Scientific paper

Experimental Design and Response Surface Modelling for Optimization of Vat Dye From Water by Nano Zero Valent Iron (NZVI)

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Abstract

In this study, NZVI particles was prepared and studied for the removal of vat green 1 dye from aqueous solution. A four-factor central composite design (CCD) combined with response surface modeling (RSM) to evaluate the combined effects of variables as well as optimization was employed for maximizing the dye removal by prepared NZVI based on 30 different experimental data obtained in a batch study. Four independent variables, viz. NZVI dose (0.1–0.9 g/L), pH (1.5–9.5), contact time (20–100 s), and initial dye concentration (10–50 mg/L) were transform to coded values and quadratic model was built to predict the responses. The significant of independent variables and their interactions were tested by the analysis of variance (ANOVA). Adequacy of the model was tested by the correlation between experimental and predicted values of the response and enumeration of prediction errors. The ANOVA results indicated that the proposed model can be used to navigate the design space. Optimization of the variables for maximum adsorption of dye by NZVI particles was performed using quadratic model. The predicted maximum adsorption efficiency (96.97%) under the optimum conditions of the process variables (NZVI dose 0.5 g/L, pH 4, contact time 60 s, and initial dye concentration 30 mg/L) was very close to the experimental value (96.16%) determined in batch experiment. In the optimization, R^2 and R^2_{adj} correlation coefficients for the model were evaluated as 0.95 and 0.90, respectively.

Keywords: Dye removal, Vat Green 1, Optimization, Response surface methodology (RSM)

1. Introduction

The colored dye effluents discharge poses a big threat to our environment and its safe handling is a challenge for scientists. These effluents are considered to be highly toxic to the aquatic biota and affect the symbiotic process by disturbing the natural equilibrium by reducing photosynthetic colourization of water.[1] Effluents contain significant level of organic contaminants, which are known to be carcinogenic and toxic in nature, as they create odour, bad taste, unsightly colour, foaming etc. These substances are inherently resistant to degradation by biological methods and conventional treatment methods are not suitable for their removal from aqueous phase.[2] Consequently, efficient removal of dyes from effluents has drown significant concern. Thus, there is a need to find alternative methods that are effective in removing dyes from large volumes of effluents. Zero-valent iron nanoparticle technology is becoming an increasingly popular choice for treatment of hazardous and toxic wastes, and for remediation of contaminated sites. Because of its small particle size, large specific surface area, high density and great intrinsic reactivity of reactive surface sites, Nano zero-valent iron (NZVI) has gained prominence for applications in environmental remediation. Based on these characteristics, the NZVI technology could become a promising approach for treating dyestuff wastewater.[3–6] The conventional approach for optimization of process variables requires determination of the dependent variable at each and every combination of independent variables just varying only one at a time and keeping all other as constant in batch studies. Thus requiring a very large number of experiments to be performed, which would be very expensive and time consuming. Moreover, it does not reveal the influence of the interactions between the process variables on the dependent variable. Such a limitation may be overcome by the statistical experimental design approach, which reduces the number of experiments as well as provides appropriate model for process optimization, allowing for the evaluation of the influence of intervariable interactions on the process outcome, Recently, several types of experimental design methods have been employed in multivariable chemical process optimization.[7] RSM is essentially a particular set of mathematical and statistical techniques beneficial for studying the effect of several variables influencing the responses by varying them simultaneously and performing a limited number of experiments.[8] The main objective of RSM is to determine the optimum operational conditions of the system or to determine a region that satisfies the operating specifications.[9,10] In the present study, nano zero valent- iron as a powerful reducing agent, was investigated for its efficiency to remove vat green 1 dye from aqueous solution and its chemical structure is shown in Fig. 1. The interaction between the parameters such as initial concentration of the dye, solution pH, NZVI dose and contact time was studied and optimized using response surface methodology.

