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E. I. Du Pont de Nemours & Company

F & F, Research & Development Division

Color Section

Interim Report

COMPUTER FORMULATION OF SOLID COLORS

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INTRODUCTION

The Formulating Computer predicts pigmentation in a color through application of the Kubelka-Munk Theory (Ref. 1, App. III) and the Duncan Equations (Ref. 2, App. III). The current procedure is to characterize each millbase using reflectance measurements on panels sprayed to complete hiding from five mixtures with a reference white millbase. Reflectances are measured on a Bausch and Lomb Spectronic 505 equipped with an integrating sphere and black light traps to eliminate specular reflection.

Results have been reasonably good in formulating light colors, permitting computer shading of the on-load formula. However, there is often a tendency to predict excessive amounts of black millbases and insufficient amounts of whites. There are also some very dark colors where the Formulating Computer fails completely.

OBJECTIVES

The objective is to achieve the full potential of the Formulating Computer in predicting solid colors. The technical objective is to determine the most accurate mathematical method of characterizing millbases.

SUMMARY AND CONCLUSIONS

(a) Characterization data generated from reflectances excluding specular reflection were found to be satisfactory in predicting pigmentation for light solid colors.

(b) Characterization data generated from reflectances including specular reflection and corrected via the Saunderson Relation (Ref. 3, App. III) were found to be more accurate in formulating dark colors, with no loss in accuracy in light colors.

(c) The current technique of using five characterization panels (at concentration levels of 10%, 20%, 40%, 80% and 100% of colorant) was verified to be the optimum.

(d) The use of separate K, S values for high and low colorant concentrations is unwarranted in view of the increased complexity of characterization and computation.

ACTION TAKEN OR PROPOSED

It is recommended that specular reflection be included in all reflectance measurements for characterization and formulation. Internal/external reflections should be corrected for by the Saunderson Relation.

Results of this study should be extended to formulation of metallic colors where feasible.

RESULTS AND DISCUSSION

(a) Inclusion of Specular Reflectance

Reflectances observed by a spectrophotometer do not account for reflection of light at the pigmented film/air interface. Black light traps may minimize errors due to external specular reflection, but make no allowance for multiple reflections within the film. Also, the percentage of external reflection trapped will be lower in the case of low gloss films. Mathematically it should be more sound to measure reflectances including specular reflection (eliminate the black traps) and correct for internal and external reflections via the Saunderson Relation (Ref. 3).

This was experimentally verified by characterizing six millbases first measuring reflectances excluding specular reflection (the old procedure) and then repeating measurements including specular reflection. These two sets of characterization data were then used to predict formulas for three light and three dark colors of known pigmentation. There was no appreciable difference between the two sets in predicting the light colors and one dark color (See Appendix I). However, on one dark color (926-93756, Appendix Ib) the first set (specular excluded) predicted excessive amounts of black and insufficient white. The second set (specular included) predicted the black and white more accurately.

The third dark color contained W-253, W-552, and W-765, all high absorption, low scatter pigments and only 4.1% of W-131. This type of color is expected to be difficult to predict since all millbases are characterized in the presence of a high scatter/low absorption white. The first set of characterization data yielded a formula which was a good tristimulus match to standard but an extremely poor curve match. The formula predicted by the second set of characterization data was close to the "on-load" formula of the standard and a good spectral match (See Appendix Ib and II).

These improvements in prediction of dark colors warrant a permanent switch to the second technique.

(b) Optimum Concentration Levels of Characterization Panels

The current characterization technique pairs reflectance curves of each concentration level (10%, 20%, 40% and 80%) with the masstone in determining K, S values and calculates averages of the four values. Instead, using ten panels at 10% concentration intervals would be expected to yield average K, S values more representative of the entire concentration range. This was found to be experimentally true. Predictions at high pigmentation levels were slightly improved. This however was at the expense of predictions at more moderate pigment concentrations. Since few colors require extremely high levels of any one millbase, it is more advantageous to retain the current technique which lays greater emphasis on the 10% to 40% range.

