MICROCOMPUTER SOFTWARE FOR COLORIMETRIC DATA MANAGEMENT AND ANALYSIS

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Abstract: Color analysis, as applied in development of new color proofing systems, requires sophistication and flexibility well beyond the computation routines normally pre-programmed in commercially available color measurement instruments.

To meet this need a complete new system, SPECTRO 1.3, was developed for processing spectral reflectance data and performing a wide variety of conventional and custom-designed calculation routines. Color properties of hypothetical new multicolor film structures can be predicted from known spectral data for single color components.

Operating convenience approaches that of popular business software. Capabilities include: storage of 1500 spectral records per disk, file search by keyword, editing and printing of finished reports.

Spectral reflectance data are transferred directly to the computer from the spectrophotometer via a communications interface. Though the present system was developed for use with the IBM Personal Computer, the programs are in BASIC and can be modified for other computers.

Background

When modern colorimetry originated, in the early

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1930's, the tristimulus values X, Y, Z were computed directly from spectrophotometric data (and the X, Y, Z tristimulus functions) by numerical integration, using mechanical calculators. The tedious calculation process essentially limited the use of colorimetry to research applications.

Later, photoelectric colorimeters simulated the tristimulus functions by means of filters and photodetectors and provided direct readings which closely approximated X, Y, Z. These instruments were sufficiently accurate for most industrial applications and have been used for many years, principally in quality control.

The past few years have brought the availability of a third type of instrument which, for want of a better name, could be called a "spectrocolorimeter." Typically, such instruments are capable of accurately measuring spectral reflectance (or transmittance) at 10 nm wave length intervals and performing fundamental calculation of X, Y, Z -- plus a variety of other colorimetric values -- directly from the spectrophotometric data. Since the calculations are performed rapidly by microcomputer devices, the spectrocolorimeter can greatly expand the role of colorimetry in the graphic arts research laboratory.

Equipment

The software described below was originally developed for use with one specific spectrocolorimeter: the IBM 7410 Color Sensor Analyzer. This instrument is equipped with a preprogrammed microcomputer which calculates and prints standard colorimetry values, including (X, Y, Z), (x, y), (L, a, b), (L*, a*, b*), etc. (These colorimetric parameters are defined and discussed in Judd and Wyszecki (1975) and other texts on color science.)

The IBM 7410 Color Sensor Analyzer can also be interfaced with the IBM Personal Computer. In the present application, the computer was configured with 64K of random access memory,

equipped with two double-sided disk drives, and connected to an Epson MX-100 Printer.

The SPECTRO 1.3 System

The SPECTRO 1.3 System was developed for use in research on new color proofing systems. Software development objectives were as follows:

1. Data Base - Efficient disk storage and retrieval of basic spectral reflectance data

2. Calculations - Wide choice of standard colorimetry calculations plus non-standard experimental routines

3. Simulation - Capability for predicting color properties of multicolor film structures from component data

4. Reports - Automated, unattended, formatted printout of results for large lists of samples

5. Ease of Use - Similar to popular business software: no programming knowledge required of user, all commands defined and prompted on-screen, all potential user errors trapped to prevent accidental termination of program

6. Documentation - Complete manual, to high quality commercial standards, with step-by-step tutorial section.

The resulting system utilizes two program disks:

Interface Disk - for transfer of data from the IBM 7410 Color Sensor Analyzer to the computer, via an RS-232 Interface

System Disk - for data management and calculation using the IBM Personal Computer

Additionally, a number of Data disks are used in conjunction with the program disks. Each Data disk contains 1500 sets of spectral reflectance data.

The principal purpose of the Interface Disk is to transfer sets of spectral reflectance readings from the spectrocolorimeter to the computer. Each set consists of 31 reflectance values (400 to 700 nm, at 10 nm intervals). Since the functional operation of the interface program is, of necessity, specific to the IBM 7410 spectrocolorimeter, it will not be discussed here.

The System Disk contains all programs necessary for data handling, calculation and reporting, in a manner which meets the above stated objectives. These programs are coded entirely in BASIC.

Though the actual program code listings are proprietary and are not disclosed here, it is felt that the following discussions of program concepts, sequence, and operating features can be of real value to those who wish to develop similar programs to meet their own specific needs.

Data Handling

Each data record consists of: a unique 5-digit Record Number, a 35-character Descriptor, a Date and a 1-character designation of Type (S for Sample or R for Reference). One two-sided disk provides random access storage for 1500 such data records. Files can be searched by Record Number or by Descriptor.