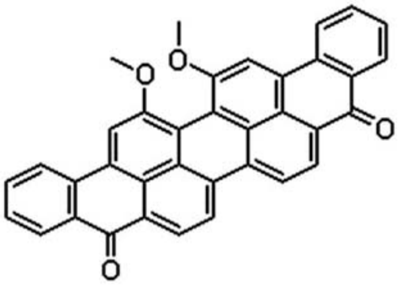

Fig. 1. Structural formula of Vat green 1 ($C_{36}H_{20}O_4$, C. I. 59825)

2. Experimental

2. 1. Materials

The Sodium borohydride ($NaBH_4$) and ferric chloride ($FeCl_3.6H_2O$) were purchased from Merck. Vat green 1 ($C_{36}H_{20}O_4$, C.I. 59825) was obtained from *Alvan Sabet* Co. and was used without further purification. All other reagents were analytical reagent grade. Deionized water was used throughout this study. Adjustment of pH of the dye solution prior to adsorption was carried out with NaOH or HCl from Merck.

2. 2. Preparation of NZVI Particles

NZVI particles were prepared by liquid phase reduction method. All solvents were degassed and saturated for 30 min with N_2 before use. Nano zero-valent iron was synthesized by adding 1M $NaBH_4$ solution into 0.5 M $FeCl_3$ solution during vigorously stirring under N_2 atmosphere. Mixture's color turned from red brown to light yellow and then eventually to black. Ferric iron (Fe^{+3}) was reduced to Fe^0 and zero-valent iron particles precipitated instantly according to the following reaction:

$$4Fe^{+3} + 3BH_4^- + 9H_2O \rightarrow 4Fe^0(s) + 3H_2BO_3^-(aq) + 12H^+ + 6H_2 \quad (1)$$

Then black NZVI particles were vaccum-filtered and washed with deionized water and 1:1 (v/v) ethanol/acetone. Then the resulting gray-black solid was dried under nitrogen atmosphere before use.[11]

2. 3. Response Surface Methodology (RSM) and Experimental Design

Response surface methodology (RSM) is an empirical statistical technique that uses quantitative data obtained from appropriately designed experiments to determine regression model and operating conditions. The main objective of RSM is to determine the optimum set of operational variables of the process. The RSM approach has widely been applied in chemical engineering and sorption process optimization.[12–15]

In this study, RSM Method was used for the experimental design and optimization of the process which were influenced by several independent variables with minimum runs of experiment. This could eliminate the time consuming phase which could not to be achieved using conventional method (one-factor-at-a-time approach). Besides, the central composite design (CCD) is well suited for fitting a quadratic surface, which usually works well for the process optimization and it requires a minimum number of experiments to be carried out.[15] By using CCD, linear, quadratic, cubic and cross-product effects of operating condition variables on the removal efficiency were investigated. NZVI dose (X_1), pH of the solution (X_2), and the contact time (X_3) and the initial concentration of the dye (X_4) were identified as the set of four independent process variables to investigate their influence on the output variable (response), the removal of the dye from aqueous solution by the prepared nano zero-valent iron.

The CCD method was adopted to decide the number of the sorption experiments to be performed for optimization of the process variables. For a design of four independent variables (n = 4), each with two different levels, the total number of experiments (N) was worked out as; N = ($2^n + 2n + n_c$) = 2^4 + (2 × 4) + 6 = 30. Here, this includes the standard 2^n factorial points with their origin at the center, 2n axial points fixed at a distance, α from the center to generate the quadratic terms, and n_c replicate points at the center.[17] After having defined the range of each of the process variables, they are coded to lie at ± 1 for the factorial points, 0 for the center points and ±α for the axial points. The numerical values of the variables were transformed into their respected coded values as:

$$X_i = \frac{2X - (X_{max} - X_{min})}{X_{max} - X_{min}} \quad (2)$$

Where X_i is the required coded value of a variable X, X_{min} and X_{max} are the low and high values of X. The selected process variables with their limits, units and notations are given in Table 1.

