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Modeling and simulation for the adsorptive removal of Cr(VI) from aqueous solution

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ABSTRACT

Cr(VI) adsorption experiments were carried out using activated carbon obtained from a waste weed *Salvinia cucullata.* The adsorbent was characterized using SEM, BET, EDAX, FT-IR, etc. Matrix method was used to develop an empirical mathematical model. Factorial design of experiments was used to minimize the number of experiments required to develop an empirical model. In the mathematical model, percentage adsorption of Cr(VI) was represented as a function of process variables like contact time, initial pH of the solution, and temperature. pH had the most influential effect on the adsorption process followed by contact time and temperature. The significance of different adsorption parameters and their combined effect on the adsorption process was established. The empirical model was simulated and solved using MATLAB and LabVIEW. The goodness of fit of the developed mathematical models to the experimental values was examined using different error analysis methods such as SSE, SAE, ARE, and ARS.

Keywords: Adsorption; Cr(VI); Factorial design; LabVIEW; Error analysis; Modeling

1. Introduction

Cr(VI) contamination of water sources is a contentious issue all over the world as it is well-known pollutant in different mining and industrial wastewater [1–5]. The adsorption process is believed to be a potential and economically feasible alternative to the wastewater treatment [6–10]. Further heavy metal adsorption using biomaterials can reduce capital cost by 20%, operational cost by 36%, and total treatment cost by 28%, as compared to other treatment processes [7]. We used carbonized *Salvinia cucullata*, a fresh water weed for the treatment of Cr(VI) contaminated wastewater in our previously reported studies [11,12]. In order to plan an adsorption process, a number of influencing parameters such as contact time, pH, adsorbate concentration, adsorbent dose, stirring speed, particle size, and temperature are need to be studied. But the process of studying each and every variance separately is quite tedious as well as time-consuming. Further, conventional and classical methods of studying the effect of different factors involved in the adsorption process at an unspecified constant level do not depict the combined effect of all the factors involved [13]. This method requires a large number of experiments to determine the optimal levels, which are unreliable. Thus, the optimization of

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all the affecting parameters collectively by using different mathematical models can minimize the above difficulties [14,15]. Therefore, as a continuation to our previous work, attempt was made in the present study to develop empirical mathematical model using matrix method. Objectives of the present study are basically to

- determine those variables which are the most influential on the response
- developing empirical models based on the independent variable so that the response is almost always near the desired maximal/minimal value
- minimize the effect of uncontrollable variable inputs
- find out the optimal process parameters

Experimental design method is an important tool in the engineering science for achieving better results with minimal effort. It has also been applied extensively in the development of new processes. Application of this method in the process development can result in improved yield, reduced variability and firm confirmation to nominal or target requirements, reduced development time, and reduced overall cost [16]. Further, predesign of experiments determines which factors have important bearings on an expected response as well as how the effect of one factor varies with the level of other factors [17–20]. A factorial experiment is the important source to quantitatively assess the individual independent terms including interaction effects of different coefficients and factors. Adsorption experiments were carried out by using a factorial design of the type 2^k. Further, which parameter has the most pronounced effect on the adsorption process was studied by developing a suitable mathematical expression using matrix method.

The MATLAB is a user-friendly tool for solving equations of various kinds by writing a proper code for the requirement. Regarded as the language for technical computing, MATLAB has also been widely used by researchers in industrial and applied mathematics, as well as engineers, scientists, and economists because of its efficiency in dealing with matrices and matrix algebra [21]. In addition, the availability of special purpose toolboxes (such as signal processing, optimization and financial toolboxes) has made it easier for researchers to use MATLAB in their work. It can be used to finish our task of solving equations easily provided the code is correct. Besides using it as a mathematical tool for solving equations, MATLAB can be used as a language to write algorithms for various softwares like LabVIEW simulation software. Also, programming languages like C can also be coded using MATLAB. In the present study, we used the matrix method to develop a mathematical model for the adsorption process. We have written a code using MATLAB to simulate the developed mathematical model.

LabVIEW is an integrated data acquisition, analysis, and presentation package for the graphical programming of scientific and engineering applications in the areas of measurement, simulation, and control using the computer. User-written LabVIEW programs are called "virtual instruments" (VIs). VIs have three main parts: the front panel, block diagram, and icon = connector. The front panel provides the user an interface for data inputs and outputs. The user operates the front panel by using the computer's keyboard and mouse. Behind the front panel is the block diagram that is responsible for the actual data flow between the inputs and outputs. The icon = connector defines data flow between subroutines. LabVIEW includes device driver functions for serial and parallel interfaces and a wide range of mathematical, logic, timing and digital signal generation, processing and analysis functions. LabVIEW has been used in areas such as simulation, automated testing, data acquisition and analysis, and process control.

It is possible for amateur programmers to design programs of high quality by using LabVIEW, and it suits the thinking methods of scientists and engineers so that it can be honored with the name of engineering language [22]. LabVIEW has wide application in the fields of aerospace, communications, automobile engineering, biomedicine, and so forth. However, to our knowledge, it has not yet been reported on frequently in the field of chemical engineering [23]. LabVIEW graphical programming relieves the user of writing and debugging code in conventional programming languages and replaces this with the simple and intuitive task of interconnecting functional blocks and control structures. The iconic presentation of blocks and structures and the familiar block diagram layout make the application almost self-explanatory with little need for additional documentation. The hierarchical nature of the VI concept allows complex systems to be divided into a set of more manageable sub-systems in a structured.

