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EXTENDED BASIC COMPUTER PROGRAM
FOR PHOTOGRAPHIC EMULSION
CALIBRATION IN EMISSION SPECTROSCOPY

Harlan N. Barton

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EXTENDED BASIC COMPUTER PROGRAM FOR PHOTOGRAPHIC EMULSION CALIBRATION IN EMISSION SPECTROSCOPY

Harlan N. Barton

Abstract: This series of programs, written in Extended Basic for a time-sharing computer, derives a polynomial representing the Seidel emulsion calibration curve and utilizes this expression in the conversion of analytical line transmittances to relative intensities. An installation library least-squares polynomial curve fitting program is applied in determining polynomial coefficients for both the Seidel preliminary and emulsion calibration curves.

INTRODUCTION:

The graphical derivation of an emulsion calibration curve is tedious and often inaccurate because of the large number of points to be plotted and the fallibility of fitting the preliminary curve by hand. A computer program representing the calibration curve by a number of linear line segments gives improved speed in application but requires considerable preparation and lacks flexibility for ready adaptation to new data of different emulsions and wavelengths.

This group of programs provides an emulsion calibration from the entry of calibration spectra transmittance data. User performed operations consist only of appropriate merging of subprograms. Data in a form convenient for plotting the preliminary curve as Seidel functions and the Seidel emulsion calibration curve are printed for graphical verification if desired.

Conversion of analytical line transmittances to intensities is accomplished by the final program after entry of the calibration constants for the specific emulsion.

PROGRAM FUNCTIONS

This series of programs performs the computations necessary to derive an expression for the emulsion calibration curve from the transmittance data of the calibration exposures, and uses this expression for experimental data conversion. The functions of the individual programs in the order of their use are:

CONVER: Convert transmittance data of emulsion calibration spectra to Seidel functions.

SEIFIL: Temporary storage of Seidel data of CONVER prior to merger with POLFIT***. Designation of AHOLD as file for POLFIT*** derived coefficients.

FILIT: Instructions to file polynomial coefficients for Seidel preliminary curve derived in POLFIT***.

POLFIT*:** Determine coefficients for polynomial fitting of Seidel function preliminary curve (A General Electric installation library program).

AHOLD: Temporary storage of polynomial coefficients for Seidel preliminary curve derived in POLFIT*** prior to merger with CURVES.

CURVES: Determine successive Seidel functions related by intensity ratio of calibration exposures and file Seidel functions and corresponding logarithm intensities in CALFIL. Present data for optional plot of preliminary and calibration curves.

CALFIL: Temporary storage of Seidel function and log intensity values derived in CURVES prior to merger with POLFIT***. Designation of BEHOLD as file for POLFIT*** derived coefficients.

FILIT: (Second Usage.) Instructions to file polynomial coefficients for Seidel emulsion calibration curve derived in POLFIT*** to BEHOLD.

POLFIT*:** (Second Usage.) Determine coefficients for polynomial representing Seidel emulsion calibration curve.

BEHOLD: Temporary storage of polynomial coefficients for Seidel emulsion calibration curve derived in POLFIT*** prior to merger with CALCUR and CALTAB.

CALCUR: Convert transmittance of analytical lines to intensity. After entry of coefficients, rename for specific calibration and save.

CALTAB: Produce table of intensities as a function of transmittance for specific calibration.

DISCUSSION:

The two-step preliminary curve method of photographic emulsion calibration is the basis for these calculations.¹ Calibration exposures of an iron arc utilizing a rotating step sector at the slit of a stigmatic spectrograph yield spectral lines of two steps, representative of intensities of unity and the step sector ratio (1.585).

Percent transmittances T , are converted to Seidel functions Δ , by

$$\Delta = \log \left(\frac{100}{T} - 1 \right)$$

to give a near linear Preliminary Curve relating the weak segment Seidel function Δ_W , to the strong, Δ_S . See Figure 1 for an example plot of emulsion calibration data and the computer derived curve.