To search files by Record Number, one simply enters the desired number. The resulting screen display appears as shown in Figure 1. (Reflectances are shown without decimal points, i. e.: displayed value = Reflectance X 10,000.)

To search files by Descriptor, the user assigns START and END record numbers and specifies up to three KEYWORDS. In SPECTRO 1.3, A KEYWORD is defined as any sequence of 11 characters, or fewer, which is included in the Descriptor. The program will search through the sequence of Record Numbers from START through END, find all records containing the KEYWORDS, and print out a list of Record Numbers, each with Type, Descriptor and Date. The user may specify an "OR" search to find every Descriptor which contains ANY of the KEYWORDS; or an "AND" search to find every Descriptor which contains ALL of the KEYWORDS. Search rate is approximately 200 records per minute.

The screen display for the Search by Descriptor function is shown in Figure 2.

SAMPLE and REFERENCE

As noted above, two types of data record are employed: sample and reference. The concept of "SAMPLE and REFERENCE" is essential for predicting color properties of multicolor structures.

In measurement of color films, 4-color printed press sheets, etc., a SAMPLE can be any area of colored material. A REFERENCE, normally, is a corresponding area of support material (either "clear" or "white") which ideally, would be spectrally nonselective, or neutral.

For every colorimetric calculation, SPECTRO 1.3 utilizes a PAIR of spectrophotometric records, one record for the SAMPLE and one for the corresponding REFERENCE. Calculations can be made for (Sample plus Reference) or (Sample minus Reference). In either case, the resultant value of reflectance is calculated at each of 31 wave lengths, and it is these resultant reflectances which are used in the subsequent colorimetric calculations. (The resultant reflectances can also be stored on the Data Disk as a "derived" record for later use.)

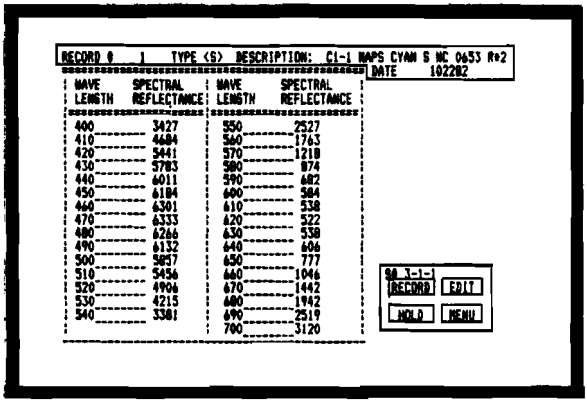

Figure 1 - Search by Record Number

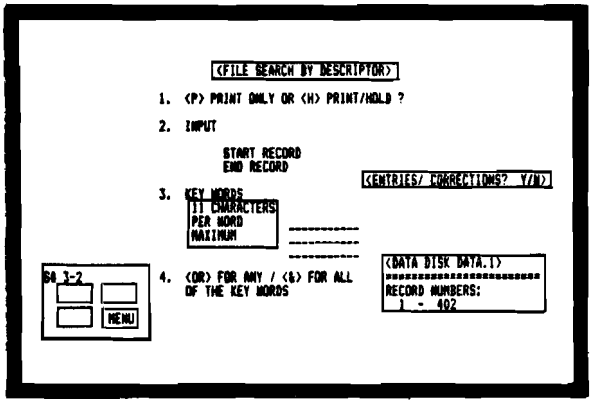

Figure 2 - Search by Descriptor

Considered in its simplest form, a (Sample minus Reference) calculation can answer such questions as: If, at a given wave length, a color film SAMPLE has a Reflectance of .17 and the "clear" base alone, or REFERENCE, has a reflectance of .85, what is the reflectance of the coating alone, "minus" the base? (It is assumed that both sample and reference films were backed up with the same "white" reference plaque during measurement.)

The (Sample minus Reference) calculation utilizes simple division at each wave length.

$$\text{REFLECTANCE OF (SAMPLE - REFERENCE)} = \frac{\text{REFLECTANCE OF SAMPLE}}{\text{REFLECTANCE OF REFERENCE}}$$

In the above example, Reflectance of (Sample - Reference) = .17/.85 = .20

The (Sample plus Reference) calculation utilizes multiplication at each wave length.

$$\text{REFLECTANCE OF (SAMPLE + REFERENCE)} = \text{REFLECTANCE OF SAMPLE} \times \text{REFLECTANCE OF REFERENCE}$$

From the (Sample + Reference) calculation we can, for example, determine the colorimetric characteristics of any two colored films or layers, when overlaid.

