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Response Surface Methodology and Genetic Algorithms Applied to Model and Optimize the Dyeing of Cotton Process with the Reactive Black 5 Dyestuff

Jorge Marcos Rosa[a], André Felipe Henriques Librantz[b*], José Carlos Curvelo Santana[c], Fábio Cosme Rodrigues dos Santos[d], Elias Basile Tambourgi[e], Ana Maria Frattini Fileti[f]

[a]Instituto SENAI -SP de Tecnologia Têxtil, Moda e Confecção, Brazil
[b]Universidade Nove de Julho, São Paulo, Brazil
[c]Universidade Federal do ABC, São Paulo, Brazil
[d]Sabesp- Companhia de Abastecimento Básico do Estado de São Paul, São Paulo, Brazil
[e,f]Faculdade de Engenharia Química da Universidade Estadual de Campinas, São Paulo, Brazil
[a]Email: jotarosa@gmail.com, [b]Email: librantz@uninove.br
[c]Email: jccurvelo@yahoo.com.br, [d]Email: fcrodrigues@sabesp.com.br
[e]Email: eliastam@feq.unicamp.br, [f]Email: frattini@feq.unicamp.br

Abstract

This work aimed to combine response surface methodology and genetic algorithms to model and optimize the dyeing process to show the influences of each component in the dyeing of cotton knit to optimize its dyeing conditions. A 2^6 design of central composite and rotational (DCCR) was used as support to execute seventy-eight dyeings with Reactive Black 5 dyestuff (RB5) on 100% knitted cotton substrate. The impacts of various dyeing process parameters were also investigated. The concentrations of [RB5] (percent), [NaCl] (g/L), [Na2CO3] (g/L), and [NaOH] (mL/L), as well as processing time (min) and temperature (°C), were employed. The K S^{-1} coefficient and the costs of each experiment were calculated as a result. The objective function was derived from the fitting of the experimental points using the least-squares method and analysis of variance (ANOVA). The findings revealed that both techniques can be efficiently applied to model and optimize the cotton dyeing, with the goal of lowering the cost and environmental impact.

Keywords: Response surface methodology; Modelling; genetic algorithms; dyeing of cotton; financial impact; environmental impact.

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* Corresponding author.

1. Introduction

Known as a strong sector with high social impact, especially the clothing manufacturers, the Brazilian textile industry employed 1.6 million professionals in 2015. The number of jobs corresponds to 16.9% of the workers at the industrial production, generating approximately U$ 67 billion in production, which corresponds to 5.5% of the industrial production. The reactive dyestuff is widely utilized in the dyeing of cellulosic fiber in this industry. It combines with the fiber and the water to produce a reaction. This type of dyestuff is a key part of the effluent due to the reaction with water; approximately 10% to 15% are not fixed and are discarded in the effluent [1,2].

As a result, optimizing dyeing operations with this class of dyestuff becomes critical to get the best coloristic intensity, decrease salt output, and promote a lower number of contaminants in the effluent created. The use of reactive dyestuffs results in high amounts of dissolved solids and oxygen demand in the effluent, both of which are undesirable. [3, 4, 5]. The usage of huge amounts of inorganic salt and alkali to ensure efficient utilization and fixation of dyestuffs that are mostly non-biodegradable and hazardous to aquatic plants and animals has resulted in this requirement. Furthermore, many commercial dyestuff preparations are mixtures of active dyestuff and other by-products that resist biological degradation and accumulate in large concentrations in the dyeing effluent. Alternative treatments should be developed because conventional wastewater treatment techniques are unable to breakdown such chemicals and detoxify the effluent.[6,7]. The dye C.I. Reactive Black 5 (RB5), which was used in this investigation, is the most sold dye on the planet. Figure 1 depicts its structure.

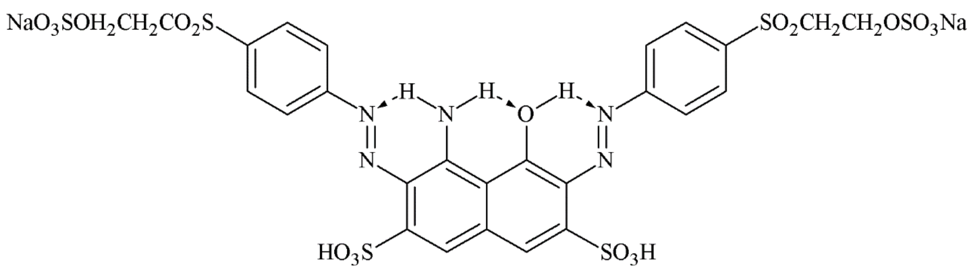

Figure 1: RB5 dyestuff structure [8].

It is an azo dyestuff, bi-homo-functional, vinyl sulphone as reactive group type, CAS Number 17095-24-8, molecular weight equal to 991.82 g mol^{-1}

1.1. Genetic algorithms applied to the textile industry

The Genetic algorithms (GA) is a metaheuristic optimization technique based on the biological natural-selection process that has been utilized to solve optimization problems in a variety of fields for decades, mostly due to its efficiency in irregular search spaces [9]. As a result, several issues involving sophisticated combinatorial optimization have been solved using this technique [10]. GA and other nonlinear techniques have been used to handle a wide range of chemical engineering challenges in the recent decade [11-17].

Reference [18] used the genetic algorithm as an aptitude function to simulate the adsorption of the hazardous methylene blue dye utilizing active carbon as an adsorbent, which is a low-cost source. The research shows that active carbon is effective at removing methylene blue dye. The greatest dye removal rate was achieved using a genetic algorithm that produced values that were close to the experimental data (96.2 %).

In order to improve the Taguchi technique's selection and removal of dyes, Neural Networks and Genetic Algorithms have been applied in the removal of several azo dyestuffs. The accuracy of the Taguchi and Neural Network models is adequate, as evidenced by high values (> 97%). Furthermore, Neural Networks and a Genetic Algorithm were used to discover the best elimination circumstances for the dyes chosen according to the Taguchi design [19,20].

In [21] the RSM and GA technique were employed to improve the removal of the blue bromophenol dye. Iron oxide, zinc oxide, and zinc ferrite oxide were utilized as adsorbents in this work, and the Langmuir model was used to improve efficiency.

Reference [22] conducted a study to compare two approaches in the prediction of Reactive Black 5 (RB5) decolorization by a crude enzyme from Pleurotus: the ANN combined to the genetic algorithm (ANN-GA) and the RSM. They determined that there was no statistical difference between the two proposed procedures based on their experiments.

