MATHEMATICAL METHOD FOR ESTIMATING COLOR OF SPAGHETTI AND MUSTARD FLOUR[1]

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ABSTRACT

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A mathematical method has been developed that allows direct calculation of dominant wavelength (DW) and percentage of purity from trichromatic coefficients if the DW lies between 550 and 600 nm. Accuracy is about ±0.23 nm for DW and ±0.5% for percentage of purity. The procedure is used with a computer to demonstrate that spectrophotometric estimations of color values of spaghetti and of mustard flour rapidly provide information that is as accurate as visual rating, and more comprehensive.

Expression of color in terms of dominant wavelength (DW), percentage of purity, and brightness according to the method of the International Committee on Illumination has been adopted as a standard procedure for estimating the color of macaroni products (1) and has been suggested as a method for estimating the color of fats and oils (2,3). Although the recent influx of small efficient calculators has allowed easy calculation of tristimulus values and trichromatic coefficients, especially using a selected ordinate procedure, using chromaticity diagrams is still necessary to obtain DW and percentage of purity of the sample.

A mathematical method has been developed that allows direct calculation of DW and percentage of purity of the sample color from the trichromatic coefficients x and y if the DW is in the range of 550 to 600 nm.

The method was programmed into a computer and was used to compare methods for estimating color of spaghetti and mustard flour by visual and spectrophotometric procedures.

DERIVATION OF MODEL

Examination of the chromaticity diagram for illuminant C (Fig. 1) shows that the area encompassing the origin and the points 550 and 600 nm (both at 100% purity) is approximately a triangle (Fig. 2), with properties as shown in Table I. (The triangle was terminated at the 600-nm point, because the relationship between the DW and the angle θ becomes increasingly nonlinear beyond this point.) All numerical constants were obtained from data in the standard work by Hardy (4).

For any point (x, y) within the triangle AOB, the angle m is given by m = arc tan

$$\frac{(y - 0.3163)}{(x - 0.3103)}$$

The angle $\theta = m - k$. Angle k = arc tan

$$\frac{(0.3725 - 0.3163)}{(0.6270 - 0.3101)} = 0.1756$$

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TABLE I
Properties of Triangle Formed by Three Points for Illuminant C[a]

Vertices	DW	% P[b]	x	y	Angles	Radius	Degrees	Sides	
A	550 nm	100	0.3016	0.6923	OAB	0.7717	44.3	a	0.3216
B	600 nm	100	0.6270	0.3725	ABO (k)	0.9523	54.6	b	0.3761
O	...	0	0.3101	0.3163	AOB	1.4176	81.2	o	0.4562

[a]See Fig. 2.
[b]% P = percentage of purity.

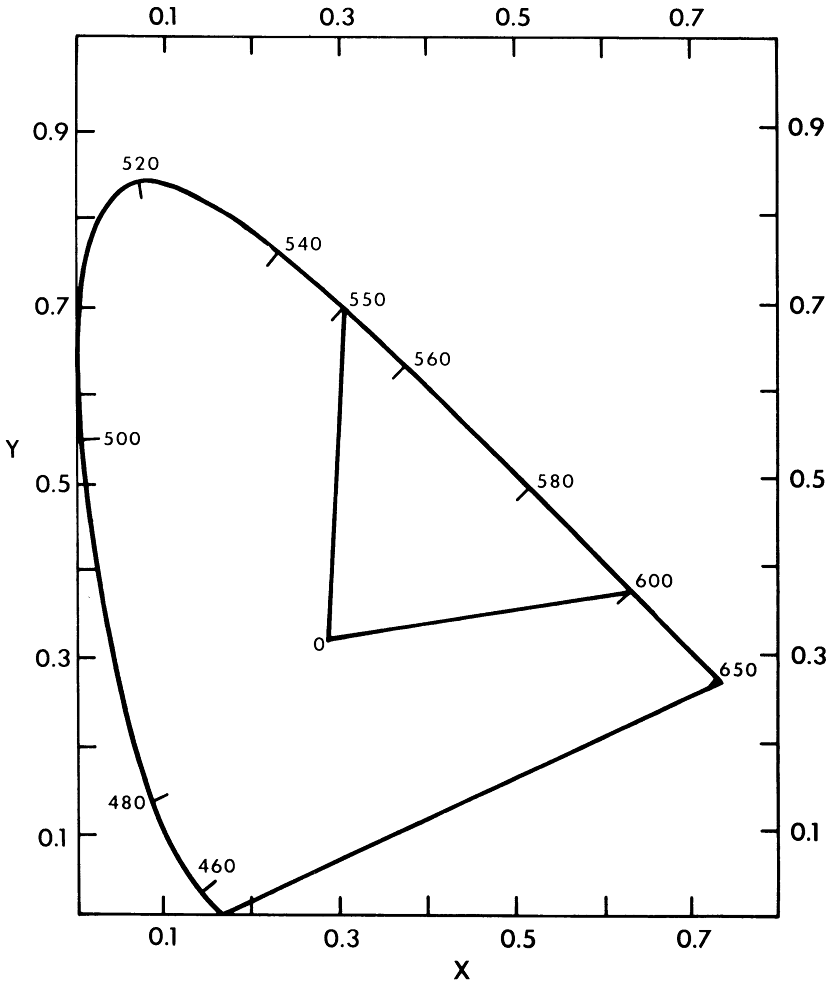

Fig. 1. Chromaticity diagram for illuminant C showing area in which model may be used.

