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A Sensitivity Model and Repeatability of Recipe Colour

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The paper briefly describes a mathematical model of the colorant mixture colour sensitivity to concentration errors and the numerical estimates of the related quantities. Features of the theoretical model are illustrated with the results of a number of numerical experiments in which the optical data of a few basic dyes applied to textile fabric were used to predict the sensitivities of recipes for sets of target colours spaced regularly in the colour solid. The rest of the article deals with the question whether the predicted values of recipe colour sensitivity provide useful information about the repeatability of recipe colour. The results of a few groups of laboratory experiments involving the textile fabric dyeing with basic dyes have been analyzed with this question in mind.

Key words: colour matching, recipe formulation, recipe colour sensitivity, repeatability.

INTRODUCTION

The prescribed target colour of a material can be achieved by the application of a set of recipes (mixtures of various colorants in appropriate proportions). Not all recipes that match the prescribed target colour are equally appropriate for use in the production. Those recipes are preferred which are the least sensitive to small random concentration errors and other inevitable small random variations in the coloration process. Using their knowledge gained from experience, colourists in industry select less sensitive ones

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among various recipes. A theoretical model of the recipe colour sensitivity to concentration errors was developed in order to enable an advanced quantitative comparison of the sensitivity of various recipes at the time of computer recipe formulation.

THEORY

According to the needs of the coloration practice, the »sensitivity« of the recipe colour is introduced as a numerical quantity. Let ΔE denote the colour difference according to the formula CMC(l:c). The explanation of the colour difference formulae and the representation of colour by triplets of numbers – cylindrical coordinates L^* (lightness, level on the vertical axis), C^* (chroma, distance from the vertical axis) and h (hue, angle of rotation around the vertical axis) can be found in textbooks.[1] For simpicity, only the case of the recipe $\boldsymbol{c} = (c_1, c_2, c_3)$, consisting of the concentrations of three colorants, will be considered. The application of the recipe $\boldsymbol{c} = (c_1, c_2, c_3)$ produces the colour position $\boldsymbol{v} = (L^*, C^*, h)$. A small concentration change $\Delta\boldsymbol{c} = (\Delta c_1, \Delta c_2, \Delta c_3)$ produces a small colour change $\Delta\boldsymbol{v} = (\Delta L^*/(lS_L), \Delta C^*/(cS_C), \Delta H^*/S_H)$. Note that the colour difference ΔE is the length of vector $\Delta\boldsymbol{v}$.

Let us introduce the directional sensitivity of recipe $\boldsymbol{c}$ in the direction of a nonzero vector $\Delta\boldsymbol{c} = (\Delta c_1, \Delta c_2, \Delta c_3)$ (in concentration space) by:

$$s_{\Delta\boldsymbol{c}} = \lim_{t\to 0+} \frac{\Delta E(t\,\Delta\boldsymbol{c})}{\left\|t\,\Delta\boldsymbol{c}\right\|} = \lim_{t\to 0+} \frac{\left\|\Delta v(t\,\Delta\boldsymbol{c})\right\|}{\left\|t\,\Delta\boldsymbol{c}\right\|}\,. \tag{1}$$

Sensitivities s_1, s_2, s_3 of the recipe $\boldsymbol{c} = (c_1, c_2, c_3)$ to particular colorants are special cases of the directional sensitivity in directions $(\Delta c_1, 0, 0)$, $(0, \Delta c_2, 0)$ and $(0, 0, \Delta c_3)$, respectively.

The overall sensitivity of the recipe $\boldsymbol{c} = (c_1, c_2, c_3)$ is defined as the highest directional sensitivity over all possible (nonzero) directions $\Delta\boldsymbol{c} = (\Delta c_1, \Delta c_2, \Delta c_3)$ of a move from the recipe position $\boldsymbol{c} = (c_1, c_2, c_3)$ in the concentration space:

$$s = \sup_{\Delta\boldsymbol{c}\neq 0} s_{\Delta\boldsymbol{c}} = \sup_{\Delta\boldsymbol{c}\neq 0}\left(\lim_{t\to 0+} \frac{\Delta E(t\,\Delta\boldsymbol{c})}{\left\|t\,\Delta\boldsymbol{c}\right\|}\right). \tag{2}$$

NUMERICAL ESTIMATES

Allen's iteration equation[2,3] used in the recipe formulation algorithms has been transformed into the form[4] that links (small) concentration errors (changes Δc_1, Δc_2, Δc_3) with the visually relevant (small) changes $\Delta L^*/(lS_L)$,