Another approach is to use separate sets of K, S data for the high and the low concentration levels. The slight improvement in results however does not warrant the increased complexity of characterization and computation.

A new characterization technique was tested which simultaneoulsly solved the Duncan Equations for three concentration levels (10%, 50% and 100%). This technique would allow characterization of a millbase using only these three concentration levels. The results were comparable to the present techniques. However, one bad characterization panel in the three could be disastrous. The current five-panel technique is more fool-proof.

REFERENCES

1. Kubelka, P. and Munk, F., Z. tech. Physik, 12, 593 (1931)

2. Duncan, D. R., Proc. Phys. Soc. London, 52, 390 (1940)

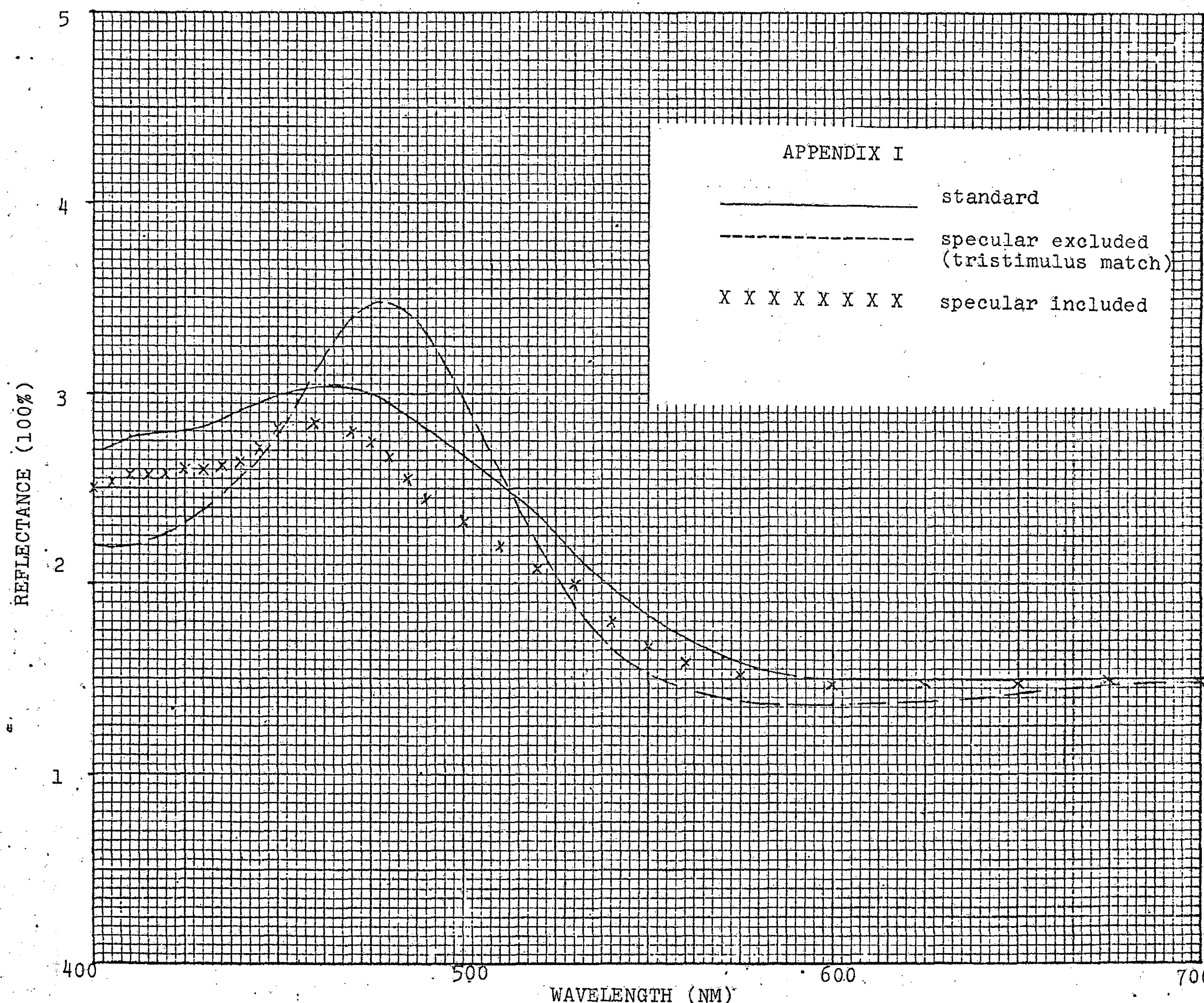
3. Saunderson, J., J. Opt. Soc. Am., 32, 727 (1942)