2. Summary of the batch and column study

Batch and column adsorption studies were carried out for the treatment of Cr(VI) contaminated wastewater using carbonized weed *Salvinia cucullata*. In the batch process, percentage of Cr(VI) adsorption was studied as a function of different adsorption

parameters such as stirring speed, contact time, pH, adsorbate concentration, adsorbent dose, and temperature. From the stirring speed variation experiments, it was found that the percentage of adsorption increased with increase in stirring speed up to 600 rpm. Therefore, it was concluded that 600 rpm is the optimum stirring speed at which we can safely assume that the bulk diffusion resistance was minimum. From the time variation experiments, it was observed that the adsorption process followed dual rate, i.e. initial faster rate followed by a slower one. It was also observed that initially faster kinetics was lasted for 30 min. The equilibrium time was found to be 720 min. In order to find out the effect of pH on the adsorption process, the initial pH was varied between 1.7 and 4.5. From the pH variation experiment, it was observed that the percentage adsorption and uptake increased with decrease in pH. The higher adsorption at lower pH may be due to ligand exchange mechanism as well as surface complexation mechanism. The optimum pH was found to be 1.7. The initial Cr(VI) concentration was varied from 400 to 700 mg/l to evaluate its effect on adsorption efficiency. The percentage adsorption decreased with increase in adsorbate concentration, whereas the uptake was found to increase with increase in adsorbate concentration. With increase in adsorbent dose, the percentage adsorption and uptake was found to increase and decrease, respectively. The temperature was varied from 30 to 60˚C and it was found that the percentage of adsorption as well as uptake increased with increase in temperature. Therefore, it was concluded that adsorption process is endothermic in nature. Four different adsorption kinetic models were employed to the experimental data to find out the best fit. From the kinetic study, it was observed that adsorption process followed pseudo-second-order rate equation. Experimental data fitted well to the Langmuir adsorption isotherm. Surface diffusion was found to be the rate controlling mechanism. The results of the batch adsorption studies are summarized in Table 1.

3. Experimental

3.1. Preparation and characterization of material

All the reagents used in this study were of analytical grade. Aqueous solution of Cr(VI) was prepared by dissolving requisite amount of $K_2Cr_2O_7$ in double-distilled water. A stock solution having concentration 1,000 mg/l of Cr(VI) was prepared and subsequently diluted to the required strengths to carry out the adsorption studies. The pH of the solution was varied using dilute hydrochloric acid and sodium hydroxide solutions.

The carbonized weed, *Salvinia Cucullata*, used in this study was collected from a lake situated about 15 km from Bhubaneswar, the capital city of Orissa. The weed grows profusely and is removed periodically to enhance the life of the lake. The weed collected from the lake was washed with tap water

Table 1
Summery of the batch adsorption study

Sl. no.	Parameters	Variation interval	Variation in %Ads.	Variation in uptake (mg/g)	Conditions
1	Agitation speed (rpm)	100–600	45.1–65.6	112.8–164.2	pH 1.7, Adsorbate conc. 500 mg/l, Adsorbent dose 2000 mg/l, Temp 30˚C, Time 12 h, Particle size 53.55 microns
2	Contact time (min)	0–720	0–65.7	0–164.2	pH 1.7, Adsorbate conc. 500 mg/l, Adsorbent dose 2000 mg/l, Temp 30˚C, Agitation speed 600 rpm, Particle size 53.55 microns
3	pH	1.7–4.5	65.7–13	164.2–232.5	Time 12 h, Adsorbate conc. 500 mg/l, Adsorbent dose 2000 mg/l, Temp 30˚C, Agitation speed 600 rpm, Particle size 53.55 microns
4	Adsorbate cons. (mg/l)	400–700	72–47	144–164	Time 12 h, pH 1.7, Adsorbent dose 2000 mg/l, Temp 30˚C, Agitation speed 600 rpm, Particle size 53.55 microns
5	Adsorbent dose (mg/l)	800–2,400	30–70	188–146	Time 12 h, pH 1.7, Adsorbate conc. 500 mg/l, Temp 30˚C, Agitation speed 600 rpm, Particle size 53.55 microns
6	Temperature (˚C)	30–60	65–84	164–212	Time 12 h, pH 1.7, Adsorbate conc. 500 mg/l, Adsorbent dose 2000 mg/l, Agitation speed 600 rpm, Particle size 53.55 microns
7	Particle size (microns)	53.5–221	66–51	164–128	Time 12 h, pH 1.7, Adsorbate conc. 500 mg/l, Adsorbent dose 2000 mg/l, Agitation speed 600 rpm, Temp 30˚C

followed by distilled water and sun-dried. Drying at 60^0C for 1hr in an oven has removed the adhering moisture. The dried material was crushed to powder. The powdered material was transferred to a muffle furnace, and activation was carried out at 500^0C under nitrogen atmosphere for 1 h. Subsequently, the carbonized mass was cooled to ambient temperature under nitrogen to prevent complete combustion. The carbonized mass thus produced was grounded and sieved to different fractions.

