Application of Information Technology to Determine the Compound of Dyeing Compositions based on Transition Metal Salts

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Abstract: Results of studies carried out with the use of digital camera and computer data processing has given; the compound of the dye compositions based on iron and copper salts for dyeing cotton fabrics has determined. It has been established that when processing of cotton fabrics by γ-aminopropyltriethoxysilane and by solution of composition based on salts of transition metals, sodium nitrite and phenol derivative in an acidic medium the stable chelate complex of nitrosophenol with the polyvalent metal cations is formed, which reacts with the modified cotton cellulose with forming a covalent bond. Based on the conducted research were designed the optimum compounds of powder dye compositions based on salts of polyvalent metals for cellulosic fibers and technology of fabric dyeing based on them. Powder dyeing compositions for textile materials based on cellulose fibers due to their interaction with the fiber contribute to the formation of salt, coordination and covalent bonds and the formation the color on the fiber having high strength to various physical and chemical influences.

Key words: Cotton fabric, amination, dyeing composition, polyvalent metal salts, phenol derivatives, technology of dyeing, dyeing mechanism.

1. Introduction

The modern level of development of computer technology and mathematical modeling methods provide a unique opportunity for the change over both the industrial production and scientific research to a new level. Digital models of complex structures, a precise description and reproduction of natural phenomena and processes, thin multiparametric optimization becomes real today.

Modern theoretical views in the field of fibrous materials dyeing by various dyes are based on the functional dependence between the values of affinity determined mainly by nature of the material being dyed and the diffusion coefficient which at this temperature for one and the same fiber depends on the geometry dimensions of the color-imparting compounds and dyeing rate. With a decrease of affinity and increase of the diffusion coefficient the rate of dyeing enhancement is observed.

The chemical structure of the fiber-forming polymer has a very large impact on the fixation of dyes considering that functional groups of building blocks, end groups of macromolecules, other circuit elements of main valences and side groups are potential active sites on which the physical and chemical adsorption of dyes can occur.

Depending on the structure of potential active sites and structure of dyes a wide range of interaction forces between them can be realized: from the physical intermolecular to the covalent chemical one. Fixing dyes by fiber as one of the major steps is include the diffusion of dyes into fiber. Herewith the very important thing is the geometric size of the molecule or ion of compound imparting color, because it largely determines the rate of diffusion into the fiber [1].
Dyeing process through synthesis on fiber of dyed nano metal complexes of low molecular compounds of simple structure is the most rational solution to the problem of intensification of the dyeing process. This is caused by that molecules of the initial compounds have virtually no affinity to the fiber and because of the small geometric dimensions show high diffusion coefficients into a fibrous substrate that promotes to achieving the maximum color penetration to fiber for a minimum duration of its stay in solution. The purpose of this research is to develop the compound of the dye compositions based on salts of iron contributing to the formation of colored metal complexes in the structure of the cotton fiber.

2. Materials and Methods

In most cases the colorimetric characteristics (color coordinates, lightness, chromaticity, colour hue, etc.) of dyed fabrics are calculated based on the absorption spectra or the diffuse reflectance [2]. With the outspread of digital photography, desktop scanners and information technology color image transformation the quick, objective and automated method of colorimetric characteristics estimating of dyed specimens has upraised [3, 4].

According to the principal law of the doctrine of color [5, 6], almost any color can be represented as the sum of three linearly independent colors. As primary colors are used red (R), green (G) and blue (B), i.e. three monochromatic radiation with wavelengths of 700.0; 546.1 and 435.8 nm, respectively. The color of any shade and intensity can be obtained by varying the relative values (intensity, brightness) of these three components. In this case we speak about the representation of color in the color system of R, G, B. In modern graphics editors which allows to carried out the various operations on the decomposition of color components and the synthesis of the color from components, information regarding the pixel color is stored in the three color channels, respectively, R, G and B, in the form of numbers from the interval 0-255. Meanwhile, the number 0 corresponds to zero brightness, and the number 255 to the maximum. Then, according to the rules of additive color synthesis a combination of 0, 0, 0 corresponds to black, combination of numbers 255, 255, 255 to white color of maximum brightness, a combination of the same number in the range 0-255 to some gray color of intermediate brightness.

Dyed Fabric samples were photographed using a digital camera Canon 40D, 28-135 lens, macro mode distance of 0.5 m, aperture value 5.6, and the focal length F-135. The external flash Canon Speeclite 430EXII in automatic mode has been used. ETTL-II-flash head was at an angle of 45° which made it possible to capture images by reflected soft light. The color separation of scales image and R-, G-, B-channels brightness determination has been performed in a graphics editor Adobe Photoshop 7.0, from the menu bar has been chosen “Image-Histogram” and brightness values of each of the three channels has been read. Mathematical processing of the results has been carried out in the editor Origin 8.0. During processing the dependence of the brightness of R-, G-, B-channels on the concentration of the determined component has been generated and the approximating function found for each dependency has been found.