Reference [23] investigated the synergistic performance of the sonophotolytic-activated ZnO/persulfate (US/UV/ZnO/PS) process in the decolorization of acid blue 113 (AB113) dye from aqueous solution, as well as its applicability in the treatment of genuine textile effluent. They used central composite design-RSM (CCD-RSM) and ANN techniques to simulate the decolorization of the AB113 solution, and CCD-RSM and genetic algorithm (GA) approaches to optimize the process parameters.

1.2. Other nonlinear techniques applied to processes optimization in the textile industry

Many authors have proposed nonlinear techniques to model and optimize dyeing process, as described in the sequence.

Reference [24] studied the decolorization and degradation of the triazo bond Direct Blue 71 (DB71) dye by mixed bacterial culture in the presence of carbon and nitrogen deficit. They used RSM and ANN techniques for modeling and optimization of the decolorization process. The authors found that the ANN model performed better than the RSM model in terms of R2 (0.99) and AAD (0.04), based on the collected findings.

Reference [25] investigated the use of central composite design (CCD) and ANN in modeling and optimization of reactive blue 21 (RB21) removal from aqueous media under photo-ozonation process. The comparison made by the authors of predicted values by CCD and ANN showed that both methods were highly efficient in the modeling of the process. In [26] the extraction of natural dye from the roots of Rubia Cordifolia was investigated using both traditional and ultrasonic extraction methods. To this goal, they created an ANN that made predictions that were compared to RSM model values.

In [27] the simultaneous ultrasound-assisted elimination of quinoline yellow (YQ) and eosin B was modeled and optimized using a combination of ANN and RSM approaches (EB). According to the authors, the results for YQ and EB were 0.55 percent and 0.58 percent, respectively, in terms of average absolute deviation (AAD). Reference [28] developed three MLP−ANN models for the prediction and simulation of the degradation of textile dyes (Reactive Orange 16 – Monoazo, Reactive Red 120 – Diazo, and Direct Red 80 - Poly azo) by high energy gamma radiation. From the conducted simulations, the authors concluded that the developed MLP−ANN models could effectively predict the behavior of radiolytic degradation of reactive dyes. Reference [29] used an MLPANN to model the deterioration of Remazol Yellow Gold and reactive Turquoise, two textile dyes. In the simulations they ran, R2 values above 0.9084 were attained, showing that the MLP was capable of making accurate predictions. In [30] Through various advanced oxidation procedures, the dye AV17, which is used in the sanitizing industry, was assessed for deterioration (AOP). They achieved R2 values more than 0.9864 in the training, testing, and validation processes by modeling an MLPANN to forecast the deterioration of AV17. Reference [31] developed an ANN model to estimate the surface temperature distributions of powered e-textile structures under various conditions, which can be useful for e-textile product designers as well as textile manufacturers, especially for cold-weather protection products like jackets, gloves, and outdoor sleeping mats, according to the authors. Reference [32] developed an MLP-ANN to predict color using tristimulus variables (X, Y, Z) that represent dye concentration. Because of its capacity to use domain-specific knowledge obtained through training, the MLPANN technique beat the traditional Kubelka–Munk model, according to the authors. To predict the dyeing effect of supercritical carbon dioxide, 33- Zhang and his colleagues (2020) used Generalized Regression (GR) and MLP neural network models (SC-CO2). As a result, mean relative error (MRE) values for MLP and GR models were determined to be 3.27–6.54 percent and 1.68–3.32 percent, respectively. Furthermore, to the best of our knowledge, no publications on the optimization of the dyeing process in the textile industry prior to waste disposal have been identified in the literature. Thus, an algorithm integrating response surface approach and genetic algorithms is suggested in this study for optimizing reactive dyeing processes to achieve enhanced coloristic intensity, decrease salt discharge, and reduce contaminants in effluents.

1.3. Genetic algorithms technique

GA is a technical optimization metaheuristic based on natural selection that has been utilized to address optimization issues in a variety of fields in recent decades. The solutions to the problem are often represented by binary strings termed chromosomes or people in this technique. Genes (representation of a parameter, which can be made up of whole, real, or binary values) are the most important components of GA. Chromosomes (a group of genes that distinguishes a person from the rest of the population); Individual (represents a solution to a problem and is also a chromosome); Population (represents a group of individuals who will compete for survival and is also a chromosome). A binary, integer, or real-valued string can be used to represent the chromosome. The more capable chromosomes of the population are selected and crossed together to generate new chromosomes that are better than those of the previous population. As a result, the likelihood of one or more individuals being a solution to the problem increases with each generation. The essential steps of the GA process are depicted in Figure 2 and will be detailed in the sequence.

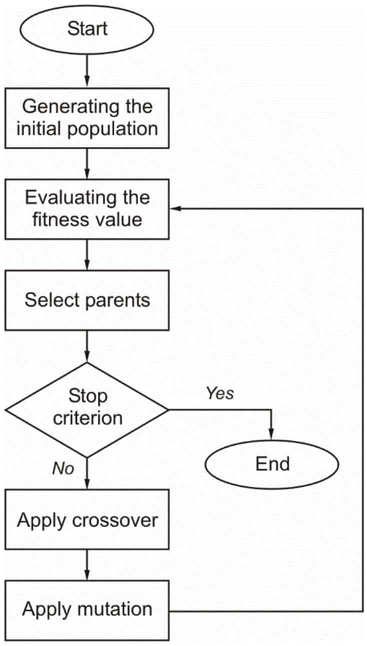

Figure 2: Flowchart of the GA process.

The process begins with the generation of the population, as shown in Figure 2. The goal function, which can be maximized or minimized, is then used to calculate aptitude. The method concludes the optimization search procedure if the solution obtained is satisfactory. Otherwise, the procedures of selection, crossover, and mutation are carried out before returning to the stage of aptitude calculation.

2. Experimental

2.1. Dyeing procedure

The 78 samples of 5 g each were bleached and dyed by exhaust method (Mathis Alt-1), at 10:1 liquor ratio, according to the process of dyestuff supplier recommendations. All steps of the process are shown in Figure 3.

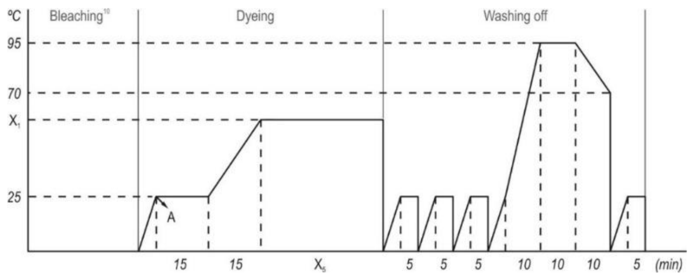

Figure 3: Scheme of dyeing process of all samples (A = addition of chemicals; independent variables being x_1 = Temperature and x_5 = Time).