Points for plotting a continuous curve relating intensity and percent transmittance, or functions

Figure 1. Preliminary Curve

thereof, are obtained by stepping the preliminary curve to obtain a series of Seidel functions related by an intensity ratio of 1.585 as shown in Figure 2.

Figure 2. Stepping of Preliminary Curve

The initial Seidel function point $\Delta_{S(1)}$ is selected at the highest reliable point of interest (2.0 in the example) and $\Delta_{W(1)}$ is determined from the preliminary curve (1.668 in the example). The succeeding $\Delta_{S(2)}$ is assigned the value of $\Delta_{W(1)}$, and $\Delta_{W(2)}$ is determined from the preliminary curve (1.348). This is continued to ensure inclusion of the entire region of interest (until the next value of $\Delta_W < -2.0$ in the example).

The emulsion calibration curve is plotted as the logarithm of intensity versus Seidel function to obtain a near linear relationship (See Figure 3).

User supplied information after entry of the transmittance data of calibration exposures is limited largely to commands merging programs. As shown in Figure 4, filed data in SEIFIL, and filing instructions in FILIT are merged with POLFIT***. Coefficients calculated are filed in AHOLD and

Figure 3. Emulsion Calibration

merged with CURVES. Data calculated in CURVES are filed in CALFIL which along with FILIT is merged with POLFIT***. Coefficients calculated are stored in BEHOLD and merged with CALCUR and CALTAB.

A discussion of the programs in order of use follows:

CONVER: (Appendix A.) This program converts percent transmittances for strong and weak segments of each line determined by a microphotometer of the calibration exposures to Seidel Functions and files these in the temporary program SEIFIL for use in POLFIT***. "T" represents percent transmittance and "S" represents Seidel function defined by $S = \log_{10}(100/T - 1)$. Consecutive line numbers beginning at 100, and the word "Data" are provided to present the data in a form acceptable to POLFIT***. Percent transmittance data are entered in the order $T(S)_1, T(W)_1, T(S)_2, T(W)_2, \dots$

SEIFIL: This temporary program is created and destroyed for each calibration. Prior to filing data from CONVER, the program contains only: 98 FILES:AHOLD. This designates the program AHOLD

to which the succeeding program POLFIT*** will file derived coefficients. After receiving data from CONVER, this program and FILIT are merged with POLFIT***.

FILIT: Modification to the installation library program POLFIT*** is effected by merger with this program. Instructions for printing to the file program AHOLD specified in SEIFIL are to print successive line numbers beginning at 1000, the word "DATA", and values for the polynomial coefficients of the Seidel preliminary curve derived by POLFIT***. The program contains the following commands:

```
1682 D = 1000
1683 PRINT #1, LNM(D); "DATA"; U(J)
```

Due to the shortness of the program, it is created and destroyed for each calibration.

POLFIT*:** (A General Electric time-sharing programming system installation library program.) This program employs a least-squares method of fitting polynomials as high as the eleventh degree to a maximum of 100 data points. Seidel function data stored in SEIFIL is entered as data lines 100 to 299. The number of points to be fitted, N, and the lowest degree polynomial for which information is desired (usually fourth), D, must be entered as data line 010. The degree of fit and coefficients for the polynomial are part of the print-out. The coefficients are filed to AHOLD as described in the preceeding paragraph. Information on higher degree polynomials is optionally available after the initial selection. The treatment of polynomials other than fourth degree required minor modification to the following CURVES program.

AHOLD: This temporary program, created and destroyed for each use, provides file storage for the polynomial coefficients of the Seidel preliminary curve derived in POLFIT***. The program is merged with CURVES to enter the coefficients into that program.

CURVES: (Appendix B.) This program determines successive Seidel functions, beginning at + 2.0 and continuing to -2.0, whose corresponding intensities are related by the step ratio of the rotating sector filter used in the emulsion calibration (1.585). These values along with line numbers, "DATA", and the logarithm of intensity values incremented by 0.2 ($\log_{10} 1.585$), are filed in CALFIL.

