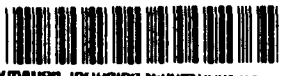


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LINEAR ESTIMATION OF HYPERSPECTRAL MIXED PIXEL COMPONENTS

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ABSTRACT

This paper presents a method to determine end members along with their relative concentration in a hyperspectral mixed pixel. The method is modeled as a linear combination of the end members reflectance spectra and a library of spectral prototypes. This method was tested with 431-band, laboratory controlled, data sets. Indications are that this method can be extended to field data observations with a small number of end members and that at least some error source can be identified and data and results adjusted accordingly.

1. INTRODUCTION

Linear estimation is a viable method for analyzing mixed pixels under the simplified assumption of accurate reflectance calibration, accurate laboratory spectral prototypes, and dominant linear mixing.

1.1 OBJECTIVE

This paper addresses a method for estimating the concentration of materials in a mixed pixel using laboratory measured hyperspectral data, a library of spectral prototypes, and a linear model. A library of spectral prototypes is simply a collection of spectra of pure materials or objects which may be components of the mixed pixel. The model is based on least squares. A basic requirement is that the spectral prototypes be linearly independent. The library can contain several hundred prototypes and each prototype can contain several hundred bands.

1.2 HYPERSPECTRAL MIXED PIXEL CONCEPT

An imaging spectrometer measures percent reflectance or radiometric values of a pixel at various frequencies. A plot of the reflectance as a function of frequency represents the spectral response of the pixel. A pixel is said to be *mixed* if its measured reflectance is a result of imaging multiple object types or materials within the pixel's footprint. In such cases the measured response will be a combination of the individual responses of the objects or materials. If the number of materials in the pixel's footprint is less than or equal to the number of measurements, and if the combination of the responses within the measuring instrument is linear, then the most probable mix of components may be estimated by a linear model and a library of spectral prototypes of materials suspected in the mixed pixel.

1.3 LINEAR ESTIMATION THEORY CONCEPTS

Estimation is defined as the process of making a decision or judgement concerning the approximate value of parameters when the decision is weighted or influenced by all available information on those parameters. The estimation is linear when the estimation characteristics are *additive* and *homogeneous*.¹ In this particular case *additive* means that the spectral response combination is the sum of the product of the individual material component responses and a scalar quantity associated with the particular material. *Homogeneous* means that the scalar quantity is dependent on the material and independent of the frequency. The spectral response ' ω ' at frequency f_0 is composed of material 'a' and material 'b', then for any frequency 'f',

$$\omega_f = k_1(\text{spectral response of 'a' at frequency 'f'}) + k_2(\text{spectral response of 'b' at frequency 'f'})$$

where:

- ω_f = total reflectance at frequency 'f'
- k_1 = scalar constant associated with material 'a'
- k_2 = scalar constant associated with material 'b'

1.4 LINEAR MODEL

Assume that there are 'p' different objects in a spectrometer's footprint and that 'n' discrete frequencies are measured, then the output reflectance measured at any frequency 'k' is given by;

$$\omega_k = \sum_{i=1}^p r_{k,i} s_i$$

where:

- ω_k = total output reflectance at frequency 'k',
- $r_{k,i}$ = response of material 'i' at frequency 'k'
- s_i = coefficient of concentration of material 'i'

The above equation in matrix form is given by;

¹ Ralph Deutsch, *Estimation Theory*, Prentice Hall

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$$\omega = \begin{bmatrix} r_{1,1} & \dots & \dots & \dots & r_{1,p} \\ \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots \\ r_{n,1} & \dots & \dots & \dots & r_{n,p} \end{bmatrix} \begin{bmatrix} s_1 \\ \cdot \\ \cdot \\ \cdot \\ s_p \end{bmatrix}$$

The above expression written in matrix notation is given by:

$$Q = Rs \tag{1}$$

The above equation represents a linear statistical measurement model in which the 'R' matrix, (nxp) is a 'laboratory prototype' spectral library of reflectance values for materials that may occur in the pixel footprint. It is important to note that these values must be obtained separately from a mixed pixel solution. These values could be obtained from measurements in the laboratory or measurements in the field under the same conditions as those employed for the mixed pixel. They represent the spectrum of a pure material or object. The column matrix 'Q' (nx1) represents the 'n' response measured by the spectrometer. The column matrix 's' (px1) is the 'coefficient of concentration' of each material and is unknown. The problem is to estimate this parameter from the 'spectral library' and from the 'n' measurements. Once determined, these coefficients can be converted to represent the relative quantity of each material.