2.2. Planning the experiments

To optimize the process variables for the highest coloristic intensity represented by its K S^{-1} coefficients (K S^{-1}) were examined the combined effect of the six different independent variables. For this, a 2^6 design of central composite and rotational (DCCR) was done. Six factors were used; they were the RB5, NaCl, Na_2CO_3, and NaOH concentrations and processing time and temperature.

The independent components, their actual values, and the six factors that were modified at these five levels (-2.83, - 1, 0, + 1, and + 2.83) are shown in Table 1. To produce the optimal K S1 settings, the factor values of the variables evaluated were determined based on preliminary testing on the effect of individual variables on dyeing and operating limits.

Table 1: Independent variables and their levels for the central composite design of dyeing.

Factors	Levels				
	-2.83	-1	0	+1	+2.83
x_1, T (°C)	22	40	50	60	78
x_2, [NaCl] (g/L^1)	-	20.00	40.00	60.00	97.00
x_3, [Na_2CO_3] (g/L)	0.425	5.000	7.500	10.000	14.575
x_4, [NaOH] (mL/L)	-	0.50	1.50	2.50	4.30
x_5, t (min)	-	30.0	60.0	90.0	145
x_6, [RB5] (%, w/v)	-	1.00	2.00	3.00	4.83

The K S^{-1} coefficient was calculated by Kubelka-Munk theory by using the Equation 1. [34]:

$$F_{k=m} = \frac{K}{S} = \frac{(1-R)^2}{2R} \quad (1)$$

Where R is the reflectance of the samples and it was assessed by visible spectrophotometry, under D_{65} illuminant, 10° (Konica-Minolta CM 3600d). The Kubelka-Munk theory has been used to a variety of industries that use pigments. It has also been used to check the composition and coloring of soils, including a study of the chromatic features of 98 soils with varying origins but an organic matter concentration of less than 2% and haematite or goethite as the major Fe oxide. According to the idea, the average soil haematite and soil goethite had hues close to their synthetic counterparts, while the rest of the soil components were simply a 'grey' matrix. It was also beneficial in predicting the amounts of haematite and goethite in soils using multiple reflectance measurements of soil-white standard blends or redness indices devised for synthetic mixtures [35].

2.3. Modeling

The least square method was used to fit each independent variable (x_i) of the experimental planning (Table 3) to a second-order polynomial equation, with the goal of correlating the response variable with the independent variables. For the early regression fits utilizing the equation, the linear, hyperbolic, and square interaction effects of the variables were evaluated. It's also utilized in the prediction equation and after second-order polynomial regression (Equation 2).

$$Y = \beta_0 + \sum_{i=1}^{n} \beta_i x_i + \sum_{i=1}^{n} \beta_{ii} x_i^2 + \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} \beta_{ij} x_j x_j \quad (2)$$

Where Y is the response variable (K S^{-1}), x_i = term of independent factor, $\square_0$= intercept, $\square_I$ = linear model coefficient, $\square_{ii}$ = quadratic coefficient for the factor i, and $\square_{ij}$ = linear model coefficient for the interaction between factors i and j (1, 2, 3, 4, 5 and 6).

Analysis of variance (ANOVA) was used to assess model fit, and RSM was used to optimize it in the Statistica6 ® for Windows software. The ANOVA is used to find significant variables, and it consists of classifying and cross-classifying statistical data. It was checked using a given classification difference, which was done using Fisher's statistical test (F-test). The F-value represents the relevance of each controllable variable on the tested model as a ratio of the mean square of regression (MRR) to the error (MRe) (F=MRR/MRe). For a model to be considered modified, the estimated F1 $\geq$ tabulated F1, while the value of the calculated $F_2 \leq$ tabulated F_2 and the R^2 value should be the closes of 1.0 [36,37].

3. Results and discussion

3.1. System modeling

The experiment planning employed in this research's assays is shown in Table 2. Using the least-squares method, the model was created using this data sheet. Figure 4 depicts the experimental data's variation in relation to the model's predictions. This table also highlights the similarity between the experimental K S^{-1} coefficient and the model's estimated K S^{-1} coefficient, as seen in Figure 1, which is supported by their comparisons.

Table 2: Planning matrix with experimental and calculated K S^{-1} coefficients.

Assay	T (ºC)	NaCl(g/L)	Na_2CO_3 (g/L)	NaOH(mL/L)	t (min)	RB5 (%)	K S^{-1} exp	K S^{-1} calc
1	40	20.0	5.000	0.50	30.0	1.00	5.2140	5.4697
2	60	20.0	5.000	0.50	30.0	1.00	11.716	10.6661
3	40	60.0	5.000	0.50	30.0	1.00	6.1280	6.9837
4	60	60.0	5.000	0.50	30.0	1.00	14.994	14.7693
5	40	20.0	10.00	0.50	30.0	1.00	6.5650	7.2513
6	60	20.0	10.00	0.50	30.0	1.00	11.804	10.7869
7	40	60.0	10.00	0.50	30.0	1.00	8.8500	9.5629
8	60	60.0	10.00	0.50	30.0	1.00	14.552	14.1301
9	40	20.0	5.000	2.50	30.0	1.00	4.8820	5.7697
10	60	20.0	5.000	2.50	30.0	1.00	6.5320	5.9161
11	40	60.0	5.000	2.50	30.0	1.00	5.6360	6.7865
12	60	60.0	5.000	2.50	30.0	1.00	11.485	10.9997
13	40	20.0	10.00	2.50	30.0	1.00	5.9030	6.4797
14	60	20.0	10.00	2.50	30.0	1.00	9.4580	9.0237
15	40	60.0	10.00	2.50	30.0	1.00	6.5030	7.8973
16	60	60.0	10.00	2.50	30.0	1.00	13.231	12.9505
17	40	20.0	5.000	0.50	90.0	1.00	11.789	12.9483
18	60	20.0	5.000	0.50	90.0	1.00	9.5110	9.1707