Table 1. Process control variables and their limits

Variable	Unit	Factors	Limits				
			–2	–1	0	+1	+2
NZVI dose	g/L	X_1	0.1	0.3	0.5	0.7	0.9
pH	–	X_2	1.5	3.5	5.5	7.5	9.5
Contact time	s	X_3	20	40	60	80	100
Initial conc. of dye	mg/L	X_4	10	20	30	40	50

2. 4. Adsorption Studies

Batch experiments were conducted to study the effect of various operating variables on the dye removal percent. All the experiments were conducted according to the CCD matrix at random, to avoid the possibility of any systematic errors in measurements. Minimum and maximum levels of each of the four process variables were defined through pre-trial experiments. Adsorption of Vat green 1 by NZVI was carried out by batch method and the influence of various parameters such as contact time (15–120 s), adsorbent dosage (0.1–0.9 g/L), pH (1.5–9), initial dye concentration (20,30,40,50 and 60 mg/L), temperature (298,308 and 318 °K) were studied. The adsorption measurements were conducted by mixing various amounts of NZVI in glass Erlenmeyer flasks containing 50 mL of dye solution of known concentration. The pH of the solution was adjusted to the desired value by adding small amount of HCl or NaOH (0.1M). At the end of determined time intervals, the samples were taken out and the supernatant solution was separated from the NZVI by centrifugation at 3500 rpm for 20 min. After that, the concentration of dye was measured based on absorbance at 630 nm using UV-VIS spectrophotometer (CARY-300, BioTech). The removal efficiency of dye is defined as follows:

$$\text{Removal efficiency (\%)} = \frac{C_0 - C_t}{C_0} \times 100 \quad (3)$$

Where C_o = initial concentration of dye (mg/L) and C_t = concentration of dye at reaction time (t) (mg/L). All batch experiments were performed in duplicate and the mean of the two are taken for all calculations. The experimental conditions and the corresponding dye removal (%) measured through the batch experiments are presented in Table 2.

2. 5. Statistical Analysis

The Design Expert Software (Version 8.0.7.1, State-Ease, Inc., USA) was used for regression and graphical analysis of the data obtained. In the optimization process, the experimental responses can be analyzed with the following second-order polynomial Eq. (4).[18]

$$Y_{Pred} = \beta_0 + \sum_{i}^{k} \beta_i x_i + \sum_{i}^{k} \beta_{ii} x_i^2 + \sum_{i}^{k-1} \sum_{j=i+1}^{k} \beta_i \quad (4)$$

Where Y_{Pred} is the predicted value, x_i and x_j are the independent variables, β_0 is the constant coefficient, β_i, β_{ii} and β_{ij} are the interaction coefficients of linear, quadratic and second-order terms, respectively, and $\in$ is the error. Response surfaces and contour plots were developed using the fitted quadratic polynomial equation obtained from regression analysis. The experiments were run changing of two variables while holding the other variable at a constant value. In this study, data for the removal efficiency of vat green 1 were processed based on Eq. (5) including analysis of variance (ANOVA). Data analysis through ANOVA is much more scientific than direct observation analysis.[19]

3. Results and Discussion

3. 1. Regression Analysis and Quadratic Model

CCD approach was adopted for investigating the individual and interactive effects of the selected process variables on the adsorption of dye the NZVI particles from aqueous solution. The measured dye removal (%) of the developed zero-valent iron nanoparticles corresponding of different combinations of selected process variables is presented in table 2. A quadratic model was selected for developing the mathematical relationship between the response and the process variables, viz. NZVI dose (g/L), pH, contact time (s) and initial dye concentration (mg/L).

Table 2. Central composite design (CCD) for four independent variables (coded values) and corresponding dye removal (%)

Serial no.	CCD term	No. of experiments	Process variables (coded values)				Removal (%)
			X_1	X_2	X_3	X_4	
1	Factorial (2^n)	16	–1,+1	–1,+1	–1,+1	–1,+1	57–98
2	Axial (2n)	8	–2,0,+2	–2,0,+2	–2,0,+2	–2,0,+2	55–96
3	Center (n_c)	6	0	0	0	0	93–98

The CCD based experiment to obtain a quadratic model, here consisted of 2^4 standard factorial runs, a star configuration ($\alpha = \pm 2$) of size, 2n, and six replicates at the center point (n_c) used to determine experimental error.