The smallest size fraction, i.e. 53.55 μm was used for adsorption studies. The physicochemical characteristics of the adsorbent are given in Table 2. X-ray diffraction (XRD) analysis was carried out using Cu Kα radiation on a computer controlled Philips 1,050 diffractometer. The scan speed was 0.5°2θ per minute and step size was 0.02°2θ. Patterns were recorded from 10 to 70°2θ. XRD analysis showed the peaks related to the major component corresponding to carbon.

The FT-IR spectra of the carbonized weed, before and after adsorption of Cr(VI), were used to determine the vibrational frequency changes in the functional groups of the adsorbents. The FT-IR spectra of the adsorbents display a number of absorption peaks, indicating the complex nature of the studied adsorbents. Table 3 presents the fundamental peaks of the adsorbents before and after use. In the carbonized weed before adsorption, the absorption peak around 2,940 cm^{-1} can be assigned to Aliphatic CH group. The peak at 1,680 cm^{-1} can be assigned to C=O stretching. The sharp peak observed at 1,600 cm^{-1} indicates the presence of secondary amino group. The other absorbance bands for the carbonized weed showed two sharp peaks at 1,555 cm^{-1} (amide bonds) and 1,361 cm^{-1} (carboxyl group); one broad band at 1,034 cm^{-1} (C−O stretching and SiO stretching) and a small peak at 885 cm^{-1} (aromatic CH). It is observed from Table 3 that the Cr(VI) adsorbed carbonized weed showed either a shift or reduction in absorption peak, suggesting the vital role played by the functional groups. These band shifts indicate that the secondary amine groups, Aliphatic CH, and carboxyl groups especially play a major role in Cr(VI) biosorption on carbonized weed. Similar observations related to Cr(VI) adsorption were observed by other researchers [24,25]. Powdered carbonized weed before and after adsorption was analyzed by scanning electron microprobe (SEM JXO-8100) at 300X magnification and the results are presented in Figs. 1 and 2. It can be seen from the figures that the carbonized weed before adsorption has irregular porous structures. It can be clearly seen from the micrographs that the surface becomes smooth after adsorption. Further, adsorption of Cr(VI) on the surface of the adsorbent was

Table 2
Physicochemical characteristics of the carbonized weed

Parameter	Values
Volatile matter (%)	28.4
Ash (%)	44.3
Fixed carbon (%)	27.3
Surface area, m^2/g	16.4
Particle size, cm	0.01875
Porosity (%)	48.9
Density, g/cc	1.44
Iodine number	1,050
XRD peak	Carbon

Table 3
The FT-IR spectral characteristics of carbonized weed before and after adsorption

IR peak	Adsorption band (cm^{-1})		Difference	Assignment
	Before adsorption	After adsorption		
1	2,940	2,948	8	Aliphatic CH
2	1,680	1,676	−4	C=O stretching
3	1,600	1,591	−9	Secondary amine group
4	1,555	1,560	5	Amide bond
5	1,361	1,367	6	Carboxyl group
6	1,034	1,038	4	C=O and SiO stretching
7	885	880	5	Aromatic CH

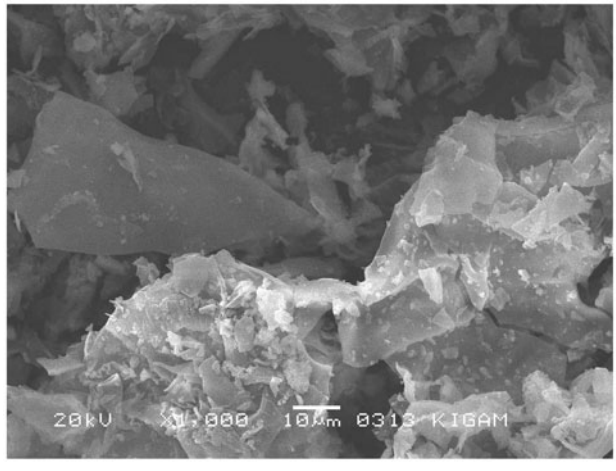

Fig. 1. SEM image of carbonized weed before adsorption.

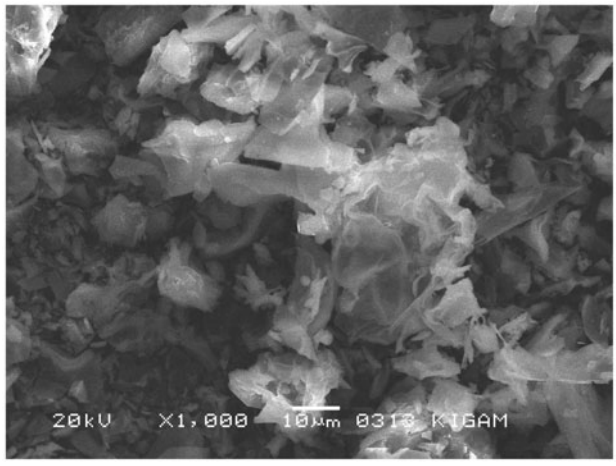

Fig. 2. SEM image of carbonized weed after adsorption.

confirmed from the elemental analysis by EDAX method. The EDAX images for the carbonized weed before and after adsorption are shown in Figs. 3 and 4. From the EDAX analysis, the mass percentage of the chromium on the adsorbent surface before and after adsorption was found to be 0.31 and 24.85%, respectively. The higher mass percentage of chromium in the used adsorbent clearly indicates the adsorption of Cr(VI) on the surface of the adsorbent.