$\Delta C^*/(cS_C)$, $\Delta H^*/S_H$, of the perceived colour of the object. The resulting linear approximation formula:

$$(\Delta L^*/(lS_L),\ \Delta C^*/(cS_C),\ \Delta H^*/S_H)^{\mathrm{T}} = \boldsymbol{J}_{\mathrm{CMC}}\boldsymbol{B}(\Delta c_1,\ \Delta c_2,\ \Delta c_3)^{\mathrm{T}} \quad (3)$$

is therefore approximately valid within a small neighbourhood of the recipe $\boldsymbol{c} = (c_1, c_2, c_3)$ in the concentration space and within a small neighbourhood of the corresponding colour position $\boldsymbol{v} = (L^*, C^*, h)$ in the colour space. This formula is then used to develop numerical estimates of the above introduced quantities.[4] It turns out that:

(a) the sensitivities s_1, s_2, s_3 of the recipe $\boldsymbol{c} = (c_1, c_2, c_3)$ to particular colorants are the lengths (norms $\|.\|_2$) of particular columns of the matrix $\boldsymbol{J}_{\mathrm{CMC}}\boldsymbol{B}$;

(b) the overall colour sensitivity of a recipe is the maximal singular value of the matrix $\boldsymbol{J}_{\mathrm{CMC}}\boldsymbol{B}$.

Usually, a larger number of recipes is treated. In order to reduce the amount of computation, the following computationally simpler upper bound

$$\sqrt{s_1^2 + s_2^2 + s_3^2}\ (=\|\boldsymbol{J}_{\mathrm{CMC}}\boldsymbol{B}\|_F) \quad (4)$$

for the overall sensitivity can be used instead of the exact value.

RESULTS

Numerical Experiments

The upper bounds (4) for the overall sensitivity s of various recipes were predicted for each of a larger set of target colours in order to investigate the dependence of the recipe colour sensitivity upon the position of the target in colour space.

Optical data of 8 basic dyes (2 yellows, 2 reds, 1 brown-red, 2 blues and 1 black) applied to textile fabric made of PAN fibres were used for match prediction. Target colours were chosen from the EUROCOLOR colour atlas, from 8 different L^*C^*-planes with hues 0, 125, 250, 350, 500, 650, 800 and 900 (per thousand), respectively. Targets were spaced uniformly by 10 units of L^* and C^* values.

For each target colour, sensitivities to particular colorants and the upper bound (4) for the overall sensitivity of all possible three-colorant recipes were calculated. The sensitivity upper bounds (4) for the recipes (containing the same combination of a yellow, a red and a blue colorant) for targets from the green L^*C^*-plane of hue $h = 350$ are presented in Table I.

TABLE I

Predicted upper bounds (4) of the overall sensitivity of the recipes (containing the same combination of a yellow, a red and a blue colorant) for each of the green targets indicated in L^*C^*-plane of hue h = 350 (EUROCOLOR 350.xx.xx)

Targets: 350.xx.xx green	C^* = 0	C^* = 10	C^* = 20	C^* = 30	C^* = 40	C^* = 50	C^* = 60
L^* = 80	3404	2246	1789	1626			
L^* = 70	1884	1192	997	898	864		
L^* = 60	994	655	545	500	498	527	564
L^* = 50	507	385	313	290	290		
L^* = 40	272	212					
L^* = 30	141	116					

Table I shows that the lightest-shade recipes are the most sensitive ones (they generally have the highest predicted (upper bound of) sensitivity) and that the recipe sensitivity rapidly decreases as the target gets darker. Furthermore, the predicted (upper bound of the) overall sensitivity is almost halved in case of a 10-unit decrease along each line parallel to the L^*-axis. The same trend was observed also for target colours in L^*C^*-planes for the 7 other hues considered. As higher lightness of a target in most cases (except *e.g.* for very saturated yellows) implies lower colorant concentration(s) in the recipe, the above observation is in agreement with the results of Alman's computer simulations,[5] suggesting that weighing errors are very important at low concentrations, whereas strength errors are more important in middle-range concentrations and that both are less important at high concentrations.