19	40	60.0	5.000	0.50	90.0	1.00	13.490	15.1071
20	60	60.0	5.000	0.50	90.0	1.00	12.159	12.0403
21	40	20.0	10.00	0.50	90.0	1.00	13.070	13.3979
22	60	20.0	10.00	0.50	90.0	1.00	11.709	11.0211
23	40	60.0	10.00	0.50	90.0	1.00	13.319	14.2255
24	60	60.0	10.00	0.50	90.0	1.00	13.314	12.6451
25	40	20.0	5.000	2.50	90.0	1.00	9.5910	11.0327
26	60	20.0	5.000	2.50	90.0	1.00	7.2760	7.4251
27	40	60.0	5.000	2.50	90.0	1.00	12.236	13.4815
28	60	60.0	5.000	2.50	90.0	1.00	9.6040	9.8527
29	40	20.0	10.00	2.50	90.0	1.00	8.9140	10.0971
30	60	20.0	10.00	2.50	90.0	1.00	7.4580	6.9247
31	40	60.0	10.00	2.50	90.0	1.00	12.394	13.4323
32	60	60.0	10.00	2.50	90.0	1.00	10.503	10.3243
33	40	20.0	5.000	0.50	30.0	3.00	9.2210	10.4621
34	60	20.0	5.000	0.50	30.0	3.00	25.855	25.0381
35	40	60.0	5.000	0.50	30.0	3.00	10.536	11.8869
36	60	60.0	5.000	0.50	30.0	3.00	31.187	31.4561
37	40	20.0	10.00	0.50	30.0	3.00	13.628	14.2497
38	60	20.0	10.00	0.50	30.0	3.00	22.715	22.0841
39	40	60.0	10.00	0.50	30.0	3.00	17.213	18.0097
40	60	60.0	10.00	0.50	30.0	3.00	31.560	30.9229
41	40	20.0	5.000	2.50	30.0	3.00	10.649	11.4937
42	60	20.0	5.000	2.50	30.0	3.00	18.489	18.6581
43	40	60.0	5.000	2.50	30.0	3.00	11.814	13.8405
44	60	60.0	5.000	2.50	30.0	3.00	26.142	26.4581
45	40	20.0	10.00	2.50	30.0	3.00	14.220	15.1201
46	60	20.0	10.00	2.50	30.0	3.00	20.241	19.6013
47	40	60.0	10.00	2.50	30.0	3.00	16.446	17.5845
48	60	60.0	10.00	2.50	30.0	3.00	27.766	27.6045
49	40	20.0	5.000	0.50	90.0	3.00	24.928	25.8771
50	60	20.0	5.000	0.50	90.0	3.00	23.678	23.7183
51	40	60.0	5.000	0.50	90.0	3.00	28.979	30.1563
52	60	60.0	5.000	0.50	90.0	3.00	28.710	28.5059
53	40	20.0	10.00	0.50	90.0	3.00	24.122	25.4007
54	60	20.0	10.00	0.50	90.0	3.00	25.453	25.4259
55	40	60.0	10.00	0.50	90.0	3.00	30.026	31.5295
56	60	60.0	10.00	0.50	90.0	3.00	30.630	30.5055
57	40	20.0	5.000	2.50	90.0	3.00	21.095	22.9283
58	60	20.0	5.000	2.50	90.0	3.00	16.342	16.3683
59	40	60.0	5.000	2.50	90.0	3.00	25.118	26.7071
60	60	60.0	5.000	2.50	90.0	3.00	23.164	23.3251
61	40	20.0	10.00	2.50	90.0	3.00	20.726	21.9771
62	60	20.0	10.00	2.50	90.0	3.00	16.888	16.6355

63	40	60.0	10.00	2.50	90.0	3.00	26.266	28.0023
64	60	60.0	10.00	2.50	90.0	3.00	23.633	24.2811
65	50	40.0	7.500	1.50	60.0	2.00	22.761	21.2098
66	50	40.0	7.500	1.50	60.0	2.00	22.147	21.2098
67	50	40.0	7.500	1.50	60.0	2.00	22.442	21.2098
68	50	40.0	7.500	1.50	60.0	2.00	21.860	21.2098
69	50	40.0	7.500	1.50	60.0	2.00	22.515	21.2098
70	50	40.0	7.500	1.50	60.0	2.00	22.345	21.2098
71	22	40.0	7.500	1.50	60.0	2.00	11.282	13.7764
72	78	40.0	7.500	1.50	60.0	2.00	14.214	20.3284
73	50	97.0	7.500	1.50	60.0	2.00	23.049	19.6585
74	50	40.0	0.425	1.50	60.0	2.00	20.288	17.3300
75	50	40.0	14.575	1.50	60.0	2.00	20.751	20.3179
76	50	40.0	7.500	4.30	60.0	2.00	15.249	11.8588
77	50	40.0	7.500	1.50	145	2.00	20.020	16.6295
78	50	40.0	7.500	1.50	60.0	4.83	31.902	28.5112

T = temperature and t = processing time

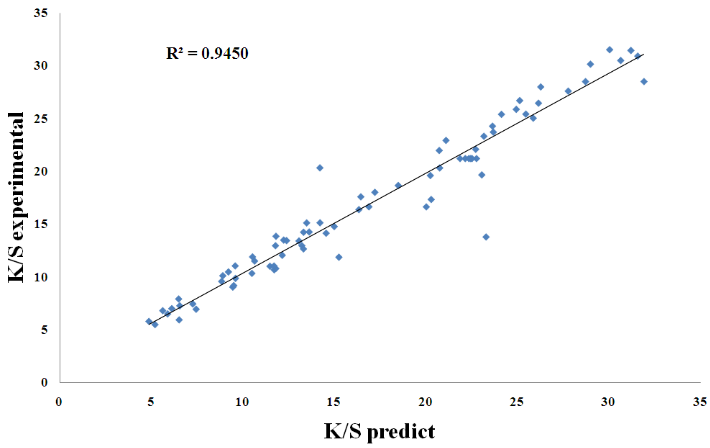

Figure 4: The behavior of the experimental data to those predicted by the model.

The ANOVA analysis is shown in Table 3. As can been seen, the variances are close to 90%, and the value of multiple correlations is close enough to the unit. At a 95% of confidence level, this number shows that the model can predict 82.50 percent of the experimental data using multiple correlations. The estimated F1- Test value was 5 times higher than the F1 tabular one, illustrating the model's importance and use in the prediction of K S^{-1} values in the examined conditions.

Table 3: Analysis of variance (ANOVA) .