1.5 LINEAR MODEL SOLUTION

The number of measurements is normally expected to be much larger than the number of components in the mixed pixel to produce an over determined system of linear equations. Methods for the solution of an over determined system of linear equations are many and are well documented. A basic least square solution is presented here.

Let,

R^t = transpose matrix of R in equation (1) above and multiply on the left both sides of the equation by it to obtain,

$$R^t Q = R^t Rs \tag{2}$$

The matrix product $[R^t R]$ produces a pxp symmetric matrix and the matrix product $R^t Q$ produces a px1 column matrix.

Let,

m = inverse of $[R^t R]$

Multiply on the left both sides of equation (2) by m to obtain,

$$m[R^t Q] = m[R^t R]s \quad (3)$$

By definition, the matrix product $m[R^t R]$ is the identity matrix and equation (3) becomes

$$m[R^t Q] = s \quad (4)$$

The matrix product $m[R^t Q]$ is $p \times 1$, a column matrix, and is the least square solution vector for 's'.

2. LABORATORY TEST

The development of an understanding of potential complications to simplified unmixing models and their ramifications may be best understood by working with laboratory controlled data.

2.1 EXPERIMENT DESIGN

A laboratory controlled experiment was designed to assess the validity of the developed model. The experiment consisted of obtaining a prototype 'spectral library' of materials and then imaging a target with a known mix of these materials. Three materials were selected for the experiment; red, green, and yellow dye. The targets were a known mix of red and green dye. Yellow was produced where the red and green overlapped in the targets. The overlap is slight but uncontrolled and the red/green interaction is not always in the same proportion. It is caused by saturation of the two dyes in the cardboard. The spectral library was obtained by imaging separately 'pure' red, green, and yellow dye on 10x10 inch cardboards and recording the spectra. These spectra constitute the library of 'spectral prototypes'.

2.2 TARGETS

A 10 x 10 inch cardboard was subdivided into 64 $1\frac{1}{2}$ x $1\frac{1}{2}$ inch squares, 8 across and 8 down. Each square was alternately dyed red and green so that the cardboard had an even mix of red and green dye, 32 red squares and 32 green squares. This constitutes a 50/50 percent red/green target. A second target was constructed like the first, except that every other green square was dyed red so that this target had a mix of 48 red squares and 16 green squares. This constitutes a 75/25 percent red/green target. A third target was constructed like the second one, except that the red and green dye are interchanged so that this target had 16 red squares and 48 green squares. This constitutes a 25/75 percent red/green target. This data set of targets was labeled 'large square' targets. A second data set was constructed just like the one above except that the cardboard was subdivided into 128 $\frac{1}{2}$ x $\frac{1}{2}$ inch squares, 16 across and 16 down.

This data set was labeled 'small square' targets. Fig. 1 shows the spectral library cardboards and the different targets.

2.3 SPECTROMETER

The instrument used for this effort was a tripod mounted, factory calibrated, Geophysical Environmental Research (GER) IRIS MkIV dual field of view spectrometer. Fig. 2 shows the spectrometer in a field environment. Radiometric values for 431 discrete spectral bands, wavelengths from 350-2500 nanometers at 5 nanometer increments, were obtained for each of the spectral prototypes and the targets. The spectrometer's raw output values, 32-bit hexadecimal numbers, were downloaded to an IBM-compatible PC for conversion to floating point numbers and percent reflectance. A Halon reflectance standard was used as a reference for the conversion to percent reflectance. Table I shows a sample of the PC output data for three of the targets. The last column of Table I is a description of the data entries. The data were collected in a laboratory with constant temperature, pressure, and lighting conditions. It was collected over two consecutive days thereby minimizing the probability of any changes which could affect the spectral information.

2.4 IMAGING PROCEDURE

The spectrometer was set up on a tripod looking straight down, one meter from the floor. The checkerboard target was placed on the level floor directly below the spectrometer. The board was constructed so that it would be larger than the spectrometer's circular field of view. The board was positioned so that its geometric center was coincident with the spectrometer's field of view center so that whatever portion of the board was imaged by the spectrometer, the color dye proportion was retained. Fig. 3 shows how a 25/75 percent checkerboard was imaged. The field of view is represented by concentric circles. The portion of the board inside each circle has the same red/green ratio as the whole board. This is true as long as the targets are symmetric about the center, the centers of the field of view and targets are coincident, and the field of view is within the board boundaries. Even if the field of view is oval or rectangular, the red/green ratio is retained as long as the above three conditions hold. The '50/50 Red/Green Large Squares Target' was imaged three times. The second data set is labeled 'repeated' and the third data set is labeled 'repeated again'. Other targets were rotated 45° for a second image and are labeled 'rotated'.