APPENDIX IA: PREDICTION OF PIGMENTATION IN LIGHT COLORS

	ON-LOAD CONCENTRATION	DEVIATION OF PREDICTED FROM ON-LOAD CONCENTRATION	
		SPECULAR EXCLUDED	SPECULAR INCLUDED
926-AF-239			
907 - 131	53.8	+ 2.9	+ 2.2
901 - 6253	0.7	+ 0.9	+ 0.8
901 - 552	40.3	- 4.2	- 2.7
901 - 765	5.2	+ 0.4	- 0.2
926-AF-240			
907 - 131	19.6	0.0	- 1.4
901 -6253	0.3	0.0	- 0.1
907 - 362	1.9	0.0	+ 0.1
907 - 630	78.2	0.0	+ 1.4
926-99944			
907 - 131	78.8	- 1.4	- 1.1
901 -6253	6.0	+ 0.3	- 1.0
907 - 362	0.2	+ 0.0	+ 0.1
907 - 630	15.1	+ 0.9	+ 1.9

APPENDIX IB: PREDICTION OF PIGMENTATION IN DARK COLORS

	ON-LOAD CONCENTRATION	DEVIATION OF PREDICTED FROM ON-LOAD CONCENTRATION	
		SPECULAR EXCLUDED	SPECULAR INCLUDED
926-93756			
907- 131	9.0	-5.5	-1.7
901-6253	42.1	+5.4	+3.0
907- 362	20.6	+2.8	+4.1
907- 630	28.4	-2.8	-5.5
DARK GREEN			
907- 131	8.5	-1.8	-1.8
901-6253	50.4	+7.5	+8.4
901- 552	11.0	-2.0	-3.8
907- 630	30.2	-3.6	-2.8
DARK BLUE			
907- 131	4.1	- 2.6	-0.9
901-6253	27.0	-18.5	+2.3
901- 552	54.0	- 9.1	+1.8
901- 765	14.9	+30.2	-3.3


APPENDIX I
standard
specular excluded (tristimulus match)
X X X X X X X X specular included
REFLECTANCE (100%)
5
4
3
2
1
400
500
600
700
WAVELENGTH (NM)

APPENDIX III: MATHEMATICAL EQUATIONS

KUBELKA-MUNK THEORY

$$\frac{K}{S} = \frac{(1-R_\infty)^2}{2R_\infty}$$

DUNCAN EQUATION

$$\frac{K}{S}_{\text{mixture}} = \frac{\Sigma c_i K_i}{\Sigma c_i S_i}$$

SAUNDERSON RELATION

$$R' = ak_1 + (1-k_1)(1-k_2)\frac{R}{1-k_2R}$$

where

K	=	coefficient of absorption.
S	=	coefficient of scatter.
R	=	true reflectance.
R'	=	apparent reflectance (as measured by a spectrophotometer).
R_∞	=	reflectance at complete hiding.
a	=	fraction of specular reflection measured.
c_i	=	concentration of component i.
k_1	=	proportion of incident light externally reflected at the surface.
k_2	=	coefficient of internal reflection for diffuse light.

ABSTRACT

It was experimentally demonstrated that the capabilities of the Formulating Computer could be expanded in the case of solid colors by taking all spectral measurements including specular reflection and using the Saunderson correction. Optimum concentration levels for characterization panels were also determined.

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