RESULTS	Statistic	ANOVA				
		gl	SQ	MQ	F_{Calc}	F_{Tab}
Regression	-	6	316.3935	58.5655	34.8416	6.71
Resídual	-					
Multiple R	0.8639	-				
Multiple R^2	0.8464					
Adjusted R^2	0.8250					

The model showed that all factors tested had square influences on the dyeing's K S^{-1} coefficients [38] produced a model that is similar to ours by verifying that the K S1 value of tiles has a quadratic relationship with the quantity of pigments and the type of color. According to [35], as a systematic relation exists between the overall color and the quantity of coloring pigment, the K S^{-1} (Y) value of a mixture of several components can be calculated by adding the weighted contribution of every single component in the mixture, as follows:

$$Y = 21.2098 + 1.1576x_1 + 1.9929x_2 + 0.5279x_3 - 1.3504x_4 + 1.9462x_5 + 6.0507x_6 - 0.5191x_1^2 - 0.8979x_2^2 - 0.2979x_3^2 - 0.6904x_4^2 - 1.2596x_5^2 - 1.2264x_6^2 + 0.5792(x_1x_2) - 0.1998(x_1.x_3) - 0.7289(x_1x_4) - 2.6617(x_1x_5) + 0.8850(x_1x_6) + 0.1362(x_2.x_3) + 0.1345(x_2.x_4) + 0.6864(x_2.x_6) - 0.3035(x_3.x_5) + 0.1613(x_3x_6) - 0.4896(x_4.x_5) - 0.3572(x_4.x_6) + 0.7686(x_5.x_6) + 0.1211(x_1x_2x_4) - 0.3977(x_1x_2x_5) + 0.2121(x_1x_2x_6) + 0.1933(x_1x_3x_4) + 0.4352(x_1x_3x_5) - 0.2686(x_1x_3x_6) + 0.2004(x_1x_4x_5) - 0.3588(x_1x_4x_6) - 0.8692(x_1x_5x_6) + 0.1811(x_2x_3x_6) + 0.1237(x_2x_4x_5) + 0.1133(x_2x_5x_6) - 0.1898(x_3x_4x_5) - 0.3587(x_4x_5x_6) - 0.1275(x_1x_2x_5x_6) - 0.3140(x_1x_3x_4x_5) + 0.2638(x_1x_3x_5x_6) + 0.1634(x_2x_3x_4x_5) - 0.1138(x_2x_3x_4x_6) + 0.1381(x_1x_2x_4x_5x_6) - 0.1027(x_1x_2x_3x_5x_6) \quad (3)$$

Several authors have confirmed these contributions of dyestuff components in ceramic glazes, such as a linear increase in the K S^{-1} with the mass of the pigment (Fe2O3-ZrSiO4) [39]. Using ground calcium carbonate as a paper pigment, [40] had a linear model of the concentration (%) of 14 components of the dye mixture measured on the K S^{-1} value.

3.2. Optimization

3.2.1. Response surface methodology

The optimization is performed in conjunction with the figures in which the factor studied coexists, as determined by an analysis of each figure, if an optimal condition for each factor is obtained, as shown in the Response Surfaces of each situation described in sequence. Figures 5 to 9 present the evaluation of the effect of the temperature (T) combined with the effects of the following factors: NaCl concentration (g L^{-1}), Na_2CO_3 concentration (g L^{-1}), NaOH concentration (mL L^{-1}), time (t) and dyestuff content, respectively. When the temperature ranges from 22 °C to 30 °C, the highest K S^{-1} values are found.

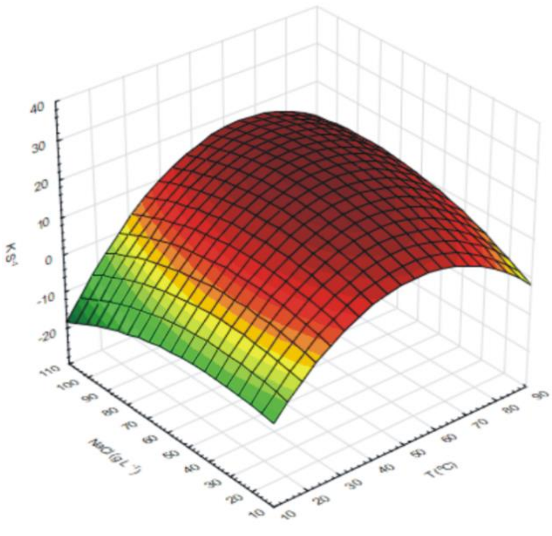

Figure 5: RS to evaluate the combined effects of NaCl and T.

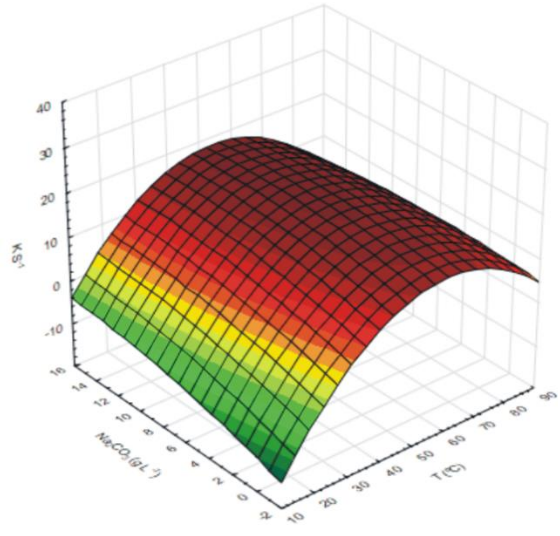

Figure 6: RS to evaluate the combined effects of Na_2CO_3 and T.

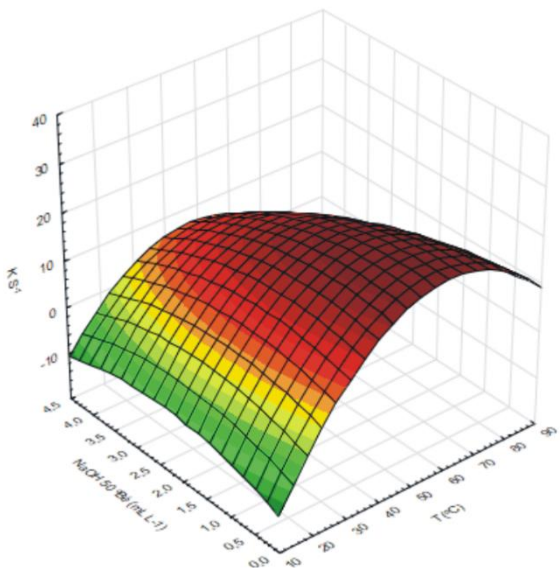

Figure 7: RS to evaluate the combined effects of NaOH and T.

Figure 8 depicts the RSM used to assess the effects of temperature and time on the K S^{-1} coefficient, in which low/medium temperature values with short process times produce the highest K S^{-1} values. Another optimal K S^{-1} response would be obtained for low-temperature values with high time values.