Contrary to the great variation of the predicted (upper bound of the) overall sensitivity with changing lightness L^*, the (upper bound of the) overall sensitivity of recipes varies considerably less when the chroma C^* of the target is increased at the constant lightness level L^*. When the target is moved radially from the grey axis, the recipe colour sensitivity moderately decreases in all directions and it can be almost halved at the gamut border (see Table I). This feature is in agreement with the observations that neutral shade recipes are generally more sensitive than other recipes.[6]

In addition, the upper bounds (4) for the sensitivity of the first 10 least metameric recipes per target were considered. These exhibited the same general trends as observed in the cases of recipes consisting of single 3-colorant combination treated above. To illustrate this, triplets consisting of the maximal (above), average (in the middle) and minimal (beneath) of the mentioned 10 sensitivity upper bounds for targets in the L^*C^*-plane with hue h = 350 are presented in Table II.

Table II shows that for some targets the sensitivity bound of the most sensitive among 10 recipes treated is up to 5-times higher than the sensitivity bound of the least sensitive one. The essential question of this paper is: does such a distinct difference in the predicted sensitivity to concentration errors also results in a significant difference in the repeatability of the (two)

TABLE II

Predicted upper bounds (4) of the overall sensitivities of the first 10 least metameric recipes for each of the green targets indicated in L^*C^*-plane of hue h = 350 (EUROCOLOR 350.xx.xx)[a]

Targets: 350.xx.xx green	C^* = 0	C^* = 10	C^* = 20	C^* = 30	C^* = 40	C^* = 50	C^* = 60
	4701	3115	2486	2148			
L^* = 80	3862	2000	1447	1139[b]			
	2590	1043	720	571			
	2660	1737	1390	1249	1150	1140	
L^* = 70	2091	1181	916	706	584[b]	564[b]	
	1211	556	415	309	261	236	
	1436	915	762	698	693	704	754
L^* = 60	1117	696	458	396	383	346[b]	434[b]
	645	396	226	171	149	140	182
	747	570	438	405	404		
L^* = 50	575	346	261	227	247[b]		
	330	178	128	93	83		
	406	318					
L^* = 40	311	232					
	179	127					
	215	176					
L^* = 30	163	102					
	93	52					

[a] Triplets consisting of the maximal (above), average (in the middle) and minimal (beneath) of the mentioned 10 sensitivity upper bounds.

[b] The average upper bound has been obtained from less than 10 values (at least from 4).

recipes (considered for a single target). As concentration errors are only one of several types of small random errors that affect the repeatability (for the case of textile see *e.g.* Sumner),[7] no simple and generally valid answer seems to exist. In situations where the relative contribution of concentration error to the total colour error is higher, the information contained in predicted sensitivity values could be useful. If so, the sensitivity values might be useful for very light targets, since in such cases the predicted sensitivities to concentration errors are the highest (see Tables I and II).

Laboratory Experiments

The recipe colour repeatability is a very important aim in coloration practice. In small-scale laboratory experiments, we wished to check whether the experimentally observed scattering of colour in the groups of samples dyed according to different recipes followed the order of the predicted sensitivities to concentration errors.

A few experiments involving laboratory dyeing of PAN fabric with basic dyes (exhaustive method) have been carried out. Standard graduated pipettes were used, each dye having it's own pipette. The concentration of the bulk solution was adjusted by measuring the solute with a measuring cylinder. All weighings of dyes and auxiliary chemicals were carried out on an analytical balance with an accuracy of ±0.0002 g. Cloth weights were always adjusted to the accuracy of 0.05 g. pH values were balanced using a pH meter, separately in each experimental tube. Dyeing apparatus Labomat (W. Mathis) was used. After the dyeing process was finished, the samples were rinsed thoroughly with warm and cold water. Ironing of the samples was then carried out using the dry heat treatment composite specimen in a heating device for 90 seconds at 100 °C.

Eight target colours were chosen from the EUROCOLOR colour atlas. Four of them were grey: Grey 50, Grey 60, Grey 70, Grey 80; and four were green: 350.50.30, 350.60.30, 350.70.30 and 350.80.30. Their positions in colour space are located approximately in the L^*C^*-plane for hue = 350 (green).

For each of the above targets, 4 recipes with different upper bounds of overall sensitivity have been determined (except for green targets 350.50.30 and 350.60.30 where only 3 recipes per target were considered). For each of the 8 targets, 20 repeated dyeing sessions have been carried out, each time producing one sample according to each of the 4 or 3 recipes. Scattering of colour positions in the respective groups of samples according to recipes for each particular target have been evaluated and compared. The RMS colour difference ΔE CMC(2:1) against the group average was used as the measure for the scattering of colour positions of samples in each 20-member group.