TABLE II
Summary of Method for Calculation of Dominant Wavelength and Percentage of Purity From Trichromatic Coefficients

1. Estimate trichromatic coefficients (x, y) by an approved procedure
2. Let $m = \arctan \dfrac{(y - 0.3163)}{(x - 0.3103)}$
3. Let $\theta = m - 0.1756$
4. Then $DW = -15.77\,\theta^3 + 33.65\,\theta^2 - 50.84\,\theta + 599.57$
5. Let $n = \pi - (\theta + 0.9523)$
6. Let $b' = ([x - 0.3103]^2 + [y - 0.3163]^2)^{1/2}$
7. Then $\%\,P = 100\,(b' \sin n/0.2241)$

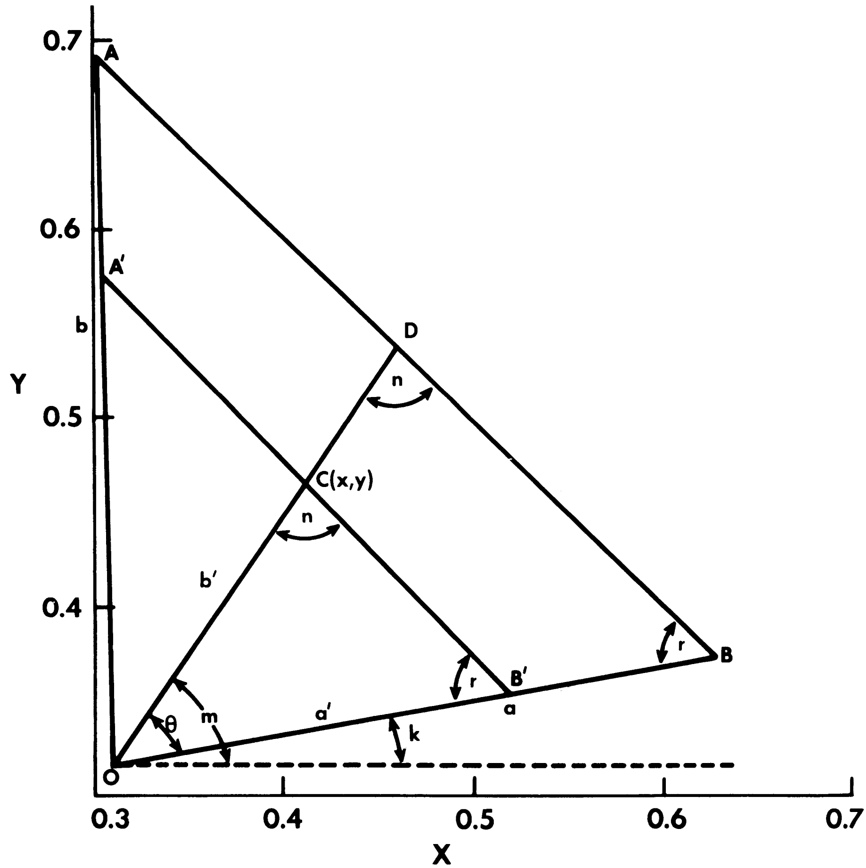

Fig. 2. Geometric constructions used in defining model.

radius (10.1 degrees) so $\theta = m - 0.1756$. Now DW = f(θ). This function may be estimated by finding the best fit curve (polynomial least squares fit) for a plot of θ versus DW (Fig. 3). This function is $DW = -15.77\ \theta^3 + 33.65\ \theta^2 - 50.84\ \theta + 599.57$, correlation coefficient r is 0.999, and standard error of estimate is 0.165.

Purity is defined as the fraction or percentage of the distance of the point C(x, y) from the origin to the outside edge of the chromaticity diagram (ie, percentage of purity = $100 \times \frac{OC}{OD}\%$). The distance $OC = b' = ([x-0.3101]^2 + [y-0.3163]^2)^{1/2}$. The distance OD may be estimated by an x sin r/ sin η (the triangles OCB′ and ODB are similar). Thus percentage of purity = $100 \times b' \sin n / 0.2241$ where $n = \pi - (\theta + 0.9523)$.