In order to establish the possibility of using a digital camera and computer software of digital image processing for determine the regularities of cotton fabric amination, the influence of $\gamma$-aminopropyltriethoxysilane concentration on the quantity of formed metal complexes of iron and copper in the structure of cotton fiber in the amination at 75 °C has been studied (Figs. 1 and 2).

It is established that in the processing of cotton fabric by 5% solution of $\gamma$-aminopropyltriethoxysilane at temperature 75 °C the highest degree of substitution is achieved and the optimum amount of metal complexes is formed on the cotton fabric. The obtained data showed that by using a digital camera and computer programs of digital image processing can be determined with high
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Precision the color properties of dyed fabrics, as well as through diffuse reflectance spectroscopy, using a laboratory spectrophotometer.

As is known by K. Venkataraman [7], the presence of initial amino groups in the polymer substrate molecules gives the possibilities of their diazotization with obtaining diazonium salts having a high activity. Diazotization has been carried out in an acidic medium in the presence of an equivalent amount of sodium nitrite which under the action of an acid passes to nitrous acid.

In combination of diazonium salt and phenols or amines the colored compounds are formed. The reaction is conducted in a weakly acidic medium in the presence of sodium acetate, which contributes to a weakly acidic medium formation. Follows from the above that textile materials containing primary amino groups may be colored dye compositions consisting of phenol or derivatives thereof, acetate and sodium nitrite; dyeing should be carried out in the presence of acid. Based on the foregoing it’s clear that the textile materials containing initial amino groups can be dyed by coloring compositions consisting of phenol or its derivatives, acetate and sodium nitrite; dyeing should be carried out in the presence of acid.

As it is known the azogroups has a low durability to light. Under the action of copper, nickel, cobalt salts [8] the azogroups are capable of forming complex compounds stable to light. Thus, for the formation of colouring on the cotton fabric durable to various physical and chemical influences, dyeing compositions should include sodium nitrite, an aromatic hydroxy compound, sodium acetate and polyvalent metal salt.

Modified cotton fiber as the functional groups contain amino and hydroxyl groups and a small number of carboxyl groups. When processing fiber by dye composition a series of processes can occur simultaneously, which contributes both to the direct dyeing of fibers and not leading to its dyeing: diazotization of the amino groups of the modified cotton fibers with the formation of diazonium salt and reacting them with phenolic derivatives, azo groups complex formation with the polyvalent metal cations, salt, formation of the cations of added salts with the carboxyl groups of fibers, the reactions between the components of the dyeing compositions with the formation of the complex compounds. In this regard, the optimum ratio of the components of dyeing compositions can not be established by the stoichiometric coefficients of the respective reactions. The most appropriate technique to establish the optimal proportions on composition components values is experimental selection. The influence of each component of dyeing composition to the color characteristics of dyed cotton fabric samples has been studied.

To study the influence of concentration of polyvalent metals salts on the color characteristics of the coloured samples of cotton fabric the dyeing was carried out at liquor ratio 25 of 3% solution of dyeing.
compositions at temperature 96 °C-98 °C. The concentration of sodium nitrite was equal to 0.5 g/L, Resorcinol-0.5 g/L. The concentration of ferrous sulfate in the dye liquor was varied from 0.25 to 1.00 g/L (Fig. 3), copper sulfate dye liquor was varied from 0.25 to 0.6 g/L (Fig. 4).

Samples of cotton fabric dyed by dyeing compositions based on iron sulphate have a blue-green color, and based on copper sulfate have gray color. Analysis of color scale images obtained by a digital camera in the coordinates R, G, B show that dyed fabric absorbs in the red region of the spectrum, therefore, the least bright channel is red (R) channel, and the brightest - green (G) and blue (B). Increasing the concentration of ferrous sulfate in the dye liquor from 0.25 to 0.5 g/L followed by increasing the color intensity of the cotton fabric, a decrease in brightness of color images of R, G, B channels caused by the decrease in the proportion of white in the color samples is observed. With further increase of the iron sulphate content there is a decrease of the color intensity which is apparently due to an increase in the rate of formation of iron metal complexes in the dye liquor. The optimum concentration of ferrous sulfate in the dye liquor is 0.5 g/L. When processing of cotton fabric with a solution of: copper sulfate, sodium nitrite, resorcinol, sulfuric acid the fabric becomes gray color having a maximum absorption in the blue region of the spectrum. Consequently, the least bright channel is blue (B), and the most bright is red (R).

One component of the dyeing compositions is NaNO₂ which during the dyeing in acidic medium becomes nitrous acid contributing the transition of modified cotton fibers amino groups to diazotized amine. The conducted studies have shown [9] that NaNO₂ also reacted with polyvalent metal cations with formation of complex compounds of various composition and appropriate strength. In this connection, the concentration of NaNO₂ in the compositions is also determined by using experimental selection (Figs. 5 and 6).