Optional graphical plotting of the Seidel preliminary curve is facilitated by a print-out of the strong and weak segments incremented by 0.2 for the strong

LEGEND:

TAPE ØR KEY

TEMPØRY PRØGRAM

CREATED PRØGRAM SAVED

SAVED PRØGRAM

INSTALLATION LIBRARY PRØGRAM

Figure 4. Program Sequence

segments. Data for optional plotting of the emulsion calibration curve are provided incremented by 0.2 log intensity. The polynomial coefficients $A(0)$ and $A(4)$ derived in the preceding POLFIT*** program are entered by merger of AHOLD with CURVES. For polynomials less than fourth degree, zeros should be entered for the missing coefficients. The expression in lines 260 and 390 must be expanded for higher degree polynomials.

CALFIL: This temporary program is created and destroyed for each use. Prior to filing of data from CURVES, the program contains only: 98 FILES: BEHOLD. This designates the program BEHOLD to which the succeeding program POLFIT*** will file derived coefficients. After receiving data from CURVES this program and FILIT are merged with POLFIT***.

FILIT: Modification to the installation library program POLFIT*** is effected by merger with FILIT as was done previously. Instructions for printing to the file program BEHOLD specified in CALFIL are line numbers beginning at 100, "DATA", and values of the polynomial coefficients of the emulsion calibration curve derived by POLFIT***.

POLFIT***: This second usage of POLFIT*** determines polynomial coefficients $B(0)$ to $B(4)$, for the Seidel emulsion calibration curve and files them in BEHOLD.

CALCUR: (Appendix C.) After receipt of the polynomial coefficients $B(0)$ to $B(4)$, representing the emulsion calibration curve by merger with BEHOLD, the program is renamed to denote the specific calibration and is saved. Percent transmittances of analytical exposures may then be converted to intensities by entry as data line numbers greater than 1004. Print-out consists of the percent transmittance entered and the corresponding intensity.

CALTAB: (Appendix D.) A table of intensities as a function of percent transmittance is generated by this program after entry of the polynomial emulsion calibration coefficients by merger with BEHOLD. Reference to the table is more convenient than using the CALCUR program when only a few conversions are to be made.

EXAMPLE

The following is a calibration of a Kodak SAI emulsion at 3000A wavelength. One hundred data points were entered in the determination of the preliminary curve.

Throughout this example explanatory material is in the lower case while computer input and print-out are in the upper case. User information entered by keyboard is shown underlined, and is box enclosed when entered by punched tape. It is assumed the following are saved programs: CONVER, CURVES, CALFIL, CALTAB.

1. Create temporary files as follows:

```
READY
NEW:SEIFIL
```

```
READY
98 FILES:AHOLD
```

```
READY
NEW:CALFIL
```

```
READY
98 FILES:BEHOLD
SAVE
```

```
READY
NEW: AHOLD
```

```
READY
SAVE
```

```
READY
NEW: BEHOLD
```

```
READY
SAVE
```

```
READY
NEW: FILIT
```

```
READY
1682 D=1000
1683 PRINT #1, LNM(D);"DATA";U(J)
SAVE
```

2. Enter a maximum of 100 transmittance points from emulsion calibration exposures into old program CONVER: The order of entry is $T(S)_1$, $T(W)_1$, $T(S)_2$, $T(W)_2$, ..., $T(S)_{100}$, $T(W)_{100}$. Use data lines greater than 999. Percent transmittances are converted to Seidel functions and filed in SEIFIL.

```
READY
OLD:CONVER
```