Experimental

Samples of spaghetti with a wide range in color were prepared and analyzed according to the AACC Standard Method 14-21. Spectrophotometry was performed using a Beckman Color DBG Reflectance Spectrophotometer, which automatically analyses 73 wavelengths from 740 to 380 nm at 5-nm intervals. A punched tape was also generated with the data for each of the samples and the

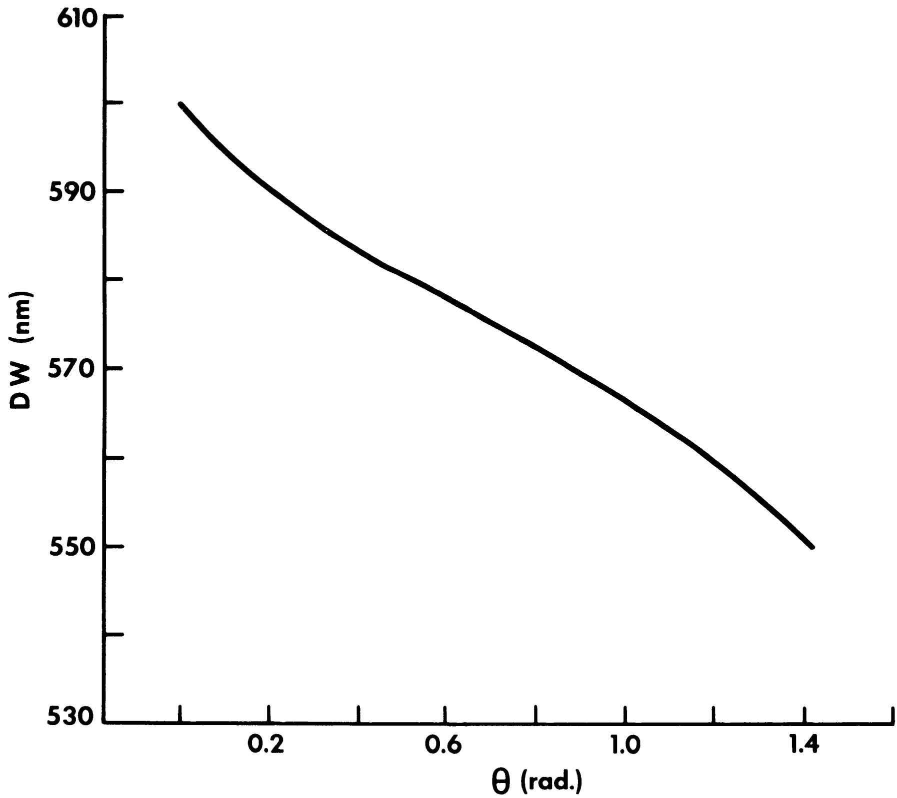

Fig. 3. Variation of dominant wavelength with angle θ.

color values were estimated using the above procedure using the Agriculture Canada Time Sharing Systems' minicomputer. A selected ordinate procedure (30 wavelengths) was used to determine trichromatic coefficients.

Samples of mustard flour were prepared by grinding samples of mustard seed in a coffee mill to an average particle size of 250 μ. V. Duke, of the Canadian Grain Commission, Inspection Division, supplied the seed, which represented good, fair, and poor specimens of each of the three grades of mustard seed. The flours were analyzed by placing them in a cell (5) and performing color analysis as with spaghetti samples. The flours were also ranked visually from lightest to darkest by a panel of nine judges.

RESULTS AND DISCUSSION

The equations derived above and summarized in Table II were used to calculate DW values and percentage of purity at 50 points of known DW and

TABLE III
Calculated Values of Dominant Wavelength (DW) and Percentage of Purity (% P) at Known Values of DW and % P

% P		Dominant Wavelength					
		550	560	570	580	590	600
	DW	552.7	560.0	570.1	580.3	590.3	599.4
10	% P	10.5	10.2	10.0	10.0	9.9	9.9
20		552.3	560.1	570.0	580.0	590.1	600.0
		20.9	20.4	20.3	20.0	20.0	19.9
30		552.2	560.0	570.1	579.9	590.2	600.2
		31.2	30.3	30.3	30.2	30.0	30.0
40		552.3	560.1	570.0	579.9	590.2	599.8
		41.8	40.3	40.3	40.2	40.2	40.0
50		552.4	560.0	570.0	579.9	590.2	599.5
		52.3	50.3	50.3	50.3	50.0	50.0
60		552.2	560.2	570.0	580.0	590.0	599.6
		62.9	60.6	60.4	60.1	60.3	59.9
70		552.4	560.0	510.0	579.9	590.2	599.6
		73.3	70.4	70.6	70.3	70.1	70.0
80		552.4	559.9	510.0	579.9	590.2	599.5
		84.0	80.4	80.6	80.3	80.2	80.0
90		552.5	560.0	570.1	579.9	590.2	599.6
		94.3	90.5	90.7	90.4	90.3	90.1
100		552.4	560.0	570.1	579.9	590.1	599.2
		104.5	100.6	100.6	100.4	99.4	100.1
	RMSD[a] DW	2.2	0.08	0.05	0.08	0.16	0.57
	% P	2.9	0.40	0.45	0.26	0.24	0.06