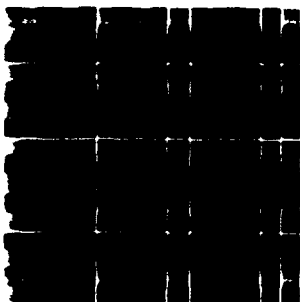
FIGURE 1. SPECTRAL PROTOTYPES AND TARGETS



SPECTRAL PROTOTYPES



TARGETS: LARGE SQUARES

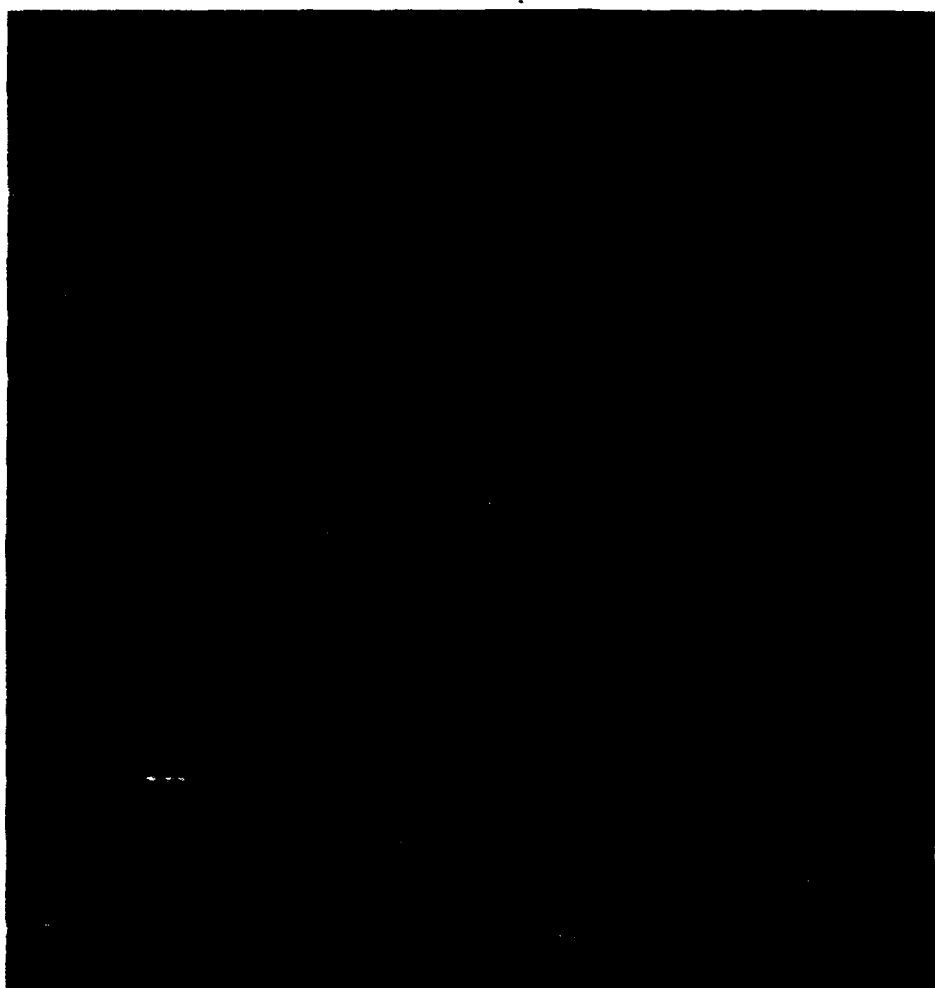


TARGETS: SMALL SQUARES

FIGURE 2. SPECTROMETER



FIGURE 3. TARGET INSTRUMENT FIELD OF VIEW DIAGRAM



Checkerboard = 25:75 Percent Red:Green Target
Concentric Circles = Spectrometer's Field of View

TABLE 1. PC OUTPUT DATA SAMPLE

8mar93tR.002	8mar93tR.003	8mar93tR.004	File Name
2	3	4	File Number
350	350	350	Start Wavelength
2500	2500	2500	End Wavelength
5	5	5	Increment
0	0	0	Separator
0	0	0	"
0	0	0	"
0	0	0	"
0	0	0	"
16.57344	13.20345	6.9677	Reflectance Data
23.66057	26.47618	37.70111	"
6.227723	4.790452	5.270441	"
18.11797	10.74448	21.21313	"
20.65312	11.15195	31.23604	"
23.36005	20.7199	34.12856	"
...	"
...	"
...	"

3. RESULTS

The results obtained embodied different factors, computer equipment, data, computations, and interpretation.