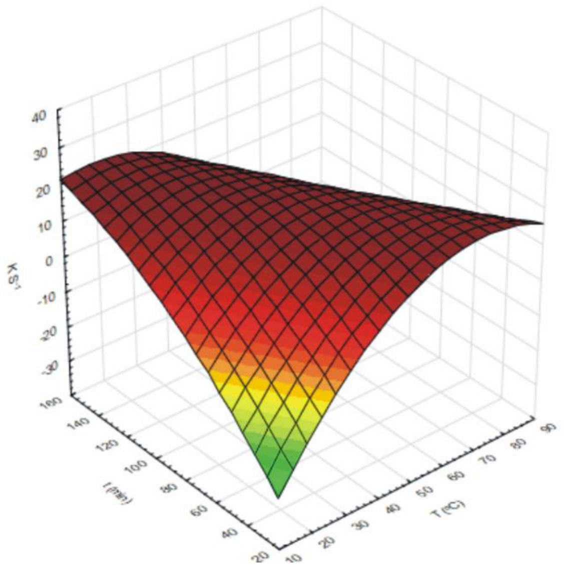

Figure 8: RS to evaluate the combined effects of t and T.

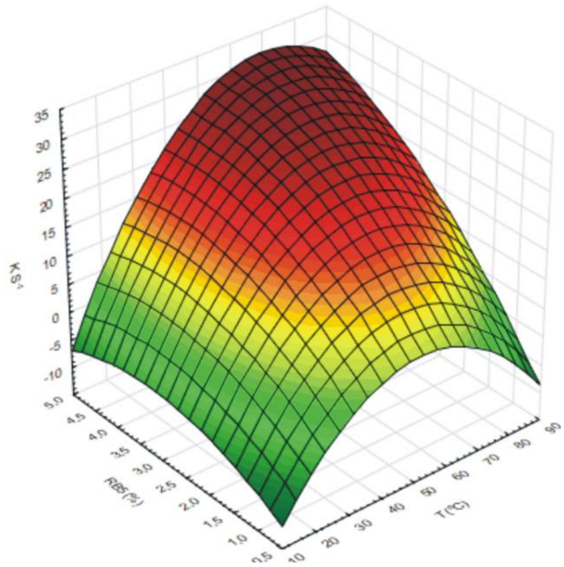

Figure 9: RS to evaluate the combined effects of RB5 and T.

Figures 5 and 10 14 show the effect of NaCl concentration combined with the effects of the following factors: T, Na2CO3, and NaOH concentrations, t, and dyestuff content, respectively. As can be seen, the behavior of K S1 under NaCl is the same in all figures, decreasing with low values of salt, but when the amounts exceed a certain level, the K S1 coefficients reach their maximum values, indicating that the concentration of this salt may be saturated in the dyeing studied. [41] also confirmed that NaCl concentrations greater than 0.2 M had no effect on the adsorption of methylene blue (MB) and reactive red (RR24) dyestuffs.

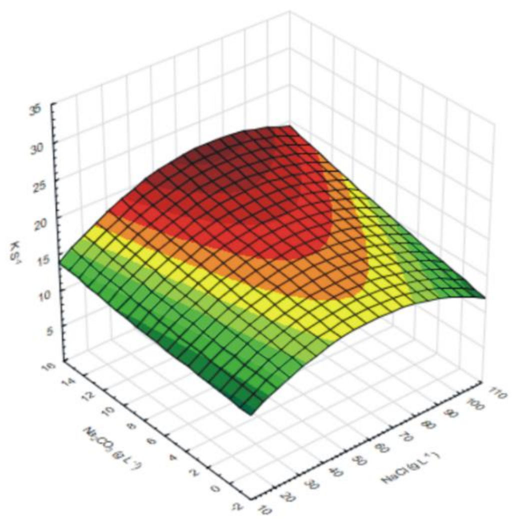

Figure 10: RS to evaluate the combined effects of Na_2CO_3 and NaCl.

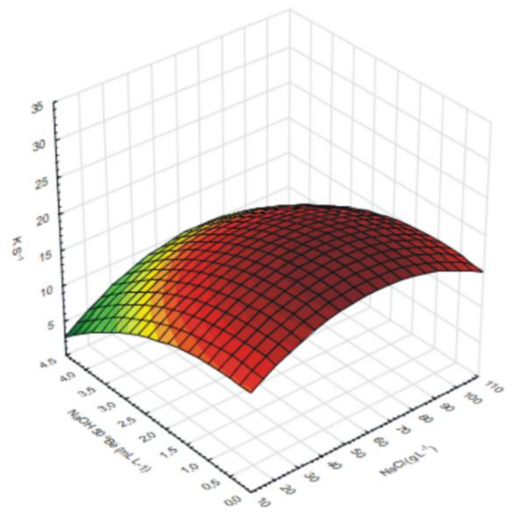

Figure 11: RS to evaluate the combined effects of NaOH and NaCl.

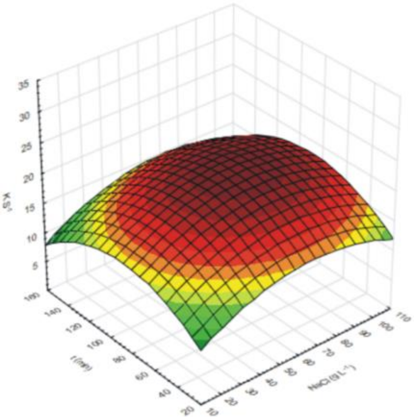

Figure 12: RS to evaluate the combined effects of t and NaCl.

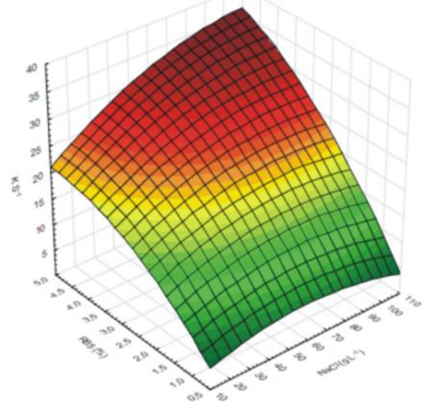

Figure 13: RS to evaluate the combined effects of RB5 and NaCl.

Figures 6, 10, and 15–17 show the effect of Na2CO3 concentration in combination with the effects of temperature, NaCl and NaOH concentrations, time, and dyestuff content, in that order. The effect of Na2CO3 concentration on the K S1 dyeing coefficient is small, but it is better explained when combined with the NaOH effect, as both contribute to the dyeing pH formation. Figures 7, 11, 15, 18, and 19 show the effect of NaOH concentration in combination with the effects of temperature, NaCl and Na2CO3 concentrations, time, and dyestuff content. These figures show that the dyeing K S1 values were highest when the NaOH content was lowest. The recommended dyeing pH range is 9 to 11, with values higher than 11 preventing dyestuff absorption in the fabric. As a result, increasing the NaOH content reduces adsorption and, as a result, the value of K S1. The effect of NaOH on the pH change in the dyeing solution and the conformation of the dyestuff structure is dependent on the type of dyestuff used in the dyeing process [42,43].