The maximum removal efficiency percent of dye by NZVI particles was observed to be 97.5%. A Polynomial regression modeling was performed between the response variable and the corresponding coded values (X_1, X_2, X_3, X_4) of the four different process variables, and finally, the best fitted model equation was obtained as,

$$Y = 96.31 + 1.05X1 - 0.66X2 + 4.74X3 - 4.37X4 + 0.95X1X2 - 5.07X1X3 + 0.03X1X4 + 1.095X2X3 - 0.88X2X4 + 3.01X3X4 - 2.26X_1^2 + 0.36X_2^2 - 2.89X_3^2 - 4.71X_4^2 \quad (5)$$

in Eq. (5), Y is the removal efficiency percent; X_1, X_2, X_3, and X_4 correspond to independent variables of NZVI dose (g/L), pH, contact time (s), and initial dye concentration (mg/L), respectively. Model Eq. (5) was used to evaluate the influence of the process variables on the removal of dye in aqueous medium by the NZVI. The quality of the model developed was evaluated based on the value of coefficient of determination (R^2). The R^2 value for Eq. (5) was 0.95 which was relatively high (close to unity). This implied that 95% of the variations for the removal efficiency of VG1 are explained by the independent variables and only 5% of the total variability in the response was not explained by the model. The high R^2 value indicated that the model obtained was able to give a convincingly good estimate of response in the studied range. The analysis of variance (ANOVA) was performed to test the significance of the model. The ANOVA results (Table 3) of the quadratic regression model (Eq. (8)) suggest that the quadratic model was highly significant, as evident from the Fisher's F-Test ($F_{model} = 21.10$) with a very low probability value ($P_{model} = 0.0001$). Furthermore, the calculated F-value ($F_{model} = 21.10$) was compared with the critical F value ($F_{0.05}$, df, (n-df-1)) for the considered probability (p = 0.05) and degrees of freedom. Since, the df for model is 14 and n = 30, Therefore, it gives (n-df-1) = 15. Hence, the critical F value ($F_{0.05,14,15} = 2.42$) is less than the calculated F-value of 21.10. It suggests that the computed Fisher's variance ratio at this level was large enough to justify a very high degree of adequacy of the quadratic model and significance of the treatment combinations.[21]

ANOVA results of this model presented in Table 3 indicate that it can be used to navigate the design space. In Table 3, the model F-value of 21.10 implies the model is significant for VG1 removal and there is only a 0.01% chance that a model F-value of this large could occur due to noise. In VG1 removal model, the adequate precision ratio 16.87 indicates an adequate signal where it measures the signal to noise ratio; a ratio greater than four is desirable.

For Eq. (5) lack of fit F-value 1.46 implied that the model of removal efficiency of VG1 developed was insignificant. The non-significant lack of fit indicates good predictability of the model. There was a 35.53% chance that a lack of fit F-value could occur due to noise. The P-values less than 0.05 indicate that model terms are significant, whereas the values greater than 0.1000 are usually considered as non-significant. Table 3 shows the results of this model when applied to contact time and initial concentration. The terms are significant according to P-values.

Table 3. The ANOVA results for the response surface quadratic model for removal of the VG1 dye.

Source	Sum of squares	DF[a]	Mean squares	P-Value	F -Value	
Quadratic model	2535.53	14	181.11	21.10	<0.0001	significant
X_1	26.50	1	26.50	3.90	0.0993	
X_2	10.35	1	10.35	1.21	0.2894	
X_3	539.11	1	539.11	62.81	<0.0001	
X_4	458.56	1	458.56	53.42	<0.0001	
X_1^2	140.58	1	140.58	16.38	0.0011	
X_2^2	3.58	1	3.58	0.42	0.5284	
X_3^2	229.62	1	229.62	26.75	0.0001	
X_4^2	609.05	1	609.05	70.96	<0.0001	
X_1X_2	14.45	1	14.45	1.68	0.2140	
X_1X_3	411.58	1	411.58	47.95	<0.0001	
X_1X_4	0.013	1	0.013	1.49	0.9696	
X_2X_3	60.77	1	60.77	7.08	0.0178	
X_2X_4	12.31	1	12.31	1.43	0.02496	
X_3X_4	144.56	1	144.56	16.84	0.0009	
Residual	128.75	15	8.58			
Lack of fit	95.58	10	9.59	1.46	0.3553	insignificant
Pure Error	32.90	5	6.58			
Corrected total	2664.28	29				

$R^2 = 0.95$; adequate precision =16.87. [a] DF-degrees of freedom.