3.1 COMPUTER EQUIPMENT

The data sets were processed on a SUN SPARC workstation using the UNIX operating system and the X-Windows windowing system. Two commercial software packages, Interactive Data Language (IDL) and Mathematica, were used for the computations and analyses. 'IDL' is a computing environment for the interactive analysis and visualization of scientific and engineering data. It provides a broad range of high quality mathematical analysis and graphical display techniques. The graphical and statistical analyses were conducted with the aid of IDL. 'Mathematica' is a general software system and language intended for matrix operations, statistical analysis, and other mathematical applications. The matrix operations and mathematical computations were conducted with the aid of Mathematica.

3.2 DATA FILTERING

High priority was given to the data filtering process to minimize the probability of using false data. The data suspected of being contaminated was filtered out. As a consequence, a significant amount of data were not used. A plot of wavelength vs. percent reflectance was made of all the data sets to analyze the characteristics of the spectra and to detect any anomalies. Figs. 4-7 show the plots made. The first few data points, around 350-500 nanometers, of all sets are irregular spikes and seem to be an idiosyncrasy of the spectrometer when it first starts to record data. These data points are obvious misreadings since reflectance values greater than 100 percent were recorded. These data points were filtered from any processing. The region around 800-1100 nanometers of all data sets deviates from the smooth spectrum curve for no readily explanatory reason other than it is an 'instrument error'. Processing with or without these data points made very little difference in the computed solutions. This is an indication that the data were valid, however the results which will be presented later do not contain these data points. Data associated with wavelengths greater than 1500 nanometers seem to be the same regardless of the dye combination, probably because at these frequencies the spectrometer was responding to the cardboard material and not the dye. These data points were filtered from processing. Additional data points were filtered out from individual data sets which accounts for the different number of data points used in the various solutions.

3.3 COMPUTATIONS

A computer routine was prepared to process the collected data and compute 'coefficients of concentrations' according to equation (4) above and to compute simple statistics of the results. Each data set was processed for a 'two vector' solution where the assumption was that the mixed pixel consisted of red and green dye and for a 'three vector' solution where the assumption was that it consisted of red, green, and yellow dye.

These coefficients were converted to percent concentration (pc) by,

$$pcc_i = [s_i / \sum_{k=1}^n s_k] 100$$

where:

- pc_i = percent concentration for material i,
- s_i = computed coefficient for material i,
- s_k = computed coefficient for material k.

FIGURE 4. PLOTS OF SPECTRAL PROTOTYPES

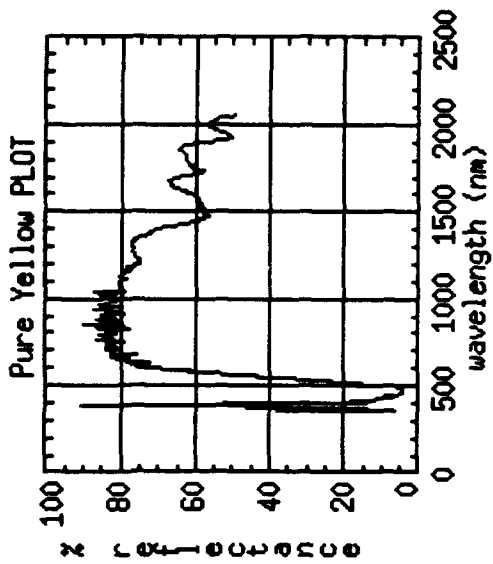
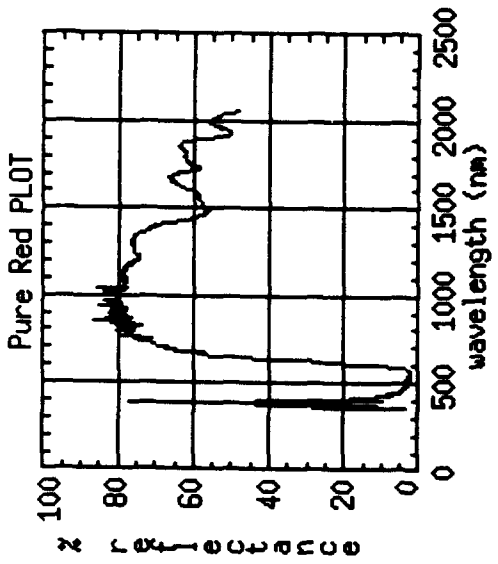
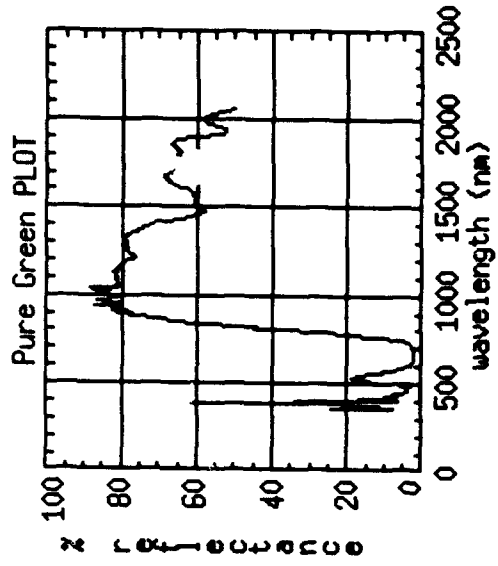