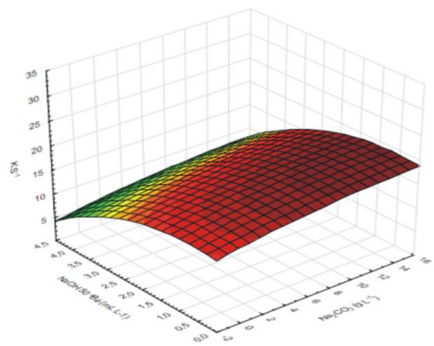

Figure 14: RS to evaluate the combined effects of NaOH and Na_2CO_3.

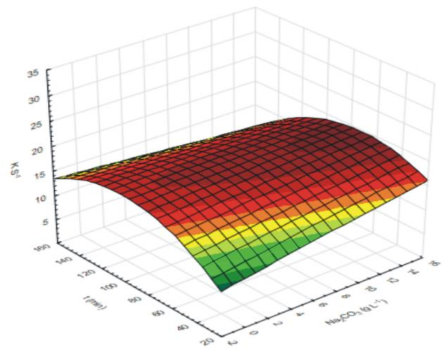

Figure 15: RS to evaluate the combined effects of t and Na_2CO_3.

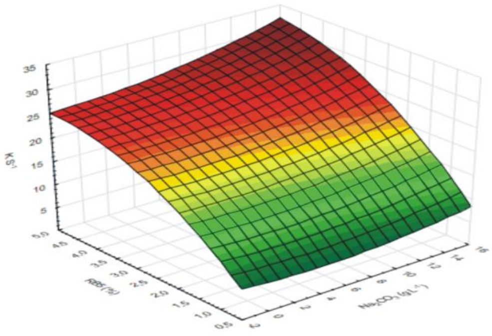

Figure 16: RS to evaluate the combined effects of RB5 and Na_2CO_3

Figures 8, 13, 16, 18, and 19 depict the effect of processing time (t) in conjunction with the effects of temperature, NaCl, Na2CO3, and NaOH concentrations, and dyestuff content, respectively. The largest K S^{-1} coefficients are achieved from the center point to the maximum value of the processing time, as shown in these figures. As previously stated in the literature, the K S1 coefficient increases with time, indicating that increasing the contact time between the dyestuff particles and the surface of the adsorbent (cotton fibers) favors adsorption which increases the absorption coefficient (K) and consequently increases the K S^{-1} value. [41,42], Figures 9, 13, 16, 18, and 19 show the effect of the dyestuff concentration in combination with the effects of temperature, NaCl, Na2CO3, and NaOH concentrations, and processing time, in that order. These graphs illustrate that as the dyestuff concentration rises, the K S-1 coefficient rises as well. As adsorption on the surface rises with increasing dyestuff concentration in dyeing, all authors agree that K S^{-1} increases with dyestuff content, as seen in our study. According to current research, greater pigment concentration tends to give deeper colors in the dyestuff due to an increase in the absorption coefficient (K) and, as a result, darker colors in the dyestuff. The reverse is true, with the lighter color of the dyestuff leading to an increase in the S value and, as a result, a reduction in the K S^{-1} value. [35, 38,44,45]

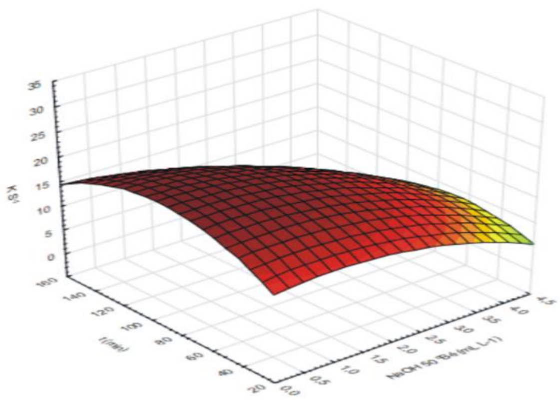

Figure 17: RS to evaluate the combined effects of t and NaOH.

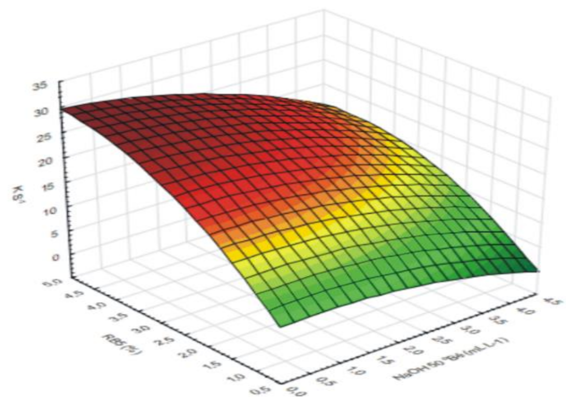

Figure 18: RS to evaluate the combined effects of RB5 and NaOH.

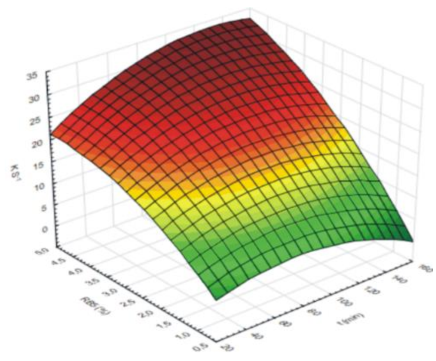

Figure 19: RS to evaluate the combined effects of RB5 and t.

The best conditions for finding the highest values of K S^{-1} coefficients are those that use a temperature of 23.5 °C combined with a NaCl concentration of 87 g L^{-1}, with a Na_2CO_3 concentration of 8.9 g L^{-1}, a NaOH concentration of 0.53 mL L^{-1}, a processing time 145 min, and a dyestuff concentration 4.83%. The optimization, on the other hand, should be based on the desired color, and then an ideal K S^{-1} coefficient should be found by adjusting the factor values under optimal conditions.