Samples with colour positions exceeding the CMC(2:1)-distance of 2 standard deviations from the group average were treated as outliers and were excluded from further calculations.

The data on the recipes matching the targets Grey 50, Grey 60, Grey 70 and Grey 80 and RMS deviations of colour positions in the corresponding groups of samples are presented in Table III. Similar data for the case of the green targets 350.50.30, 350.60.30, 350.70.30, and 350.80.30 are presented

TABLE III

Data on recipes matching the grey targets with lightness levels $L^*=80$, $L^*=70$, $L^*=60$ and $L^*=50$, and the data on the observed scattering of colour positions in groups of samples according to these recipes (4 recipes per each target)

	Recipe 1	Recipe 2	Recipe 3	Recipe 4
		Grey 80		
conc.(%)	0.0011 Yellow 1	0.0067 Yellow 1	0.0015 Red 1	0.0021 Yellow 2
conc.(%)	0.0111 Blue	0.0031 Red 1	0.0024 Yellow 2	0.0012 Red 2
conc.(%)	0.0058 Brown	0.0094 Blue	0.0056 Marine	0.0056 Marine
Sens. upp. bound	2134	3404	3771	4701
RMS ΔE	1.08	1.20	1.23	1.24
		Grey 70		
conc.(%)	0.009 Yellow 1	0.030 Yellow 1	0.005 Red 1	0.015 Yellow 2
conc.(%)	0.026 Blue	0.011 Red 1	0.015 Yellow 2	0.004 Red 2
conc.(%)	0.016 Brown	0.027 Blue	0.016 Marine	0.015 Marine
Sens. upp. bound	1211	1884	2126	2660
RMS ΔE	1.07	1.27	1.06	1.40
		Grey 60		
conc.(%)	0.026 Yellow 1	0.078 Yellow 1	0.010 Red 1	0.036 Yellow 2
conc.(%)	0.056 Blue	0.025 Red 1	0.035 Yellow 2	0.007 Red 2
conc.(%)	0.036 Brown	0.056 Blue	0.034 Marine	0.035 Marine
Sens. upp. bound	645	994	1142	1436
RMS ΔE	0.78	0.96	0.61	1.36
		Grey 50		
conc.(%)	0.066 Yellow 1	0.178 Yellow 1	0.019 Red 1	0.081 Yellow 2
conc.(%)	0.128 Blue	0.053 Red 1	0.076 Yellow 2	0.012 Red 2
conc.(%)	0.083 Brown	0.124 Blue	0.071 Marine	0.075 Marine
Sens. upp. bound	330	507	589	747
RMS ΔE	1.21	0.59	0.50	0.56

in Table IV. The RMS ΔE against the average colour position of a group of 20 dyeings with no colorants added was 0.39.

The observed scattering of colour (precisely: RMS colour difference ΔE against the group average) in the obtained 20-member groups of samples is presented also in Figure 1. Each of the diagrams in that figure relates to a particular one of the above 8 targets and it presents the observed RMS col-

TABLE IV

Data on recipes matching the green targets 350.80.30, 350.70.30, 350.60.30, and 350.50.30 with lightness levels L^*=80, L^*=70, L^*=60 and L^*=50, respectively, and the data on the observed scattering of colour positions in groups of samples according to these recipes (4 or 3 recipes per each target)

	Recipe 1	Recipe 2	Recipe 3	Recipe 4
		350.80.30		
conc.(%)	0.0625 Yellow 1	0.0846 Yellow 1	0.0925 Yellow 1	0.0981 Yellow 1
conc.(%)	0.0158 Blue	0.0095 Blue	0.0146 Blue	0.0015 Red 1
conc.(%)	0.0133 Yellow 2	0.0071 Black	0.0028 Brown	0.0142 Blue
Sens. upp. bound	571	616	892	1626
RMS ΔE	0.39	0.39	0.50	0.51
		350.70.30		
conc.(%)	0.0999 Yellow 1	0.1878 Yellow 1	0.1817 Yellow 1	0.2156 Yellow 1
conc.(%)	0.0405 Blue	0.0359 Blue	0.0213 Marine	0.0061 Red 1
conc.(%)	0.0446 Yellow 2	0.0091 Brown	0.0034 Brown	0.0348 Blue
Sens. upp. bound	309	496	617	898
RMS ΔE	0.51	0.57	0.70	0.57
		350.60.30		
conc.(%)	0.0721 Yellow 1	0.2230 Yellow 1	0.2668 Yellow 1	
conc.(%)	0.0863 Blue	0.0750 Blue	0.0157 Red 1	
conc.(%)	0.1206 Yellow 2	0.0309 Brown	0.0740 Blue	
Sens. upp. bound	171	279	500	
RMS ΔE	0.36	0.49	0.31	
		350.50.30		
conc.(%)	0.1254 Yellow 1	0.4498 Yellow 1	0.5607 Yellow 1	
conc.(%)	0.1668 Blue	0.1439 Blue	0.0307 Red 1	
conc.(%)	0.2402 Yellow 2	0.0602 Brown	0.1418 Blue	
Sens. upp. bound	93	160	290	
RMS ΔE	0.36	0.51	0.55	