FIGURE 5. PLOTS OF TARGETS

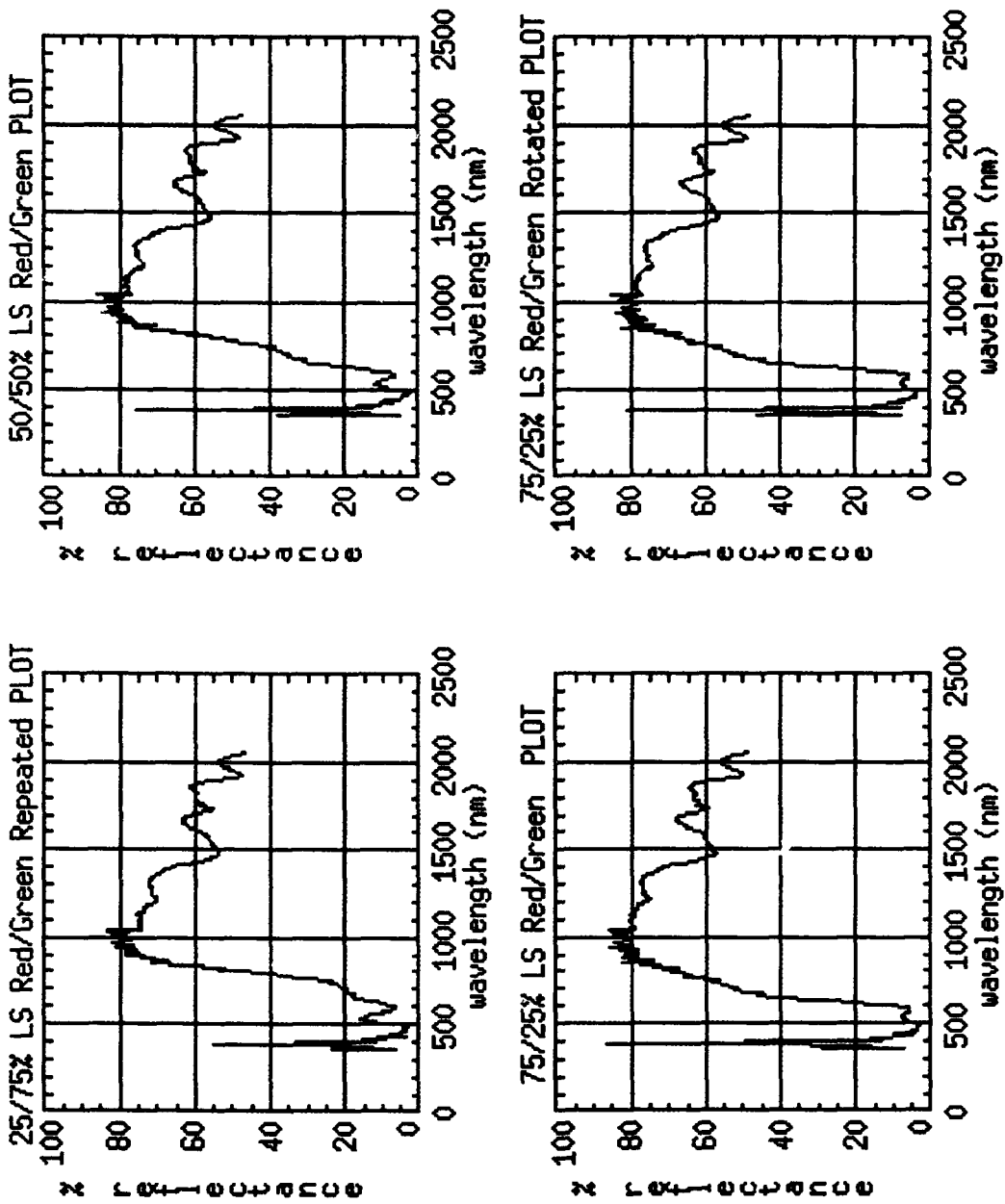


FIGURE 6. PLOTS OF TARGETS