3.2. Methods

Adsorption studies were carried out in batches using 250 ml of Cr(VI) solution taken in 500 ml beaker and stirred in Rime make mechanical stirrers where the temperature can be maintained within ±0.5°C of the desired value. For higher temperatures, the adsorption studies were carried out in a sealed unit to avoid the evaporation loss. 5 ml of representative samples was drawn from the reaction mixture at regular interval and filtered. The residual Cr(VI) concentration was analyzed spectrophotometrically using diphenyl carbazide in a PE LAMBDA 35 UV–visible spectrophotometer [26].

4. Results and discussion

4.1. Design of experiments

In order to minimize the number of experiments required to develop empirical mathematical model for adsorption of Cr(VI) on the treated weed, a full-factorial design of the type n^k has been used, where n is the number of levels and k is the number of factors under verification. Here time, pH, and temperature were chosen as three independent factors/variables ($k=3$ and $n=2$) and the percentage of adsorption as the dependent output response variable. A 2^3 full-factorial experimental design [19] with number of three triplicates at the center point and thus a total of 11 experiments were employed in this study. For statistical calculation, the base level, which is the average of two level, was calculated using the following relation

$$x_i = \frac{X_i - X_0}{\delta X} \quad (1)$$

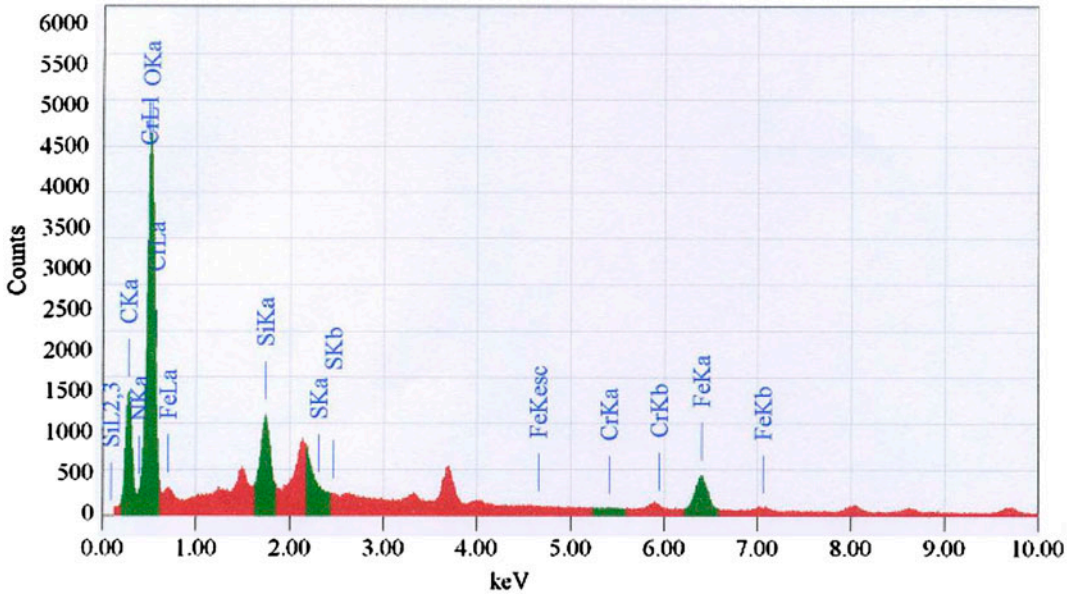

Fig. 3. EDAX plot for carbonized weed before adsorption.

