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Optimization and Mathematical Modelling of Sodium Hypochlorite Mediated Decolorization of DIAZO DYE (Direct Blue 14)

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Abstract

Synthetic organic textile dyes are recalcitrant compounds released directly by the textile processing units into water bodies are important class of water pollutants. Decolourization of textile diazo dye Trypan Blue (Direct Blue 14) was investigated using a strong oxidative agent sodium hypochlorite using chemometric tools. Statistical tools such as Box-Behnken Design was applied for the study and optimization of decolourization process by investigating three important process operating variables such as pH (X_1), incubation time (minutes) (X_2) and dye concentration (mg/L) (X_3). A total of 17 experiments were conducted in the study towards the construction of a second order quadratic model. Among the three variables, incubation time (X_2) and dye concentration (X_3) were found to be influencing factors towards the response. Statistical indicators such as ANOVA, Fischer's Test and student's t- value support and explain model adequacy. Under optimized conditions of pH 3.0, incubation time of 32 minutes and 150 mg/L of dye concentration, sodium hypochlorite was able to decolorize 93% of Trypan Blue. The predicted conditions were subsequently validated to ensure reproducibility and validity of the statistical model. Experimental and predicted values were found to be in close agreement with each other.

Keywords: Response Surface Methodology (RSM), ANOVA, Prototypical textile dye, Trypan Blue, Degradation.

1. Introduction

Dyes are finding vast and wide application in textile garment manufacturing industries. Spent wash from textile processing industries contains substantial amount of unused dyes (10 to 15% of dye), which has to be detoxified/remediated before being discharged into water bodies (Ravikumar et al 2005). Soluble dyes in aqueous bionetwork diminishes the photosynthesis process, hindering light penetration, thereby abating water quality, leading to changes in chemical oxygen demand (COD), biological oxygen demand (BOD), mass transfer and solubility of gases in aqueous systems (Asad et al 2007). Azo dyes account for more than 50% of all the dyes produced annually (Kusic et al., 2011). Highly substituted ring structures present make azo dyes recalcitrant, where conventional wastewater treatment processes fail to degrade azo dyes effectively (Wang, 2010).

Response Surface Methodology is combinatorial methodology amalgamating both mathematical and statistical approaches, towards designing experiments, generating models, evaluating the relative contributing of individual process parameters and predicting optimal working conditions for desirable responses (Box and Draper, 1987; Draper and John, 1998; Zhang and Zheng, 2009). RSM based on Box-Behnken design has been widely used to identify the optimum conditions for a multivariable system. Recent literatures have reported optimization of many process parameters influencing wastewater treatment using RSM (Murugesan et al 2007; Li et al 2009). The present study targets optimization strategies such as Response Surface Methodology (RSM) using Box-Behnken Design (BBD) to investigate the effect of three influencing variables such as pH (X_1), incubation time (minutes) (X_2) and dye concentration (mg/L) (X_3) towards decolourization of diazo dye.

2. Materials and Methods

2.1 Chemicals

Synthetic organic dyes such as Trypan Blue (TB) from Hi media and Merck Limited. All other chemicals used in the study were of analytical grade and procured from SD Fine Chemicals limited, India.

2.2 Methodology

Batch experiments were performed with reaction conditions as follows; 0.5 mL of textile dye solution of desired concentration (W/V %),followed by addition of 9.5 mL of double distilled water and 0.5 mL of sodium hypochlorite. The dye solutions are stirred and 3 mL samples are withdrawn at regular time intervals and the dye decolorization was measured spectrophotometrically using a UV-Visible spectrophotometer (Elico, India). Dye decolorization is expressed as follows:

$$\text{Decolorization (\%)} = \left(\frac{[A_{\text{Initial}} - A_{\text{Final}}]}{A_{\text{Initial}}}\right) \times 100 \quad (1)$$

3. Optimization

Three level factorial Box-Behnken Design was chosen to study interactions, prediction and modelling of optimal conditions influencing the textile dye decolorization, as it requires fewer experimental runs than a central composite design (Box and Benhnken, 1960). Three influencing variables such as pH, dye concentration (mg/L) and incubation time (minutes) were selected for sodium hypochlorite assisted decolourization studies. Backward regression was applied to investigate the effect of influencing variables towards the response and the final optimized response equation are represented in equation 2 and equation 3. Variance analysis such as ANOVA, Fisher's Test and Student test (t-value) explains the model statistics.