The HOLD BUFFER Concept

As will be evident from later discussion, calculations can be performed by manual entry of SAMPLE and REFERENCE record numbers. This process can be repeated by keying in many successive pairs of record numbers and the results can be printed out, one line at a time.

Where more than a very few samples are involved, however, the HOLD BUFFER provides a much faster and more convenient method of operation.

SPECTRO 1.3 provides the capability for accumulating a list of up to 100 pairs of record numbers (Sample and Reference) in a HOLD BUFFER, in the computer memory. Calculation can be set up for automatic input from the hold buffer. In this mode, the computer automatically reads the record numbers in the hold buffer, retrieves the corresponding records from the Data Disk, performs the calculations and prints the results. These operations are performed in relatively quick succession, and can continue without operator attention until the entire hold buffer listing has been completed.

SPECTRO 1.3 includes Hold Buffer functions which permit the user to create a hold buffer listing by entering Sample and Reference Record Numbers, and to edit by inserting or deleting record numbers anywhere in the list. Hold buffer information in the computer memory can be saved on disk as a HOLD FILE. Conversely, HOLD FILES saved on disk can be loaded into the computer memory hold buffer.

Additional capability for compiling a hold buffer is provided by the file search functions (discussed above) which include a search-and-hold option. With this option, all record numbers found in a search can be automatically added to the end of the hold buffer.

Calculations

The main purpose of SPECTRO 1.3 is to perform calculations and print tabulated reports, as illustrated by Figure 3.

The Calculation Set-Up Display, depicted in Figure 4, offers the user a wide choice of calculation procedures:

1. Results of calculation can be printed, or displayed only.

2. Input can be manual or automatic.

3. Calculations can be (Sample + Reference) or (Sample - Reference).

4. Five different "Standard Observer" functions are available.

Standard Observer options 1 and 2 are the well known 1931 Illuminant C and 1964 Illuminant D65 (Judd and Wyszecki, p. 153). Option 3 uses experimental block filters. Option 4 will provide for calculation of ANSI color densities when the approved standard factors become available. Option 5 uses factors developed by Hensel (1984).

If manual entry is selected, the Record Number - Manual Entry display (Figure 5) prompts for entry of SAMPLE and REFERENCE Record Numbers. (A calculation for SAMPLE ALONE can be obtained by entering "N" as the Reference Record Number.) After about 7 seconds calculation time, results are displayed on the screen as shown in Figure 6. If the PRINT option was selected, the results are also printed out as one line of the report. The user may then recall the Record Number - Manual Entry display (Figure 5) and enter another pair of Record Numbers, or return to the Calculation Set-Up display (Figure 4).

Figure 3 - Format of Printed Report

1931 ILLUMINANT C
SAMPLE MINUS REFERENCE

EXHIBIT A
TUTORIAL - CALCULATION USING THE HOLD BUFFER
***** SAMPLE MINUS REFERENCE *****

SAMPLE	DESCRIPTION	TYPE	DATE	X	Y	Z	L	a	b	ANG	RAD	L*	a*	b*	DX	DY	DZ
3	C1-3 MAPS MAGENTA S MM0472 R#4	S	102282	49.58	25.92	42.77	50.91	+84.73	-14.16	-9.49	85.91	57.96	+79.56	-15.04	0.296	0.586	0.441
4	*C1-4 MAPS MAGENTA CLEAR MM 0472*	R	*102282*														
1	C1-1 MAPS CYAN S MC 0653 R#2	S	102282	27.20	33.44	94.68	57.83	-17.25	-56.56	-106.96	59.13	64.52	-20.96	-46.97	0.557	0.476	0.096
2	*C1-2 MAPS CYAN CLEAR MC 0653*	R	*102282*														
3	C1-3 MAPS MAGENTA S MM0472 R#4	S	102282	39.15	20.55	32.61	45.33	+74.84	-10.91	-8.29	75.63	52.45	+73.15	-12.21	0.399	0.687	0.559
1	C1-1 MAPS CYAN S MC 0653 R#2	S	102282	20.63	25.94	71.26	50.93	-16.82	-47.28	-109.58	50.18	57.98	-21.47	-41.45	0.677	0.586	0.219