The actual and predicted VG1 removal percent are shown in Fig. 2. Actual values are the measured response data for a particular run, and the predicted values are evaluated from the model are generated by using the approximately functions.

In Fig. 2, the values of R^2 and R^2_{adj} were found to be 0.95 and 0.90, respectively. From this figure, it is noted that the values calculated using the predictive second-order model was in good agreement with the experimental values with satisfactory correlation between these values. Thus, the model developed is suitable for predicting the removal efficiency of VG1 in the conditions investigated. The fair correlation coefficients might have resulted by the insignificant terms in Table 3, and most likely due to four different variables selected in wide ranges with a limited number of experiments as well as the nonlinear influence of the investigated parameters on process response.[22]

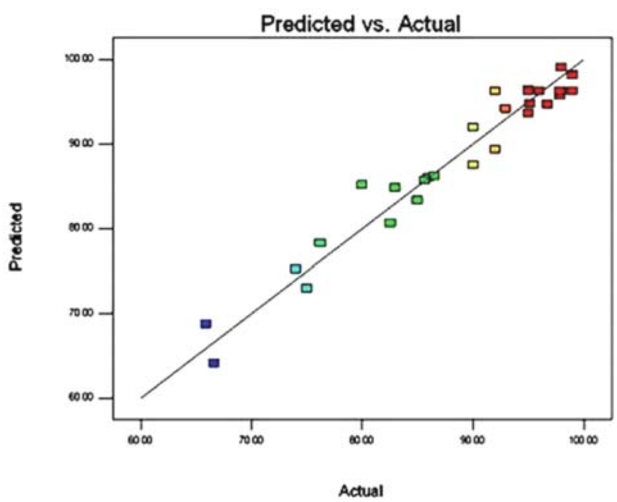

Fig 2. Actual and predicted values of removal of Vat green 1 by NZVI ($R^2 = 0.95$).

3. 2. Three-dimensional Response Surface Plots

The three-dimensional (3D) response surface plots of the dependent variable as a function of two independent variables, maintaining all other variables at fixed levels can provide information on their relationships and can be helpful in understanding both the main and the interaction effects of these two independent variables.[22,23] Therefore, in order to gain better understanding of the effects of the independent variables and their interactions on the dependent variable, 3D response surface plots for the measured responses were constructed based on the quadratic model. The influence of the four different process variables on the response factor (removal %) are visualized in the 3D response surface plots (Figs. 3–8).

3. 2. 1. Effect of pH and NZVI Dose

The effect of pH and NZVI dose on VG1 removal is shown in Fig. 3. Vg1 removal increased with increasing NZVI dose and decreasing pH. Such a behavior may be due to the reversal in ionic structure of the dye in acidic and basic medium. The VG1 molecule acquires a positive charge in acidic pH medium, whereas, a negative charge in alkaline medium. So, despite an increase in number of binding sites with the dose, repulsive forces at the NZVI-dye interface may lead to a decreased uptake. A maximum dye removal (95.5%) was observed at NZVI dose (0.7 g/L) and pH (3.5).

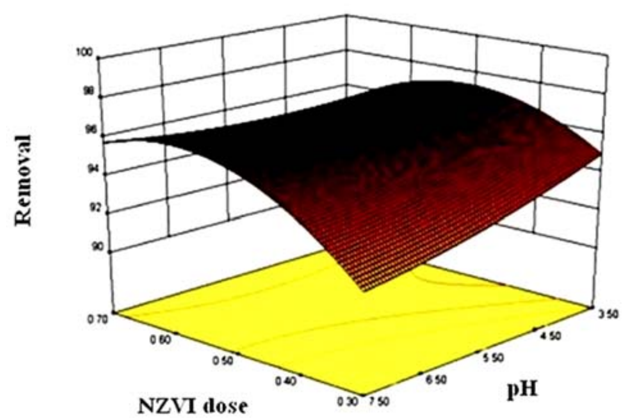

Fig. 3. Combined effect of NZVI dose and pH on removal of the Vat green 1 dye.