4. Results

Table 1 and **Table 2** represent Box-Benhken Design matrix and ANOVA table. Statistical indicators such as determination coefficient (R^2), multiple correlation coefficients(R) and ANOVA analysis of the quadratic equation helps us to navigate through space and predict the optimal conditions. The high value of R (0.922) demonstrates a high degree of agreement between the experimental observations and predicted values. The optimized equation influencing the response (Decolourization) is represented in the equation 2 and the final optimized equation after backward regression algorithm is represented in equation 3;

$$\text{Response} = 92.010 - 4.112X_1 + 0.611X_2 + 0.052X_3 + 0.005X_1X_2 + 0.001X_1X_3 - 0.001X_2X_3 + 0.422X_1^2 - 0.007X_2^2 + 0.000061X_3^2 \quad (2)$$

$$\text{Response} = 83.114 + 0.629X_2 + 0.046X_3 - 0.001X_2X_3 - 0.007X_2^2 \quad (3)$$

5. Discussion

Table 2 represents the ANOVA test, where the determination of coefficient was found to be 0.922, recommending that 92.2% variance can be explained by the model. Literatures have recommended that, R2 should be close to 1, the stronger the model and better the prediction of the response (Joglekar and May, 1987, Haaland, 1989). The model F-value of 9.28 and value of p of less than 0.0039 indicated that the model was highly significant.

Backward regression analysis was performed to predict the significant contributing variables towards the response. Among the three variables, incubation time (X_2) and dye concentration (X_3) was found to have positive influence towards the response, whereas pH (X_1) was found to have negative influence towards response (Decolourization). As reported in **Table 2**, incubation time (X_2), dye concentration

(X_3), the individual linear term incubation time (X_2^2) are the most significant factors towards decolourization. All other terms was found to be insignificant.

After performing backward regression analysis, the optimized predicted conditions was found to be pH 3.0, incubation time of 32 minutes and 150 mg/L of dye concentration. Under the above optimized conditions, sodium hypochlorite was able to decolorize 93% of Trypan Blue. The predicted conditions were subsequently validated to ensure reproducibility and validity of the statistical model.

Table 1: Box-Benhkhen Design to study decolourization of Trypan Blue by Oxidative Process.

Run	pH (X_1)	Incubation time (X_2) (Minutes)	Dye concentration (X_3) – (mg/L)	Decolourization (%)	
				Actual	Predicted
1	4	15	50	92.87	92.52
2	3	45	100	97.91	96.90
3	5	45	100	97.49	96.90
4	3	30	50	96.91	96.30
5	5	30	150	97.83	97.99
6	4	30	100	97.83	97.14
7	4	45	50	96.16	96.82
8	4	45	150	96.06	96.99
9	4	30	100	96.71	97.14
10	3	15	100	94.28	94.11
11	4	15	150	95.78	95.70
12	5	30	50	95.72	96.30
13	4	30	100	96.08	97.14
14	3	30	150	98.71	97.99
15	4	30	100	97.11	97.14
16	5	15	100	93.52	94.11
17	4	30	100	97.39	97.14

Table 2: ANOVA analysis of Box-Benkhen Design.

Source	Sum of Squares	df	Mean Square	F Value	p-value Prob > F
Model	34.874	4	8.718	16.705	< 0.0001*
(X_2)	15.614	1	15.614	29.919	0.0001*
(X_3)	5.653	1	5.653	10.833	0.0064*
(X_2X_3)	2.262	1	2.262	4.335	0.0594
(X_2^2)	11.343	1	11.343	21.736	0.0005*
Residual	6.262	12	0.521		
Lack of Fit	4.475	8	0.559	1.251	0.4416
Pure Error	1.787	4	0.446		

Cor Total	41.137	16			
Statistical indicators before and after backward regression analysis					
Before			**After**		
R2	90.11		R2	84.77	
Adjusted R2	77.41		Adjusted R2	79.70	
Std.deviation	0.762		Std. deviation	0.722	
*statistically significant at 95% confidence limit					

6. Conclusion

Literatures have reported the strong oxidizing potential of sodium hypochlorite in the past, but we report, the decolourization/degradation of Trypan Blue (Direct Blue 14), a diazo dye by sodium hypochlorite applying a chemometric statistical methodology like Box-Benkhen Design. RSM was successfully applied to determine the optimal operational conditions for maximum decolouration of Direct Blue 14 at pH 3.0, incubation time of 32 minutes and 150 mg/L of dye concentration. Further validations have to be carried out to authenticate the mechanism through analytical probes.

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