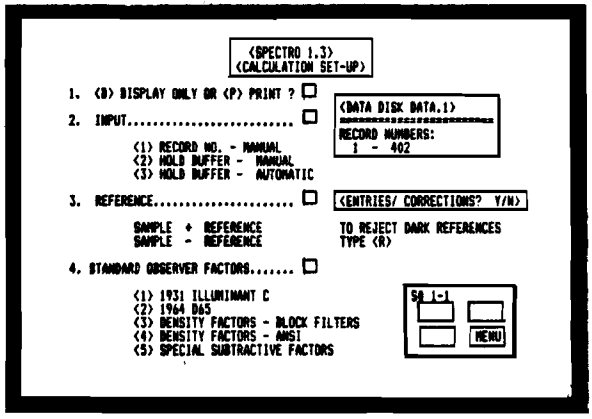

Figure 4 - Calculation Set-Up

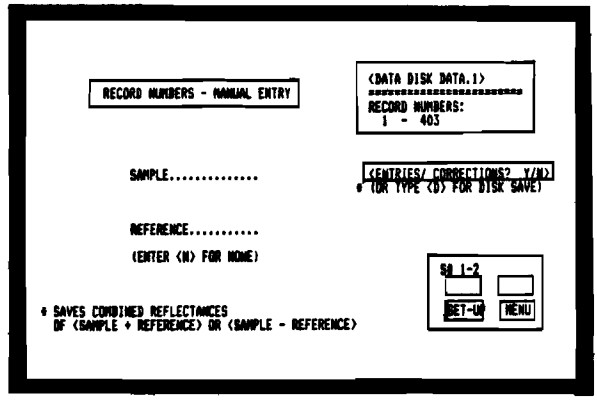

Figure 5 - Calculation - Manual Entry of Record Numbers

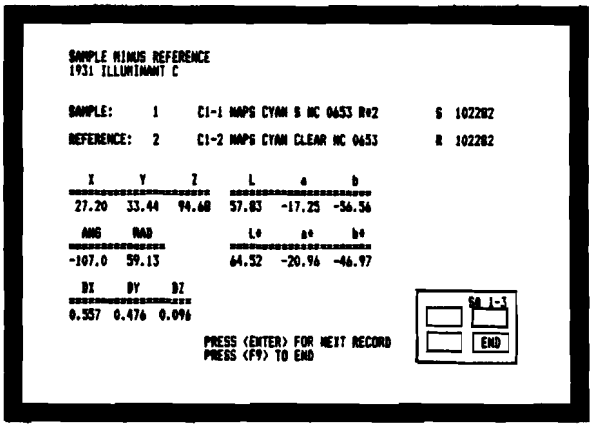

Figure 6 - Calculated Results

If automatic input is selected the computer will automatically access each successive pair of Sample and Reference Record Numbers listed in the HOLD BUFFER, and display and print the calculated results. A full 100-Item hold buffer will produce a five page report. After the last calculation, the program automatically returns to the Calculation Set-Up display (Figure 4). The user can quickly obtain additional reports, with changes in (Sample +/- Reference) or in Standard Observer, simply by changing the Calculation Set-up choices.

Each printed report, as illustrated by Figure 3, includes a 3-line title entered by the user, and is identified by (Sample + Reference) or (Sample - Reference) and by Standard Observer. For easy reading, SAMPLE information is printed in normal type, and REFERENCE information in italic type. Reports longer than one page are automatically page numbered.

Support Functions

The principal SPECTRO 1.3 operations of data management and calculation are supported by the following essential functions and features:

1. The Enter New Record function - provides for manual entry of spectrophotometric data. This capability is needed at start-up of a new system, in emergency if the normal spectrophotometer interface is out of service, or for use with data from alternate spectrophotometers.

2. Data Editing features - incorporated in the File Search and Enter New Record functions; permit the user to edit any portion of any data record: Record Number, Descriptor, Type, Date and spectral reflectance values. (Though editing of spectral data is rarely required, it can be useful for correcting erroneous results due to minor errors in spectrophotometer calibration.)

3. The Hold Buffer Editor (discussed below) - enables the user to select up to 100 different Samples, assign to each a Reference and arrange the listing of Record Numbers in any desired order for subsequent calculation and report printing.