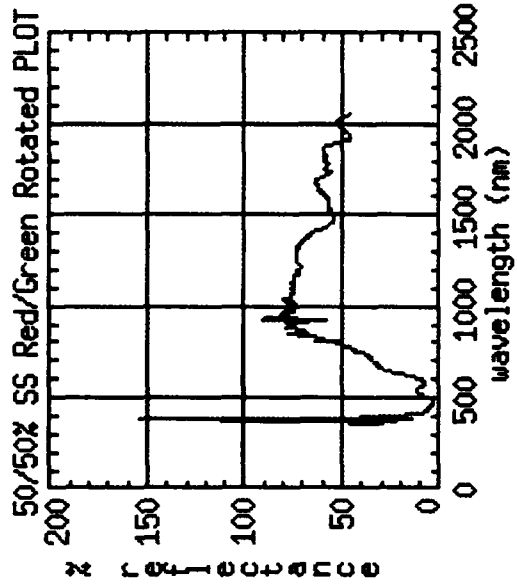
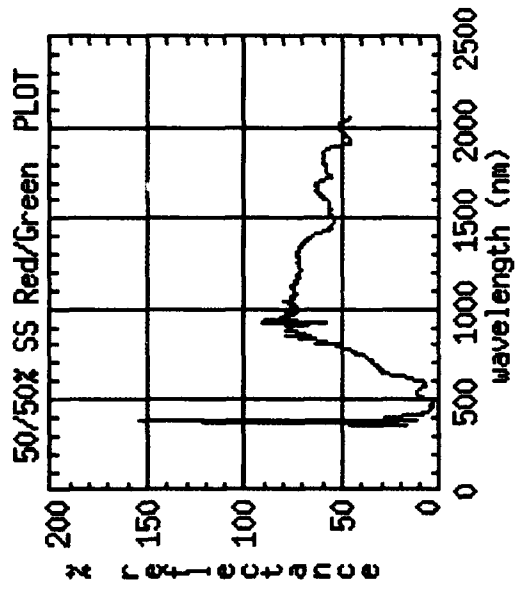
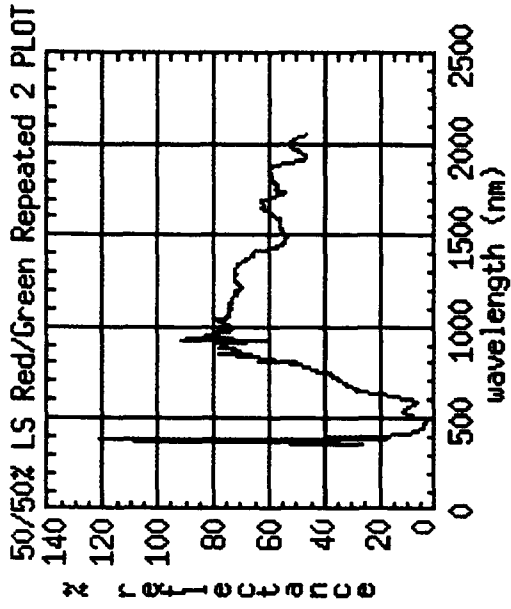