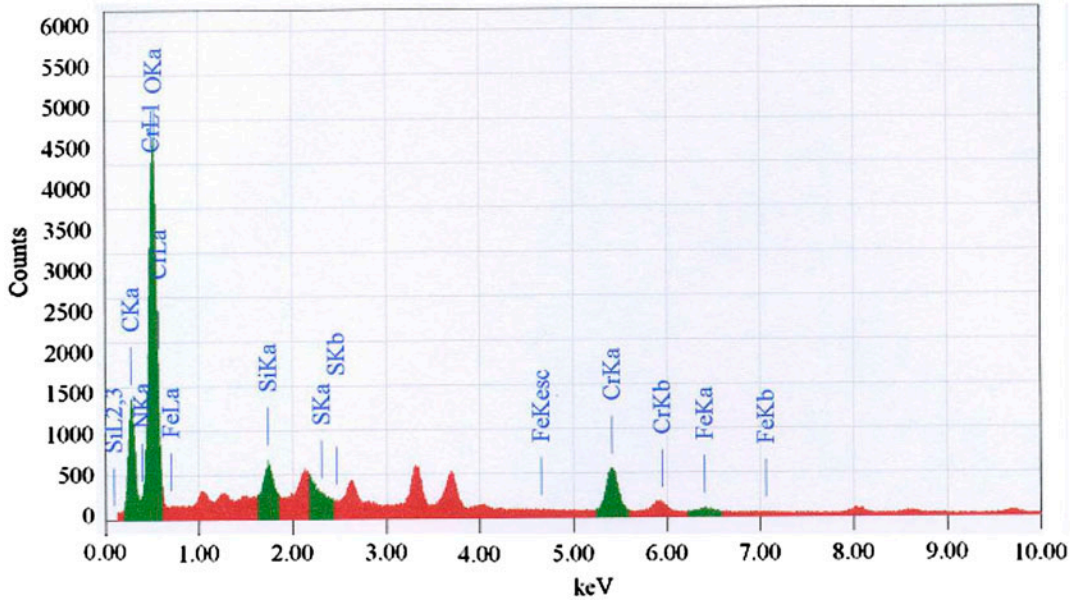

Fig. 4. EDAX plot for carbonized weed after adsorption.

The behavior of the system was explained by the following equation:

$$Y = b_0 + b_1x_1 + b_2x_2 + b_3x_3 + b_{12}x_1x_2 + b_{23}x_2x_3 + b_{31}x_3x_1 + b_{123}x_1x_2x_3 \quad (2)$$

where b_0, b_1 … b_{123} are the regression interaction coefficients of the concerned variables; and x_1, x_2, and x_3 are the dimensionless coded factor affecting the process. Here, x_1 = time, x_2 = pH, and x_3 = temperature. The factorial levels and variation interval of the coded factor are shown in Table 4.

The parameters varied were time (5–15 min), pH (1.6–1.8), and temperature (30–400˚C). The variable parameters in two levels, their coded values and the condition for the base level experiments, are given in Table 5. The +, −, and 0 designations were given to the higher, lower, and base levels, respectively.

Table 4
Factorial levels and variation intervals

x_1 = Time in min, x_2 = pH, x_3 = Temperature in ˚C

Factors	−1	0	1	Variation interval
x_1	5	10	15	5
x_2	1.6	1.7	1.8	0.1
x_3	30	35	40	5

4.2. Development of mathematical model

Eq. (3) is a representation of Table 5. X is obtained by interpolating columns 2–8 of Table 5 into matrix

Table 5
Design of trial runs (in coded form) for adsorption of Cr(VI)

Trial no	x_1	x_2	x_3	x_1x_2	x_2x_3	x_3x_1	$x_1x_2x_3$	Y
1	+	+	+	+	+	+	+	38.84
2	−	+	+	−	+	−	−	35.94
3	+	−	+	−	−	+	−	51.13
4	−	−	+	+	−	−	+	45.95
5	+	+	−	+	−	−	−	35.38
6	−	+	−	−	−	+	+	27.03
7	+	−	−	−	+	−	+	41.43
8	−	−	−	+	+	+	−	35.43
9	0	0	0	0	0	0	0	27.14
10	0	0	0	0	0	0	0	27.1
11	0	0	0	0	0	0	0	27.15

form excluding the base values. Thus, X is an 8×8 matrix obtained for all the possible combinations of x_1, x_2, and x_3, as shown in Eq. (5). Further, the regression coefficients are represented by an 8×1 matrix B as shown in Eq. (6). Thus, the product of X and B is the matrix Y with values corresponding to 9th column of Table 5.

$$[Y] = [X] \times [B] \tag{3}$$

where

$$[Y] = \begin{bmatrix} Y_1 \\ Y_2 \\ Y_3 \\ Y_4 \\ Y_5 \\ Y_6 \\ Y_7 \\ Y_8 \end{bmatrix} \tag{4}$$

$$[X] = \begin{bmatrix} 1 & +x_1 & +x_2 & +x_3 & (+x_1)\times(+x_2) & (+x_2)\times(+x_3) & (+x_3)\times(+x_1) & (+x_1)\times(+x_2)\times(+x_3) \\ 1 & -x_1 & +x_2 & +x_3 & (-x_1)\times(+x_2) & (+x_2)\times(+x_3) & (+x_3)\times(-x_1) & (-x_1)\times(+x_2)\times(+x_3) \\ 1 & +x_1 & -x_2 & +x_3 & (+x_1)\times(-x_2) & (-x_2)\times(+x_3) & (+x_3)\times(+x_1) & (+x_1)\times(-x_2)\times(+x_3) \\ 1 & -x_1 & -x_2 & +x_3 & (-x_1)\times(-x_2) & (-x_2)\times(+x_3) & (+x_3)\times(-x_1) & (-x_1)\times(-x_2)\times(+x_3) \\ 1 & +x_1 & +x_2 & -x_3 & (+x_1)\times(+x_2) & (+x_2)\times(-x_3) & (-x_3)\times(+x_1) & (+x_1)\times(+x_2)\times(-x_3) \\ 1 & -x_1 & +x_2 & -x_3 & (-x_1)\times(+x_2) & (+x_2)\times(-x_3) & (-x_3)\times(-x_1) & (-x_1)\times(+x_2)\times(-x_3) \\ 1 & +x_1 & -x_2 & -x_3 & (+x_1)\times(-x_2) & (-x_2)\times(-x_3) & (-x_3)\times(+x_1) & (+x_1)\times(-x_2)\times(-x_3) \\ 1 & -x_1 & -x_2 & -x_3 & (-x_1)\times(-x_2) & (-x_2)\times(-x_3) & (-x_3)\times(-x_1) & (-x_1)\times(-x_2)\times(-x_3) \end{bmatrix} \tag{5}$$

$$[B] = \begin{bmatrix} b_0 \\ b_1 \\ b_2 \\ b_3 \\ b_{12} \\ b_{23} \\ b_{31} \\ b_{123} \end{bmatrix} \tag{6}$$