[a]RMSD = root mean square deviation.

percentage of purity shown in Table III. The results indicate that the equations can be used to calculate DW to within ±0.2 nm (1 standard deviation [SD]) and percentage of purity to within ±0.3% (1 SD). Much of this inaccuracy is due to difficulty in finding accurate values for x and y from the published chromaticity diagram.

Results were significantly different at 550 nm. This is possibly due to decreasing linearity of f (θ) from 560 to 550 nm, or more likely to errors in calculation caused by use of the absolute value of tan m where $m > \pi/2$ but $\simeq \pi/2$. The calculation procedure would thus seem most suited for calculations in the region of 555 nm $\leqslant$ DW $\leqslant$ 600 nm.

Table IV compares results from 13 samples of spaghetti analyzed by two

TABLE IV
Results From Manual and Computer Assisted Procedures for Determining Color of Spaghetti[a]

Sample	Visual Rating	Brightness		Purity		Dominant Wavelength	
		Manual	Computer	Manual	Computer	Manual	Computer
1	1	50.4	51.1	67.2	67.8	577.2	577.2
2	1	49.9	50.4	66.5	66.6	577.2	577.2
3	1	51.8	51.7	67.0	67.4	577.0	577.1
4	1	52.7	52.6	67.8	67.6	576.8	576.7
5	1	50.4	50.4	68.5	68.4	577.2	577.2
6	1	50.4	49.8	65.3	65.9	577.3	577.2
7	2	55.0	54.8	62.1	62.8	576.6	576.5
8	3	51.6	51.5	53.0	53.6	576.5	576.6
9	4	46.7	46.9	54.6	54.1	577.5	577.7
10	5	42.8	42.5	75.5	75.7	578.5	578.6
11	6	54.0	53.8	38.9	39.1	577.0	577.0
12	7	54.3	53.8	35.5	36.3	577.0	577.0
13	7	42.8	43.3	57.3	57.4	578.6	578.6
	RMSD[b]	0.39		0.46		0.09	

[a]Separate spectra obtained for manual and computer calculations.
[b]RMSD = root mean square deviation.

TABLE V
Color of Mustard Flour Samples

Sample	Rank[a,b]	Brightness	Purity	Dominant Wavelength
1 Can. G	1.50 ± 0.58 A	56.6	36.1	578.0
1 Can. F	2.55 ± 0.80 B	57.8	35.8	577.9
1 Can. P	1.95 ± 0.81 A B	57.0	35.3	578.0
2 Can. G	6.25 ± 0.85 C	53.1	41.7	578.5
2 Can. F	4.15 ± 0.34	56.5	42.9	578.2
2 Can. P	6.35 ± 0.67 C	56.5	41.0	578.6
3 Can. G	5.45 ± 0.76	53.5	42.7	578.4
3 Can. F	8.1 ± 0.32	50.5	45.5	578.4
3 Can. P	8.9 ± 0.32	51.7	46.6	577.8

[a]Rank order correlation (with grade) = 0.91.
[b]Samples with same letters not different at 5% level.

different procedures. The time required for analysis of the 13 samples by the manual procedure was about 8 man hours. This time is reduced by about 50% when using the computer to process the data. Results were not significantly different between the two sets of samples. Slightly higher results in brightness and purity obtained using the computer procedure are likely due to the two different operators using the spectrophotometer.

The 13 samples were also evaluated using a visual rating scale. Samples were rated against a sample having desirable color characteristics. A good correlation (multiple $r^2 = 0.89$) was found between visual ranking and color values. The spectrophotometric procedure seems to be slightly more sensitive than is the visible rating procedure in differentiating between samples.

Table V shows a comparison between the spectrophotometric procedure and a visual grading procedure for differentiating between different samples of mustard flour. A good correlation (multiple $r^2 = 0.88$) was again observed between visual ranking and color values. As with the spaghetti, the spectrophotometric procedure seems more sensitive to color changes than does visual scoring.

CONCLUSIONS

The color of grain products is often evaluated by simple visual scoring. Spectrophotometric procedures, which express color in terms of the internationally recognized color values (brightness, purity, and DW), are not in common use both because of the relatively unusual equipment required and because of the complexity of the mathematical calculations and other bookwork required to produce the final results. This study demonstrates that when using a relatively inexpensive reflectance spectrophotometer coupled indirectly with a computer, color values may be produced rapidly. These values may provide more accurate, comprehensive information than does visual screening.

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