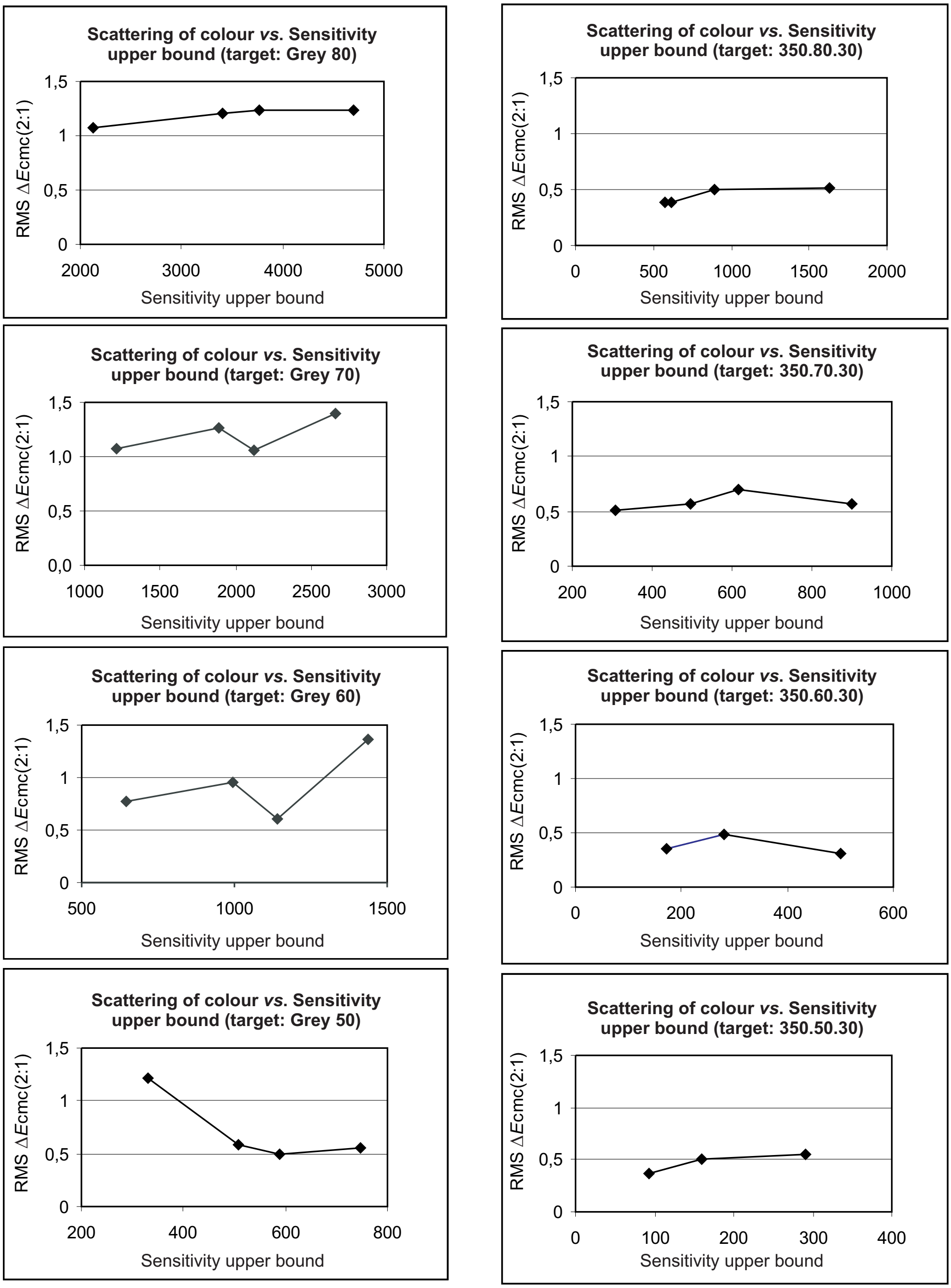

Figure. 1. Scattering of colour in groups of samples *vs*. sensitivity upper bounds (4) of the corresponding recipes. Each diagram relates to recipes for one of the 8 chosen target colours.