4.3. Simulation using MATLAB

Simulation of adsorption process would best be implemented with a tool that can perform matrix computations efficiently, carry out numerical analysis conveniently, and produce a desired output accurately. MATLAB is one such tool that can do all these computations concomitantly. In the succeeding section, the development of code using MATLAB for solving Eq. (3) is outlined.

Matrices developed in section 4.2 were solved to obtain the regression interaction coefficients $b_0, b_1 \ldots b_{123}$ of Eq. (2). Eq. (3) was solved using MATLAB and the corresponding code is given in Table 6. The variation levels of parameters obtained from Table 4 were defined as x_p, x_o and x_n where p, n, and 0 represents +, −, and base values. Eq. (5) as discussed earlier is defined for all the possible combinations of the adsorption parameters obtained from Table 5. By executing the code as given in Table 6, we obtain the values of regression interaction coefficients $b_0, b_1, \ldots b_{123}$. Thus, Eq. (2) can be represented as:

$$Y = 38.89 + 2.8x_1 - 4.593x_2 + 4.073x_3 + 0.0087x_1x_2 - 0.9812x_2x_3 - 0.7837x_3x_1 - 0.5787x_1x_2x_3 \tag{7}$$

4.4. Simulation using LabVIEW

The block diagram was developed with an assumption that the adsorption parameters are variables. Considering the matrix approach as discussed earlier in Section 4.2, the equations were solved using block diagram approach. Generally, LabVIEW accepts variables in array format only. To obtain a constant or a variable in an array format, a function for formatting these constants and variables into arrays was needed. For this, LabVIEW has a built in application that is used for array formation. A window called "FUNCTIONS" panel which appears in the block diagram has several mathematical applications and tools required for developing a block diagram. A tool called "ARRAY" from the functions panel was used for formatting these variables and constants into arrays. Later by using matrix-templates obtained from the same panel, these arrays were arranged into their corresponding matrix forms.

Table 6
MATLAB code

```
≫x1o = 0;
≫ x1p = 1;
≫ x1n = − 1;
≫ x2o = 0;
≫ x2p = 1;
≫ x2n = − 1;
≫ x3o = 0;
≫ x3p = 1
≫ x3n = − 1;
≫ a = [1 x1p x2p x3p (x1p × x2p) (x2p × x3p)(x3p × x1p)(x1p × x2p × x3p)];
≫ b = [1 x1n x2p x3p (x1n × x2p) (x2p × x3p)(x3p × x1n)(x1n × x2p × x3p)];
≫ c = [1 x1p x2n x3p (x1p × x2n) (x2n × x3p)(x3p × x1p)(x1p × x2n × x3p)];
≫ d = [1 x1n x2n x3p (x1n × x2n) (x2n × x3p)(x3p × x1n)(x1n × x2n × x3p)];
≫ e = [1 x1p x2p x3n (x1p × x2p) (x2p × x3n)(x3n × x1p)(x1p × x2p × x3n)];
≫ f = [1 x1p x2p x3n (x1p × x2p) (x2p × x3n)(x3n × x1p)(x1p × x2p × x3n)];
≫ g = [1 x1p x2n x3n (x1p × x2n) (x2n × x3n)(x3n × x1p)(x1p × x2n × x3n)];
≫ h = [1 x1n x2n x3n (x1n × x2n) (x2n × x3n)(x3n × x1n)(x1n × x2n × x3n)];
≫ x = [a; b; c; d; e; f; g; h];
≫
≫ y = [38.84;35.94;51.13;45.95;35.38;27.03;41.43;35.43];
≫ B = x^−1 × y
```

Thus, a block diagram as shown in Fig. 5 was developed.