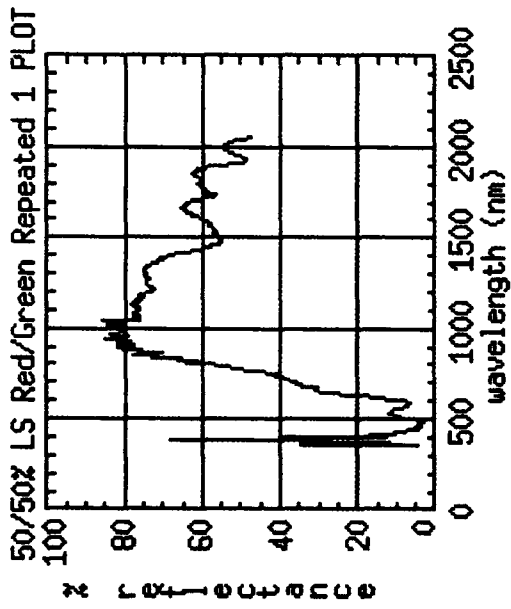
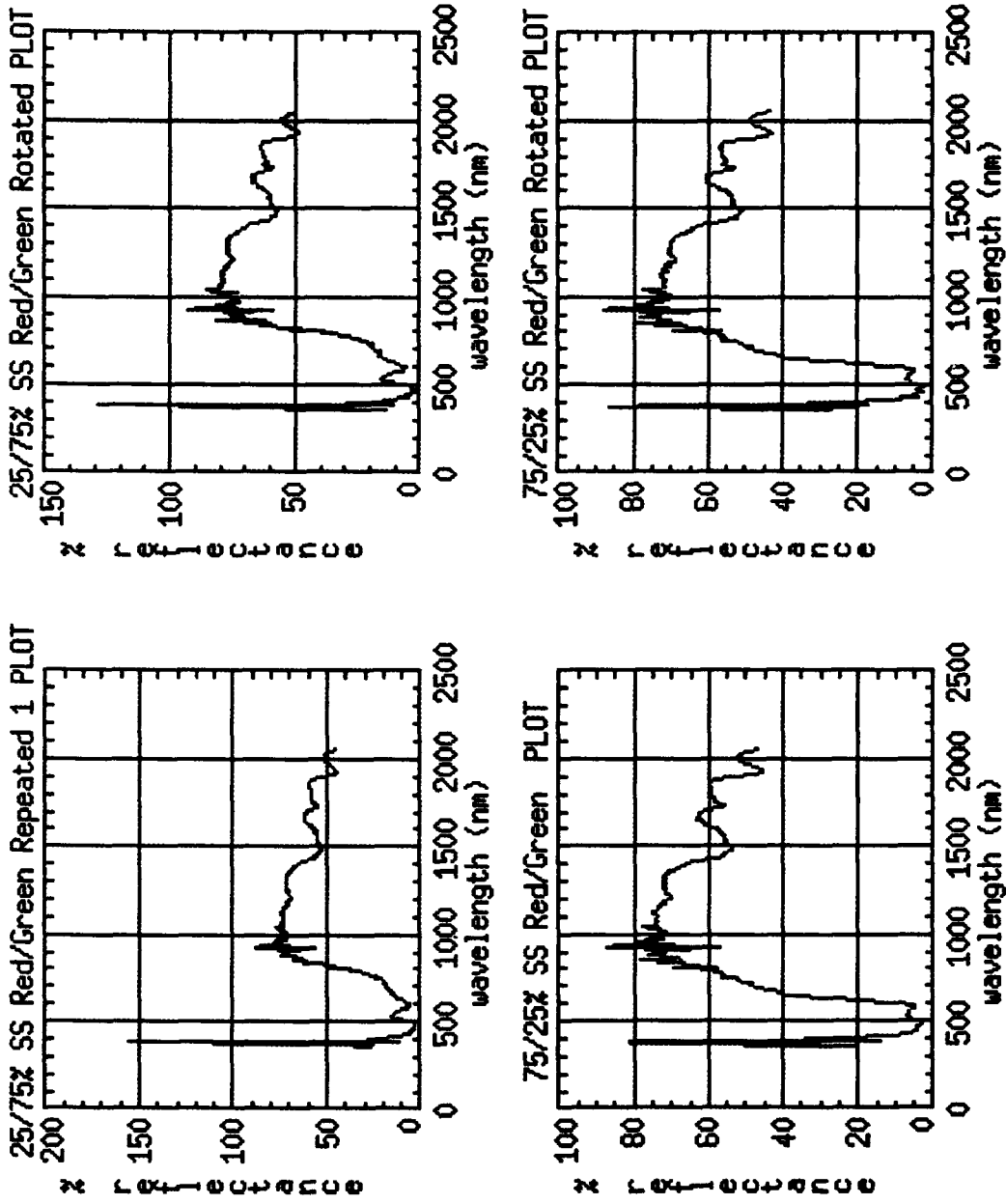