READY
TAPE

READY

1000 DATA 86,97,86,96,80,96,68,89,64,88,59,76,63,87,48,70,19,45,16,35
1001 DATA 30,58,28,56,24,48,16,33,20,40,14,32,13,29,16,32,04,08,05,11
1002 DATA 06,11,52,75,33,56,34,60,28,52,18,36,06,13,12,25,08,16,88,97
1003 DATA 78,95,68,85,55,79,20,44,35,65,21,43,19,41,20,39,06,10,75,92
1004 DATA 31,58,38,66,74,92,49,74,69,90,39,61,35,53,24,47,18,30,43,72
1005 DATA 76,91,54,78,58,83,51,76,34,61,10,24,22,47,61,85,56,81,27,53
1006 DATA 16,36,16,32,03,08,01,02,31,56,02,05,03,05,56,84,17,37,18,37
1007 DATA 32,62,53,81,33,61,34,59,11,24,24,44,23,48,41,70,62,85,39,65
1008 DATA 20,40,07,13,08,17,24,47,17,36,28,50,14,28,13,26,27,52,12,25
1009 DATA 36,64,12,25,26,65,40,66,39,63,31,56,37,65,38,65,42,67,42,68

RUN

CØNVER 13:37 C-S-S THU-02/26/70

ØUT ØF DATA LINE #110

CØMPUTER UNITS 12.6

3. Merge SEIFEL and FILIT with POLFIT*** to enter Seidel function data and instructions for filing coefficients to AHØLD. Specify EBASIC system. Specify N, number of data points and D, the degree of polynomial to fit, as data line 010. Provide responses to computer questions.

READY

EDIT MERGE POLFIT***:SEIFEL-96:FILIT-1681

COMPUTER UNITS 07.2

READY

SYSTEM: EBASIC

READY

010 DATA 100,1

RUN

PØLFIT 13:39 C-S-S THU-02/26/70

DØ YØU WANT DATA SHIFTED TØ ZERØ MEANS
(1=YES 2=NO) ? 2

LEAST-SQUARES PØLYNØMIALS

NUMBER ØF PØINTS = 100

MEAN VALUE ØF X = .38846

MEAN VALUE ØF Y = -7.53574E-2

STD ERROR ØF Y = .624479

NØTE: CØDE FØR 'WHAT NEXT?' IS:

0 = STØP PRØGRAM

1 = CØFFICIENTS ØNLY

2 = ENTIRE SUMMARY

3 = FIT NEXT HIGHER DEGREE

POLYFIT ØF DEGREE 4 INDEX ØF DETERM = .990925 WHAT NEXT? 1

TERM

CØEFFICIENT

0	-.50721461075
1	1.1352727158
2	-.04154031744
3	.05507442808
4	-2.3108735076E-2

WHAT NEXT? 0

COMPUTER UNITS 25.1

4. Merge AHØLD with CURVES to enter preliminary curve polynomial coefficients. Seidel function and logarithm of intensity data for the emulsion calibration curve will be filed to CALFIL. Data for optional plots of preliminary and emulsion calibration curves will be printed out.

READY

EDIT MERGE CURVES: AHØLD - 999

COMPUTER UNITS 02.6

READY

RUN

CURVES 13:42 C-S-S THU-02/26/70

DATA FØR PLØT ØF PRELIMINARY EMULSION
CALIBRATION CURVE AS SEIDEL FUNCTION

X SEIDEL FUNCT. STRØNG	Y SEIDEL FUNCT. WEAK
-2.0	-3.75
-1.8	-3.25
-1.6	-2.81
-1.4	-2.42
-1.2	-2.07
-1.0	-1.76
-0.8	-1.48
-0.6	-1.22
-0.4	-0.97
-0.2	-0.74
0.0	-0.51
0.2	-0.28
0.4	-0.06
0.6	0.17
0.8	0.39
1.0	0.62
1.2	0.84
1.4	1.06
1.6	1.28
1.8	1.48
2.0	1.67

DATA FOR PLOT OF SEIDEL EMULSION CALIBRATION CURVE

	S	LOG I
1	2.000	1.8
2	1.668	1.6
3	1.348	1.4
4	1.006	1.2
5	0.625	1.0
6	0.196	0.8
7	-0.286	0.6
8	-0.837	0.4
9	-1.530	0.2

COMPUTER UNITS 08.1

5. Merge CALFIL and FILIT with POLFIT*** to enter Seidel functions and corresponding intensities, and to provide instructions for filing derived coefficients for emulsion calibration curve to BEHOLD. Specify EBASIC system. Specify N, the number of data points read from above print-out (9) and D, the degree of polynomial (4) as data line 010. Provide responses to computer questions.