The front panel of the virtual instrument is an interface between user and computer. Besides friendly

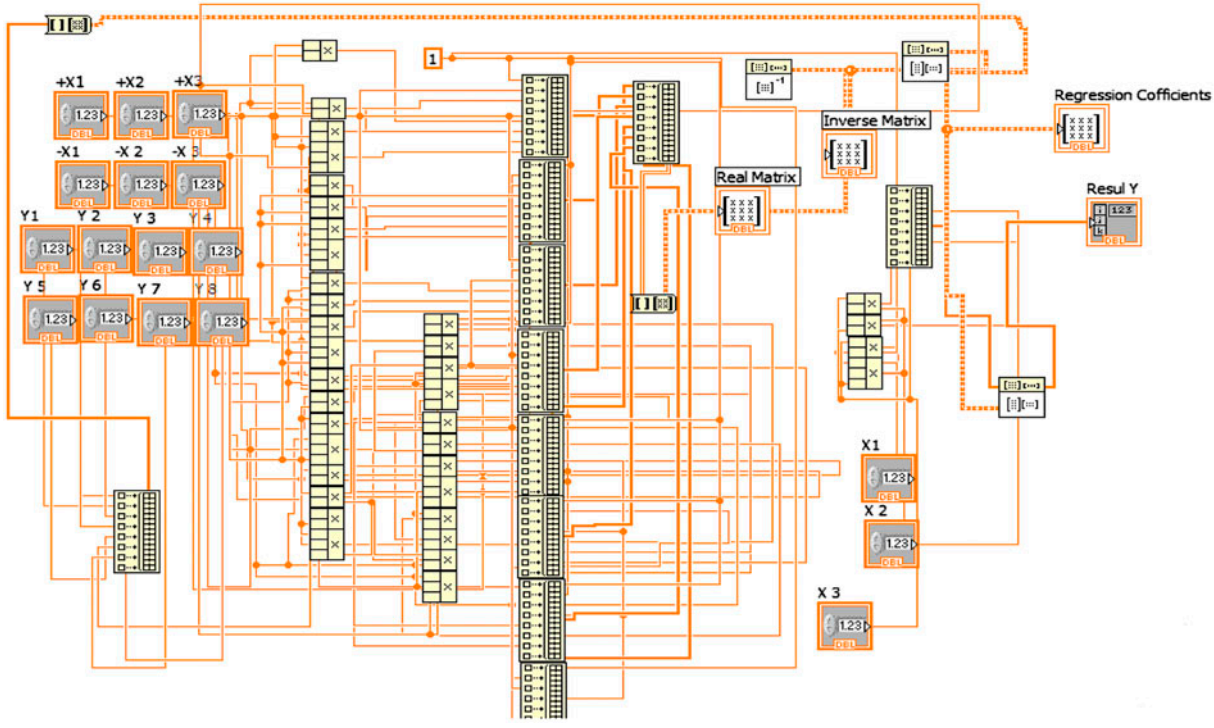

Fig. 5. The configuration of the VI system.

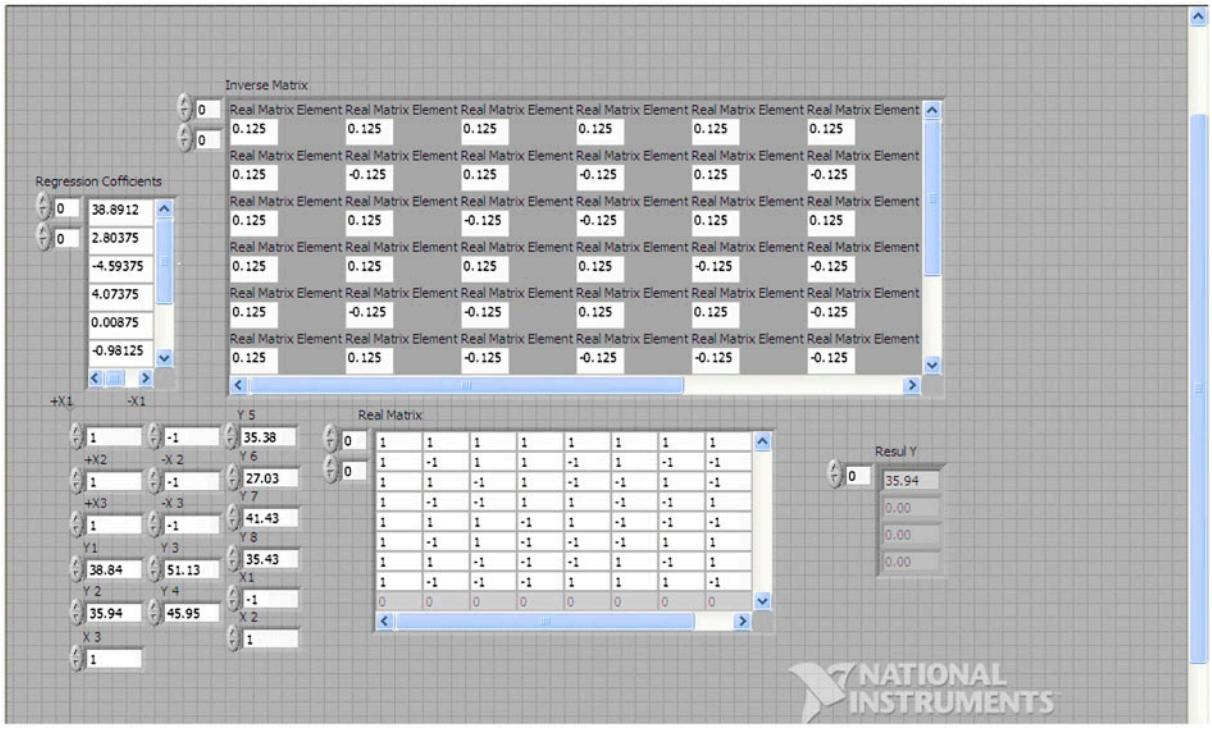

Fig. 6. The configuration of front panel window input/output.

interface and easy control, the corresponding test function can be started up by a simple manipulation. It should also be able to finish user's task successfully. Software is a key section of the virtual instrument. Fig. 6 shows the front panel window where provision for the three adsorption parameter x_1, x_2, and x_3 is provided. The values of $(+x_1, +x_2, +x_3)$ and $(+x_{12}, +x_{22}, +x_{32})$ correspond to the variation values as given in Table 4. The real matrix and the inverse matrix obtained are shown in Fig. 6. Result icon in the front panel window of Fig. 6 is the desired output Y. The block diagram of the process between the inputs and output is delineated in Fig. 5.