The obtained data shows that with increasing sodium nitrite concentration in the composition the intensity of coloration is increased and reach its maximum value when the concentration of sodium nitrite is 0.4 g/L-0.5 g/L. Further increase in the concentration of sodium nitrite in the dye liquor does not lead to significant changes in the intensity of the obtained colors.

The diazonium salts are capable to interact with polyvalent metal cations with the formation of complex compounds. By itself the azo group is not capable to give stable complexes with metals, if in this case a chelate bond does not form. For formation a chelate bonds is required a presence of hydroxyl or amino groups in the o-position to the azo group. For formation of stable dyed complexes of cotton fibers a resorcinol is
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Fig. 5 The dependence of R-, G-, B- components of cotton fabrics dyeing containing the metal complexes of iron on the concentration of NaNO2 in the solution.

Fig. 6 The dependence of R-, G-, B- components of cotton fabrics dyeing containing the metal complexes of copper on the concentration of NaNO2 in the solution.

Fig. 7 The dependence of R-, G-, B- components of cotton fabrics dyeing containing the metal complexes of iron on the concentration of resorcinol in the solution.

Fig. 8 The dependence of R-, G-, B- components of cotton fabrics dyeing containing the metal complexes of copper on the concentration of resorcinol in the solution.

Added into the composition. Resorcinol concentration in the dye liquor was varied from 0.15 g/L to 1.00 g/L. The concentration of ferric sulfate and sodium nitrite was equal to 0.5 g/L.

The concentration of resorcinol in complex forming solution changed from 0.15 g/L to 1.0 g/L. The most saturated colors are formed when the concentration of resorcinol is 0.5 g/L in complex forming solution comprising a cation Fe$^{3+}$-0.75 g/L in solutions containing cations Cu$^{2+}$. A further increase of resorcinol concentration in the dye liquor leads to reducing the intensity of color and has little effect on the color tone (Figs. 7 and 8).

3. Results and Discussion

In a significant number of studies the crucial role of pH solutions of metallochelates formation has shown. Variations of pH may impact on the surface charge of the adsorbent and the degree of ionization and speciation of the metal adsorbate. In connection with this the influence of pH of the treated solution on cotton fabric color coordinates has been studied (Fig. 9).

It was established that changing the pH of the treated solution has a strong influence on the number of metal complexes formed in the cotton fiber structure. While maintaining the pH of the treated solution from 3.6 to 4.0 the fabric becomes more intense color, indicating the formation of the maximum amount of metal complexes in the cotton fiber structure. Increasing the intensity of cotton fabric color is accompanied by a decrease in brightness of the color image of R, G, B, caused by a decrease in the proportion of white in the color of the sample.
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At very low pH of the solution the binding sections on modified cellulose of cotton fibers and resorcinol, probably will be protonated, leading to low levels of metal communication. The optimum range of pH 3.6-4.0 leaving the binding sections unprotonated maximizes the binding of metal with nitrosoresorcinol and further binding of the formed complex with the modified cellulosic fiber.

The data obtained (Fig. 9) testifies to the fact that when treating the cotton fabric by a composition solution the pH of solution increases, which seems to be the indication of binding of cobalt cations in complex and H⁺ ions of the treated solution neutralization by released Cl⁻ ions.

The effect of temperature on the formation process of metal complexes in the structure of aminated cotton fiber has been studied (Fig. 10). The processing of cotton fabric was carried out at temperatures of 20, 50, 80 and 98 °C. The kinetic curves shown in Fig. 2 show that the formation of metal complexes in the structure of aminated cotton fiber is occur very intensively. With increasing temperature the rate of formation of metal complexes increases significantly.

Increasing the processing temperature contributes to increasing the rate of components of the treated solution penetration into the fiber and the formation of metal complexes in the structure of fiber. The optimum temperature is 98 °C: as the formation of complex compounds in solution, the formation of metal complexes in the structure of the cotton fiber at 98 °C is occurred with a very high speed (for 5-7 min).

4. Conclusion

On the basis of conducted studies it was established that compositions based on iron and copper salts, sodium nitrite and phenols are capable to dye the aminated cotton fiber. The optimum ratio of the components of the dyeing compositions contributing to the formation of the maximum amount of metal complexes in the structure of the cotton fiber depends on the nature of the polyvalent metal cations, and for the composition of ferrous sulfate, sodium nitrite, resorcinol compound is 1:1:1; for compositions of copper sulfate, sodium nitrite, resorcinol is 1:5:7.5.

By means of digital camera and computer software of digital image processing can accurately determine the color characteristics of dyed fabrics. The usage of special programs will improve the accuracy and speed of parameters determination.

References