READY

EDIT MERGE POLFIT***:CALFIL-96:FILIT-1681

COMPUTER UNITS 05.5

READY

SYSTEM:EBASIC

READY

010 DATA 9,4

RUN

POLFIT 13:44 C-S-S THU-02/26/70

DO YOU WANT DATA SHIFTED TO ZERO MEANS
(1=YES 2=NO) ? 2

LEAST-SQUARES POLYNOMIALS

NUMBER OF POINTS = 9

MEAN VALUE OF X = .465582

MEAN VALUE OF Y = 1.

STD ERROR OF Y = .547723

NOTE: CODE FOR 'WHAT NEXT?' IS:

0 = STOP PROGRAM

1 = COEFFICIENTS ONLY

2 = ENTIRE PROGRAM

3 = FIT NEXT HIGHER DEGREE

POLYFIT OF DEGREE 4 INDEX OF DETERM =

.999962 WHAT NEXT

? 1

TERM COEFFICIENT

0	.71200085663
1	.42166266085
2	.06729633176
3	2.8035695038E-3
4	-2.7683091761E-3

WHAT NEXT ? 0

COMPUTER UNITS 09.6

6. Merge BEHOLD with CALCUR to enter emulsion calibration curve coefficients. Rename and save. Program is ready for conversion of percent transmittance to intensity.

READY

EDIT MERGE CALCUR: BEHOLD-999

COMPUTER UNITS 02.7

READY

RENAME:SA1556

READY

SAVE

7. Merge BEHOLD with CALTAB to provide table of intensity as a function of percent transmittance (only beginning and end of table is shown here for brevity).

READY

EDIT MERGE CALTAB:BEHOLD-999

COMPUTER UNITS 02.5

READY

RUN

CALTAB 13:50 C-S-S THU-02/26/70

CONVERSION %T TO INTENSITY,...CALIB.....A

%T	0.0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9
1	63.08	59.34	56.12	53.32	50.85	48.66	46.70	44.94	43.34	41.88
2	40.54	39.31	38.17	37.12	36.14	35.22	34.36	33.56	32.81	32.09
3	31.42	30.78	30.18	29.61	29.06	28.54	28.05	27.57	27.12	26.69
98	1.43	1.41	1.39	1.37	1.34	1.32	1.30	1.27	1.24	1.21
99	1.18	1.15	1.11	1.07	1.02	0.97	0.91	0.83	0.73	0.57

COMPUTER UNITS 02.5

8. Unsave the temporary programs to clear for future use and avoid charges for saving.

READY

UNSAVE:SEIFIL

READY

UNSAVE:CALFIL

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READY
UNSAVE:AHOLD

READY
UNSAVE:BEHOLD

READY
UNSAVE:FILIT

9. Conversion of percent transmittance data to intensity is accomplished by recall of saved specific emulsion calibration program and entry of %T data.

READY
OLD:SA1556

READY
2000 DATA 19.7,14.2,12.8,10.0,10.8,09.3
RUN

SA1556 13:52 C-S-S THU-02/26/70

CONVERSION PERCENT TRANSMITTANCE TO
INTENSITY

%T	I
19.7	9.88
14.2	12.10
12.8	12.89
10.0	14.99
10.8	14.30
9.3	15.67

OUT OF DATA LINE # 170

COMPUTER UNITS 01.3

REFERENCE

1. American Society for Testing Materials, "Methods for Emission Spectrochemical Analysis," 5th Edition, pp. 148-151 (1968).