For further verification of the model developed, we defined three different variables x_1, x_2, and x_3 and their respective experimental Y value known in preempt. The new matrix X and the matrix B obtained from earlier calculations were used in Eq. (3) to evaluate the corresponding theoretical value of Y. Next, the values of all the adsorption parameters were inputted in the front panel window and by execution we obtained the theoretical value of Y.

4.5. Comparison between MATLAB and LabVIEW

In the MATLAB method of solution, our main aim was to obtain the values of regression interaction coefficients. There were a few disadvantages with MATLAB approach of solving the mathematical model. If there is a need to change the parameters which are considered as the basis for this mathematical model, the coded matrix has to be changed followed by the complete change in values of Table 5. This indeed requires a complete change of the code given in Table 6. To avoid this tedious approach of solving Eq. (2), a much user-friendly method was developed using LabVIEW. In this model, the values of parameters were inputted in the front panel window. The results were immediately obtained without any manual calculation in the same front panel window.

4.6. Error analysis

In order to verify the goodness of fit of the developed mathematical models to the experimental values, it is necessary to examine the data using error analysis. A number of error analysis methods such as the sum of the square of the error (SSE), the sum of the absolute error (SAE), average relative error (ARE), and the average relative standard error (ARS) were used in the present study to verify which mathematical model is best fit to the experimental observations.

Table 7
Validation of the mathematical model by error analysis

Time (min)	pH	Temp. (°C)	Y_e	Y_c	SSE	SAE	ARE	ARS
1	1.7	30	31.73	28.36	326.86	45.33	0.11	0.20
3	1.7	30	34.30	29.79				
5	1.8	40	35.94	35.94				
5	1.6	40	45.94	45.95				
5	1.8	30	27.03	27.03				
5	1.6	30	35.43	35.43				
10	1.7	30	38.94	34.82				
10	2	30	32.34	23.98				
10	2.5	30	14.50	5.92				
10	1.7	50	40.21	51.11				
15	1.8	40	38.83	38.84				
15	1.6	40	51.12	51.13				
15	1.8	30	35.37	37.38				
15	1.6	30	41.42	41.43				
30	1.7	30	45.73	49.17				

The expressions for the above said error functions are as follows [27–30]:

$$\mathrm{SSE} = \sum_{i=1}^{n} (\mathrm{y}_c - \mathrm{y}_e)_i^2 \tag{8}$$

$$\mathrm{SAE} = \sum_{i=1}^{n} |\mathrm{y}_c - \mathrm{y}_e|_i \tag{9}$$

$$\mathrm{ARE} = \frac{1}{n}\sum_{i=1}^{n} \left|\frac{\mathrm{y}_c - \mathrm{y}_e}{\mathrm{y}_e}\right| \tag{10}$$

$$\mathrm{ARS} = \sqrt{\frac{\sum_{i=1}^{n} [(\mathrm{y}_c - \mathrm{y}_e)/\mathrm{y}_e]^2}{n-1}} \tag{11}$$

where "n" is the number of experimental data points, "y_c" is the predicted (calculated) data, "y_e" is the experimental data, and "y" represents the percentage of adsorption. The above statistical error expressions were applied to the mathematical model developed for different values of time, pH, and temperature. The values of the statistical parameters along with the predicted values from the mathematical models are shown in Table 7. It can be concluded from the values of the statistical parameters that the experimental data fit well to the mathematical model.

5. Conclusions

Thermally treated waste weed *Salvinia cucullata* was used as an adsorbent to treat Cr(VI) contaminated water. X-ray diffraction analysis showed that the major component of the activated weed was carbon. The FT-IR studies indicated that the secondary amine groups, Aliphatic CH, and carboxyl groups especially play a major role in Cr(VI) adsorption. Scanning electron microscope images showed the change in morphology of the surface of the adsorbent after adsorption. EDAX analysis showed an increase in Cr(VI) concentration on the surface of the adsorbent. Empirical mathematical model was developed using matrix method. The significance of different adsorption parameters along with their combined effect on the process was studied. Error analysis using statistical method indicated that the experimental values were well fitted to the mathematical model. Later, the empirical model was simulated using MATLAB and LabVIEW. Among the two simulating tool, the latter one was found to be much user friendly. From the analysis, it was concluded that pH had the most influential effect on the adsorption process followed by contact time. Temperature had the least influential effect on the adsorption process. Among all possible combined effects, the effect of pH and contact time was the most influential one.

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