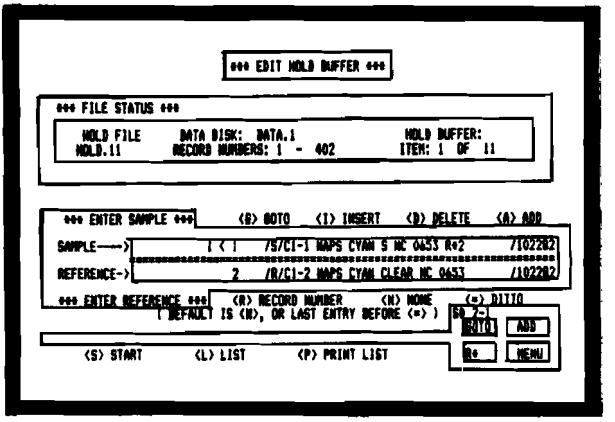

Figure 7 - Hold Buffer Editor

Figure 7 represents the HOLD BUFFER EDITOR display.

The upper portion of the display shows file status: name of Hold File loaded from disk (HOLD.11), name of Data Disk (DATA.1) and Record Numbers which it contains (1-402), and also the displayed Hold Buffer Item Number (1) and the total number of Items in the Hold Buffer (11).

The displayed Hold Buffer Item (consisting of SAMPLE and REFERENCE) is seen in the Sample and Reference windows, midway down the display, and shows Sample Record Number 1, Reference Record Number 2.

The user can display-list the entire Hold Buffer sequentially, one Item at a time, in the Sample and Reference windows; display any individual Hold Buffer Item by number; or print out a complete listing.

Any Item can be deleted, or a new Item can be inserted anywhere in the listing, or added to the end. (With any of these changes, all Hold Buffer Items are automatically renumbered.)

A separate Reference Record Number can be assigned, corresponding to each Sample Record

Number, or one Reference Record Number can be assigned to correspond to a group of Samples, or "N" can be assigned as a Reference Record Number where calculation for SAMPLE ALONE is desired.

User Convenience

Throughout the program development, an effort was made to anticipate and avoid problems due to program or user error.

To prevent terminal errors, or "crashes," all user inputs are examined for format and validity, e. g.: Record Numbers may not exceed 5 digits or contain non-numeric characters, and must be within the range of numbers stored on the particular Data Disk. Inappropriate commands are rejected, and an explanation displayed if necessary.

All calculation routines have built-in checks to prevent accidental division by zero, over-load, underload, or other errors which would terminate a BASIC program.

Warnings are displayed if the number of records on the Data Disk, the number of Items in a Hold Buffer, etc., have reached the maximum values allowable in SPECTRO 1.3.

To facilitate user choice of program options, each display which requires more than one input utilizes an "Edit Prompt," displayed in the form <ENTRIES/CORRECTIONS? Y/N>. In Figure 4, Calculation Set-up, for example, the <ENTRIES/CORRECTIONS? Y/N> prompt is seen toward the right, midway down the display. When this display first appears, the user must respond by entering <Y> before any further inputs will be accepted. After all of the 4 required choices have been entered, the user must again respond to the <ENTRIES/CORRECTIONS? Y/N> prompt. This time, he can either enter <N> and proceed with execution of the program or enter <Y> and edit any of the entries.

This edit cycle can be repeated as many times as desired.

Throughout SPECTRO 1.3, user commands are simplified by maximum utilization of the IBM Personal Computer function keys. Figure 8 shows the layout of the 10 function keys and also a typical SPECTRO 1.3 "Command Prompt." This type of Command Prompt appears in many of the SPECTRO 1.3 displays (including Figures 1, 2, 4, 5, 6, and 7) and is keyed to the BOTTOM 4 function keys: F7, F8, F9, F10. Any of the commands shown in the Command Prompt can be executed with one key stroke.

Since the upper 6 of the function keys are used for one-stroke menu choice inputs, control of most user commands is concentrated in one easy-to-remember section of the computer keyboard.

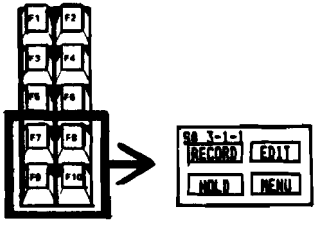

Figure 8 - Function Keys and Command Prompt

Conclusions

During six months of actual use to date, the SPECTRO 1.3 system has performed well in a variety of color research laboratory applications ranging from mass evaluation of color samples to exploration of new color measurement criteria. All software development objectives, for functional operation and ease of use, have been fulfilled.

Enhancement of the system is planned, to provide faster data base handling. The computer random access memory will be increased to 512K and appropriate program changes will be made to substitute faster, electronic memory search for slower, mechanical disk drive access.

References

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Color in Business, Science and Industry, John Wiley and Sons, New York 1975