3.2.2. Genetic algorithms application

The GA technique was also used to obtain the best values for the variables involved in the dyeing process in the presented problem. The objective function is derived from the regression model itself, subject to the following constraints: $22°C \leq T \leq 78°C$, $20 \leq$ NaCl concentration ≤ 97 , $0.425 \leq Na_2CO_3$ concentration ≤ 14.575 , $0.5 \leq$ NaOH concentration ≤ 4.3 , $30min \leq t \leq 145min$, $1 \leq$ RB5 concentration ≤ 4.83.

The parameters used in this work are from MatLab® default values, as follows: Population = 200 individuals; Mutation rate = 1%; Maximum generations = 200; Function tolerance = 1×10^{-6} (stop criterion); Crossover fraction = 0.8. After 300 trials, it was obtained the best performance of the dyeing process of 81.90 % (optimal process value) for the following variables parameters (Table 4). The best performance has obtained after 136 generations.

Table 4: Optimal process values obtained from GA.

Parameter	Value
T (°C)	22.0
NaCl (g L^{-1})	97.0
Na_2CO_3 (g L^{-1})	73.876
NaOH (mL L^{-1})	0.5
t (min)	145.0
RB5 (%)	4.83

Figure 20: shows the evolution of the convergence of GA as function of generation number.

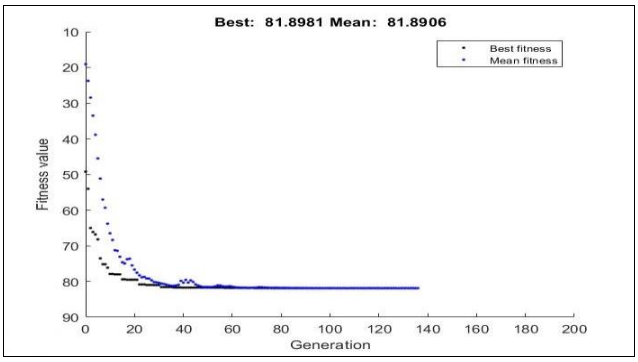

Figure 20: Performance of GA algorithm.

The black line is the best performance among existing populations, whereas the blue line represents the population's average convergence. In generation 136, the tolerance defined in the GA parameters was achieved, and the algorithm was stopped. Table 5 indicates the average number of generations required to attain the best outcome of 81.90 percent for the convergences constructed as intermediaries. 60 %, 70%, and 80%t were chosen as intermediate values, yielding 62.6 %, 71.47% t, and 80.33%, respectively. Ten trials were carried out for each percentage that was chosen as an intermediate.

Table 5: Process values obtained from different KS values.

KS	Fitness obtained	Generations	Process values					
			T (ºC)	NaCl (g/L)	Na_2CO_3 (g/L)	NaOH (mL/L)	t (min)	RB5 (%)
60	626.329	2	24.0	70.0	59.035	1.2	139.5	4.62
70	714.467	5	23.7	78.2	33.992	0.7	141.7	4.63
80	803.293	24	22.2	89.6	55.040	0.5	144.4	4.81
max	818.981	136	22.0	97.0	73.876	0.5	145.0	4.83

According to Table 5 and Figure 20, one can see a decrease in the values of temperature and NaOH as the convergence of GA increases. Likewise, the values of NaCl, duration and RB5 increase as the convergence value increases. These behaviors are observed from the first convergence established value to the optimized values, showing the decreasing and increases of the inputs to obtain the optimized dyeing process.

3.3. Formulations comparison

Two dyeings were prepared, which are described in Table 6: one with formulation provide by RSM technique and other with formulation provided by GA technique.

Table 6: Formulations data.

Formulation	RB5 (%)	NaCl ($g\ L^{-1}$)	Na_2CO_3 ($g\ L^{-1}$)	NaOH ($mL\ L^{-1}$)	Time (min)	Temp (ºC)	$K\ S^{-1}$
RSM Model	4.83	87	8,9	0.53	145	23.5	32.523
GA Model	4.83	97	7.4	0.5	145	22	31.985

The difference between the values was less than 0.54, indicating that both techniques could be used to improve dyeings using RB5 dyestuff. Colorfastness to water, that is a requirement for all dyeings produced by all formulas. [46], perspiration [47] and rubbing [48] were evaluated. Table 7 summarizes the findings.

Table 7: Formulations data.

Color fastness		RSM model		CA model	
		C	S	C	S
Water		4/5	4/5	4/5	4/5
Rubbing	Dry	5	4/5	4/5	5
	Wet	4	4/5	4/5	4/5
Perspiration	Acid	4/5	4/5	4/5	4/5
	Alkaline	5	4/5	4/5	4/5

OBS: C = color change; S = staining

In a scale from 1 (poor) up to 5 (excellent), both colors presented similar values of color fastness.

4. Conclusion

The use of Response Surface Methodology and Genetic Algorithms to model and optimize the dyeing of cotton with the Reactive Black 5 dyestuff is given in this paper. The $K\ S^{-1}$ function is shown as a sum of the contributions of each compound used in the dyeing formulation in the fitting model, and the model that best fit the experimental data presented square influences of all factors on the K S1 coefficient of the dyeing under investigation. Temperature of 23.5 ^{o}C, NaCl concentration of 87 g L^{-1}, Na2CO3 concentration of 8.9 g L^{-1}, NaOH concentration of 0.53 mL L^{-1}, processing time of 154 min, and RB5 concentration of 4.83 g L^{-1} are the optimal RSM settings for obtaining the greatest values of K S-1 coefficients. In addition, when applying GA, the best conditions for finding the highest value of $K\ S^{-1}$ coefficients are obtained Furthermore, while using GA, the optimal circumstances for obtaining the greatest value of $K\ S^{-1}$ coefficients are 22 ℃ , 97 g/ L for NaCl, 7.387 g/ L for Na2CO3, 0.50 mL L NaOH, 145 min processing time, and 4.83 g/L RB5, which are all in good agreement with the response surface results. Model - based dyeing formulations has shown that it is possible to reduce production costs without reducing product quality. Using this model, an approach for creating a computational tool to support the dyeing process was designed, allowing both the saving of chemical, water, and costs involved with these inputs for cotton dyeing with RB5 dyestuff. Furthermore, this computational tool could be used to reduce the environmental impacts of dumping chemical reagents and dyes, as well as the consumption of water, in addition to the economic impacts, since the Brazilian textile industry uses a lot of inputs and energy, which leads to high production costs and high environmental fines, that can affect the company's reputation. As can be shown, both color matching techniques can assist the textile industry in the prediction or formulation of a specific color based on the Kubelka-Munk theory. As a limitation of this work, it was carried out for only one dyestuff (Reactive Black 5). For future researches, the methodology can be applied to other dyestuffs, alone or together with, using bi or trichrome combination.

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