3. 2. 2. Effect of pH and Contact Time

The plot for combined effect of pH and contact time (Fig. 4.) shows that dye removal increased with pH and increasing contact time decreasing. At lower pH, the dye removal increases with increasing contact time. It may be attributed to the fact that the uptake would be higher due

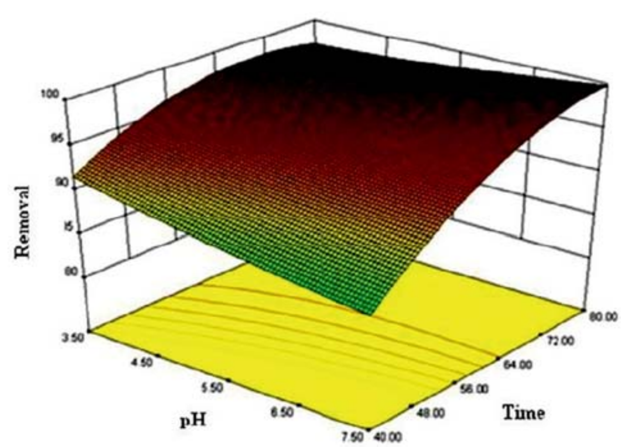

Fig. 4. Combined effect of time and pH on removal of the Vat green 1 dye.

to availability of more active binding sites and may be due to the formation of oxide film of surface of the particle at higher pH, whereas, at Lower pH, constant dissolution of NZVI particles does not allow such inactive layer formation. Cissoko et al. reported similar influence of the pH and Cr(VI) concentration on reduction efficiency of iron nanoparticles in aqueous medium.[24] At pH (3.5) and contact time (80 s), a maximum dye removal of 97% was determined.

3. 2. 3. Effect of pH and Initial Dye Concentration

The plot for combined effect of the solution pH and dye concentration (Fig. 5.) suggests that increasing dye concentration results in a decreasing removal of the dye, whereas, it increases with decreasing the pH value. Ascending trend in dye uptake with decreasing pH may be attributed to the positive charges on the dye molecules in the acidic medium, and the trend reverses where the dye adsorption decreases with increasing concentration. This behavior can be understood as the increasing adsorbate concentration with fixed NZVI dose would result in saturation of the binding sites on the surface and subsequently declining of the adsorbate uptake with increasing concentration. A maximum dye removal (97%) was determined at pH (3.5) and dye concentration (20 mg/L).

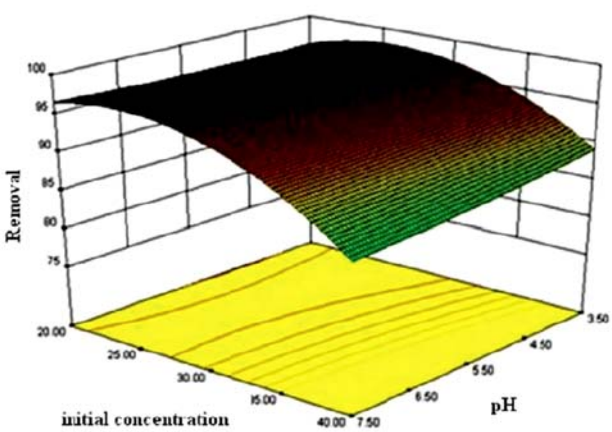

Fig. 5. Combined effect of pH and initial concentration on removal of the Vat green 1 dye.

3. 2. 4. Effect of NZVI Dose and Contact Time

Fig. 6. shows the interactive influence of NZVI dose and contact time on the dye removal from aqueous phase. It is evident that the dye removal increased with the increase in both the NZVI dose and contact time. The observed trend may be understood the increase in NZVI dose would make higher number of adsorption sites available. At NZVI dose (0.7 g/L) and contact time (80 s), a maximum dye removal of 93.5% was determined.