our difference ΔE (against the group average) in 4 (or 3) groups of samples *vs*. the predicted sensitivity bounds of recipes treated for this same target. The diagrams are arranged in a similar way as the corresponding targets are positioned in the mentioned L^*C^*-halfplane with hue h = 350.

DISCUSSION

Although neither the number of recipes nor the number of repeated dyeings were large, let us state the following observations. In the chosen case of laboratory dyeing of PAN fabric with basic dyes, a lower recipe sensitivity to concentration errors did not generally lead to lower scattering of colour in the corresponding group of samples, but when it did, it was just in the cases of light neutral target colours, which are known to be most difficult to reproduce in practice. It is also worth to mention that the least sensitive recipe performed the best or the second best in 7 out of 8 treated cases.

Especially interesting is the case of recipes which produced the lowest scattering of colour for targets Grey 50, Grey 60 and Grey 70 although their sensitivities were the second highest. All the three recipes consisted of the same colorant combination. It seems that this colorant combination has an additional quality and that the resulting advantage diminished only in the case of the lightest target Grey 80.

The big colour scattering of samples according to the least sensitive recipe for target Grey 50 is also a surprise. The corresponding RMS ΔE is 1.21, which is considerably more than all the RMS ΔE's 0.78, 1.07 and 1.08 produced by the recipes (consisting of the same colorant combination) for the lighter targets Grey 60, Grey 70 and Grey 80. The other 3 colorant combinations used in recipes for grey targets, exhibited approximately halving of the RMS of ΔE's, when moving from the target Grey 80 to the target Grey 50. This suggests that the above unexpected irregularity should be additionally checked.

In spite of the mentioned exceptions, in 4 cases out of 8 (Grey 60, Grey 70, Grey 80 and green 350.50.30), we notice a considerable difference in colour scattering between samples dyed according to the least sensitive recipe and the most sensitive one. In practice, such a difference would be a good reason for the use of the less sensitive recipe.

CONCLUSIONS

In the small-scale experiment described, the lower recipe sensitivity to concentration errors generally did not result in lower colour scattering in the corresponding group of samples, but a tendency of that kind was observed just in the cases of light neutral target colours, which are known to be the most difficult to reproduce in practice. The level of correlation between the predicted sensitivity of a recipe colour to concentration errors and the repeatability of a recipe colour will have to be studied on a larger set of target colours using a larger number of recipes (and, of course, separately for different coloration processes). Need for extension of the sensitivity model to other sources of error might emerge, but the practical application of such extended models for prediction of the relationship between repeatabilities of various recipes (for a given target) would require a great deal of additional calibration dyeing.

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SAŽETAK

Teorijski model za osjetljivost i ponovljivost boje mješavine bojila

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Ukratko je izložen matematički model i numeričke procjene osjetljivosti boje mješavine bojila na pogreške u koncentracijama bojila. Svojstva toga teorijskog modela ilustrirana su rezultatima numeričkih eksperimenata, u kojima su optički podaci za nekoliko baznih bojila, koja se upotrebljavaju za bojenje tekstilne tkanine, iskorišteni da bi se iz njih predvidjele osjetljivosti mješavinâ bojilâ, tj. receptura, za svaku iz skupa standardnih boja, pravilno raspoređenih u sustavu boja. Kako izneseni model uzima u obzir samo neke od izvora pogrešaka u procesu bojenja, pitanje glasi je li predviđene osjetljivosti na pogreške u koncentracijama bojila pružaju korisnu informaciju kada želimo predvidjeti onu recepturu koja bi, između više njih, u kasnijoj primjeni pokazala najbolju ponovljivost boje. Prodiskutirani su rezultati nekoliko skupina laboratorijskih eksperimenata s obzirom na ovo važno pitanje.