted	Error %	qe Predicted	Error %
110.3074	109.0056	1.3018	108.2564	2.0510	110.8693	0.5619	107.9900	2.1023
86.8930	87.6725	0.7795	88.5359	1.6429	89.5515	2.6585	88.0300	1.3040
72.1787	73.5172	1.3385	71.2665	0.9122	71.8618	0.3169	71.3700	1.1203
43.1130	41.9008	1.2122	43.0647	0.0483	43.2090	0.0960	41.1200	4.6243
92.2380	95.4412	3.2033	88.8610	3.3770	99.2552	7.0172	97.7100	1.0811
107.7400	107.0978	0.6422	105.4656	2.2744	107.7475	0.0070	110.4300	3.2400

In the prediction section, it is seen that there are modified data in which the data is estimated closer (as range 0.048-7.01%error) than raw data (as range 0.14-27.08%).

In the analysis of the models which were created 20 times and took average values, the predicted values of raw (0.09-8.94%) were closer but one data showed an excessive deviation.

The models show two trends; in the first, it shows all errors around 3.05-.9.1% and in the second case, there are one or two values that deviate too much in the estimation while the other values deviate errors 0.007-3.24%.

6. CONCLUSIONS

In this study, experimental adsorption data obtained previously (Duranoğlu, 2008) were modelled. . This study consists of two different modeling methods; nonlinear regression analysis and ANN modelling.

For the first part of the modelling, theoretical adsorption isotherm constants, were calculated using non-linear regression method via MATLAB and R programming. The results of the first part of the study are as follows:

- It was observed that the values obtained in R and MATLAB were compatible.
- Freundlich (R^2:0.9907) in two-parameter adsorption isotherms; Sips(R^2:0.9959) in three-parameter adsorption isotherms are optimal values for all pH conditions. Compared to these two isotherms, Sips isotherm was found to be more suitable for total experimental data.

In the second part of modelling, Adsorption data was predicted using the ANN model. Data from the adsorption experiments, whose properties are known (pH, amount of activated carbon, temperature and initial concentrations), have been studied to be able to predict their future values (qe). Therefore; modeling of raw data, modified data and average of raw data repeated 20 times and average of modified data repeated 20 times has been run and their results are as follows:

- After the analysis of the raw data used, logarithms, squares, squared roots, cube and inverse values of inputs were added to find out if replicating the number of data in models affected modeling. However, R^2, Chi-square and % error values remained in the previous range.
- The average results of the ANN models by trying 20 times predicted more closely than the raw data and modified data.
- In ANN studies conducted by averaging 20 models, compared to modified data and raw data, raw data seems more appropriate. But, the situation varies, when the predicted variables are examined.

The models show two trends; in the first, it shows all errors around 3.05-.9.1% and in the second case, there are one or two values that deviate too much in the estimation while the other values deviate errors 0.007-3.24%.

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[1] https://www.r-project.org/about.html