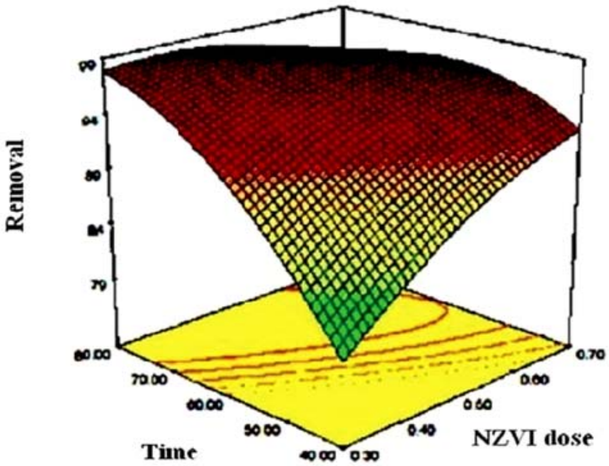

Fig. 6. Combined effect of NZVI dose and time on removal of the Vat green 1 dye.

3. 2. 5. Effect of NZVI Dose And Initial Dye Concentration

The combined effect of NZVI dose and initial dye concentration on removal dye is shown in Fig. 7. It may be noted that the dye removal increased with increasing NZVI dose and decreasing dye concentration. This is due to increase in initial dye concentration, adsorption sites, surface area of the NZVI are saturated, resulting in decrease in the adsorption efficiency. At NZVI dose (0.7 g/L) and dye concentration (20 mg/L), a maximum dye removal of 97.5% was determined.

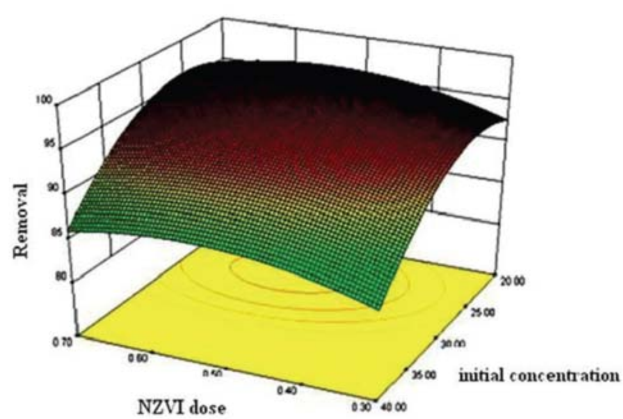

Fig. 7. Combined effect of NZVI dose and initial concentration on removal of the Vat green 1 dye.

3. 2. 6. Effect of Initial Dye Concentration and Contact Time

The interactive effect of initial dye concentration and contact time on dye removal is shown in Fig. 8. It is evident that the dye removal increases with the increase contact time and decreases with the increase the dye concentration. This is very obvious due to the fact that at lower time, dye removal process would not be completed. A maximum dye removal (97%) was determined at dye concentration (30 mg/L) and contact time (60 s).

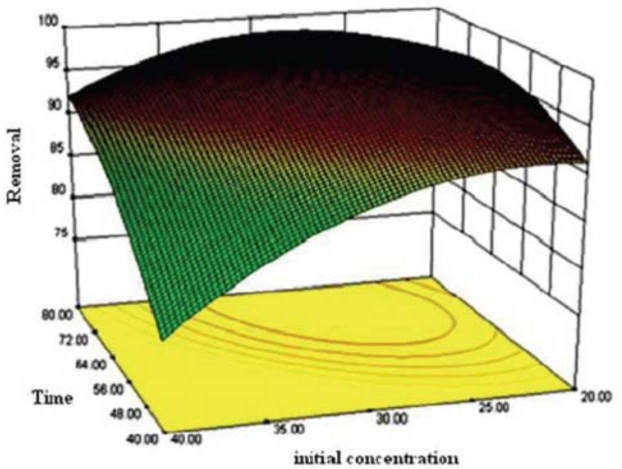

Fig. 8. Combined effect time and initial concentration on removal of the Vat green 1 dye.