APPENDIX A.
CONVER PROGRAM

```
100 FILES:SEIFIL  
110 READ T  
120 S=CLG(100/T-1)  
130 I=100  
140 PRINT#1,LNM(I);"DATA";S  
150 GO TO 110  
9999 END
```

APPENDIX B.
CURVES PROGRAM

```
100 FILES:CALFIL
110 PRINT"DATA FOR PLOT OF PRELIMINARY EMULSION CALIBRATION CURVE"
120 PRINT"AS SEIDEL FUNCTION"
130 ENTER VALUES FOR A(0)-A(4) AS DATA LINES 1000-1004
140 PRINT
150 PRINT USING 160
160: X      Y
170 PRINT USING 180
180:SEIDEL SEIDEL
190 PRINT USING 200
200:FUNCT.  FUNCT.
210 PRINT USING 220
220:STRONG WEAK
230 PRINT
240 READ A(0),A(1),A(2),A(3),A(4)
250 FOR X=-2 TO 2 STEP.2
260 Y=A(0)+A(1)*X+A(2)*X^2+A(3)*X^3+A(4)*X^4
270 PRINT USING 280,X,Y
280: ##.##      ##.##
290 NEXT X
300 PRINT
310 PRINT"DATA FOR PLOT OF SEIDEL EMULSION CALIBRATION CURVE"
320 PRINT
330 PRINT USING 340
340:      S      LOG I
350 X=2
360 K=1
370 I=100
380 Z=2
390 Y=A(0)+A(1)*X+A(2)*X^2+A(3)*X^3+A(4)*X^4
400 Z=Z-.2
410 PRINT #1,LMN(I),"DATA",X,Z
420 PRINT USING 430,LMN(K),X,Z
430: ##      ##.###      #.#
440 X=Y
450 IF X>-2 THEN 390
9999END
```

APPENDIX C.
CALCUR PROGRAM

```
100 PRINT"CONVERSION PERCENT TRANSMITTANCE TO INTENSITY"  
110 ENTER VALUES FOR B(0)-B(4) AS DATA LINES 1000-1004  
120 ENTER %T VALUES AS DATA LINES >1004  
130 PRINT USING 140  
140: % T I  
150 PRINT  
160 READ B(0),B(1),B(2),B(3),B(4)  
170 READ T  
180 IF T<0 THEN 9999  
190 S=CLG(100/T-1)  
200 Y=B(0)+B(1)*S+B(2)*S^2+B(3)*S^3+B(4)*S^4  
210 I=EXP(2.30259*Y)  
220 PRINT USING 230,T,I  
230:##.## ##.##  
240 GO TO 170  
9999END
```

APPENDIX D.
CALTAB PROGRAM

```

100 PRINT USING 110
110: CONVERSION %T TO INTENSITY, --- CALIB ----, ----A
120 ENTER VALUES FOR B(0)-B(4) AS DATE LINES 1000-1004
130 PRINT
140 PRINT USING 150
150: %T      .0      .1      .2      .3      .4      .5      .6      .7      .8      .9
160 PRINT
170 READ B(0),B(1),B(2),B(3),B(4)
180 FOR U=1 TO 99
190 FOR I=0 TO 9
200 T=U+.1*I
210 S=CLG(100/T-1)
220 Y=B(0)+B(1)*S+B(2)*S^2+B(3)*S^3+B(4)*S^4
230 X(I)=EXP(2.30259*Y)
240 NEXT I
250 PRINT USING 260, U, X(0), X(1), X(2), X(3), X(4), X(5), X(6), X(7), X(8), X(9)
260: ##      ##.## ##.## ##.## ##.## ##.## ##.## ##.## ##.## ##.## ##.## ##.## ##.##
270 NEXT U
9999 END

```