3. 3. Model Validation and Optimization of Dye Removal

In order to confirm the validity of predicted model and optimize the variables, 10 solutions for the optimum conditions were generated by the design of experiments (DOE) software according to the order of suitability.[24,25] The first five solutions for the optimum conditions were chosen as shown in Table 4. The experimental values obtained for removal efficiency of vat green 1 were found to be within 5% accuracy to those predicted values using Eq. (5). Optimization of the process variables were performed using the quadratic model within the studied experimental range of various process variables to obtain the highest possible removal efficiency of vat green 1 by using NZVI dose.

The process of optimization modeling suggested the optimum values of different process variables (viz. NZVI dose 0.5 g/L, pH 3.5, contact time 60 s, and initial dye concentration 30 mg/L) to achieve the maximum removal (96.97%) of the VG1 dye from the aqueous solution. The corresponding experimental value of the dye adsorption was determined as 96.16%, which is very close to the optimum value predicted by the model. The experimental value obtained was in good agreement with the value predicted from the quadratic model. This result confirmed that the RSM was an effective and reliable method for optimizing the removal of vat green 1.

4. Conclusions

The present study aimed to develop and determine the application of NZVI particles for removal dye. The NZVI particles appeared to be very active reducing agent for removal of vat green 1 dye in aqueous solution. The RSM based on CCD combining was used to determine the effect of four different process variables, viz. NZVI dose, pH, contact time, and initial dye concentration on the dye removal efficiency of the NZVI particles from the aqueous solution. Relative effects of interaction between process variables were successfully analyzed. The optimized variables for the removal efficiency of VG1 determined in this study were found at NZVI dose 0.5 g/L, pH 3.5, contact time 60 s, and initial dye concentration 30 mg/L to achieve the maximum removal (96.97%) of the VG1 dye from the aqueous solution. The corresponding experimental value of the dye adsorption was determined as 96.16%, which is very close to the optimum value predicted by the model. The experimental design and RSM approach successfully determined the removal efficiency of the NZVI particles for VG1 dye from the aqueous solution and optimization of process variables for maximum dye removal.

5. Acknowledgement

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Table 4. Experimental results for model validation conducted at the optimum conditions as obtained from RSM.

Runs	X_1	X_2	X_3	X_4	Experimental values	Predicted values
1	0.52	3.38	63.86	24.96	95.42	98.29
2	0.28	3.26	84.16	26.36	92.68	96.32
3	0.72	3.52	62.46	26.28	94.34	97.41
4	0.41	4.25	74.67	23.29	92.53	96.85
5	0.84	4.67	52.16	22.88	95.14	98.54

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Povzetek

V okviru raziskave smo pripravili in preučevali NZVI delce za odstranjevanje barvila Vat Green 1 iz vodnih raztopin. Središčni kompozitni načrt (CCD) s štirimi faktorji smo uporabili skupaj z modeliranjem odzivne površine (RSM) in optimizacijo za povečevanje obsega odstranjevanja barvila s pripravljenimi NZVI na podlagi 30 različnih izmerjenih podatkov, pridobljenih s pomočjo šaržnih eksperimentov. Štiri neodvisne spremenljivke, vsebnost NZVI (0,1–0,9 g/L), pH (1,5–9,5), čas izpostavitve (20–100 s) in začetno koncentracijo barvila (10–50 mg/L), smo pretvorili v kodirane vrednosti ter postavili kvadratni model za napovedovanje odzivov. Rezultati ANOVA so nakazovali, da lahko predlagani model uporabljamo, če se nahajamo v prostoru načrta eksperimentov. Z uporabo kvadratnega modela pa je bila izvedena tudi optimizacija spremenljivk za doseganje največje vezave barvila na NZVI delce. Napovedana največja učinkovitost vezave (96,97 %) pri določenih optimalnih pogojih spremenljivk pri postopku (vsebnost NZVI 0,5 g/L, pH = 4, čas izpostavitve 60 s in začetna koncentracija barvila 30 mg/L) je bila zelo blizu izmerjeni vrednosti (96,16 %), določeni s šaržnim poskusom. Pri optimizaciji sta bila korelacijska koeficienta modela, R^2 in R^2_{adj}, ocenjena kot 0,95 ter 0,90.