FIGURE 7. PLOTS OF TARGETS



Tables 2-7 show the results of the various tests. The tables show the percent red, green, and yellow, the statistics variance, standard deviation (std), mean, maximum and minimum residuals for the various targets. The percent concentration is the most fundamental test of the computed information because if this value is not close to the true concentration, the rest of the statistical information is meaningless. As can be seen from the tables, all the computed concentrations are very close to the known concentrations. It was pointed out earlier that yellow was produced in the targets where red and green came together. It is not possible to accurately determine the true concentration of yellow in the targets, but all the red/green targets have a little yellow. The small square targets should contain twice as much yellow as the corresponding large ones, but only if the red/green dyes overlap exactly in the same constant manner in the different targets. In the computations, the yellow dye in the targets varied from 1.56 to 5.16. Table 8 list-ranks the computed yellow in each of the targets. The higher values, except for one, belong to the 'small square' target group. This seems to confirm the fact that 'small square' targets contain more yellow than 'large square', but not in the expected proportion. The targets and spectral prototypes were computer generated and printed with a Kodak XL7700 color printer. Although the quality of the printer is excellent, small variations in paper quality and idiosyncrasies of the printer can account for some of the yellow differences in the targets. It was noted that hard copy prints of the generated spectral prototypes contained slight, but noticeable, color variations. Similar variation in the targets could exist, but in a much smaller scale which would be very hard to detect and correct. Also, yellow is defined as a homogenous mixture of equal amounts of pure red and pure green. The yellow spectral prototype was generated with this definition. In the targets equal amounts of red and green produced yellow, but any deviation in the red/green ratio would produce a shade of yellow whose spectra is different from pure yellow. The model then would not detect all of these shades as yellow. Residual vectors were computed for each data set by;

$$\text{residual vector} = \text{measured vector} - \text{computed vector}$$

The computed vector is the matrix product of the computed coefficients and the spectral library. A large residual variance or large residuals would indicate that the data does not fit the model, or in other words, that the model is not valid. As seen from the tables, the residual variances vary from 0.229514 to 2.07936 percent. These low values are indications of a valid model. The size and distribution of the residuals are shown in Fig. 8-13. The distribution is balance, but residuals at the higher frequencies seem to have a different pattern than those at the lower ones.

TABLE 2. PERCENT CONCENTRATION RESULTS

Large Squares 50/50 Red/Green Mix
62 Data Points Used

Red = 48.3615%
Green = 51.6385%
Residual Variance = 0.399593
Residual Standard = 0.632134
Residual Mean = 0.117161
Residual Max Value = 1.328410
Residual Min Value = -1.40322

Large Squares 50/50 Red/Green Mix
62 Data Points Used

Red = 47.6452%
Green = 50.7926%
Yellow = 1.56212%
Residual Variance = 0.229514
Residual Standard = 0.479076
Residual Mean = -0.0542426
Residual Max Value = 1.07
Residual Min Value = -1.30296

Large Squares 25/75 Red/Green Mix
71 Data Points Used

Red = 27.9018%
Green = 72.0982%
Residual Variance = 0.717481
Residual Standard = 0.847043
Residual Mean = 0.412358
Residual Max Value = 2.098570
Residual Min Value = -2.58418

Large Squares 25/75 Red/Green Mix
71 Data Points Used

Red = 24.9470%
Green = 72.3506%
Yellow = 2.70239%
Residual Variance = 0.349629
Residual Standard = 0.591294
Residual Mean = 0.042242
Residual Max Value = 1.204380
Residual Min Value = -2.17339

TABLE 3. PERCENT CONCENTRATION RESULTS

Large Squares 75/25 Red/Green Mix
73 Data Points Used

Red = 75.3445%
Green = 24.6555%
Residual Variance = 0.546755
Residual Standard = 0.739429
Residual Mean = 0.326348
Residual Max Value = 1.585870
Residual Min Value = -2.00696

Large Squares 75/25 Red/Green Mix
73 Data Points Used

Red = 73.1665%
Green = 24.5850%
Yellow = 2.24847%
Residual Variance = 0.271439
Residual Standard = 0.520998
Residual Mean = 0.0251939
Residual Max Value = 1.576690
Residual Min Value = -1.59279

Large Squares 75/25 Red/Green Mix (Rotated)
72 Data Points Used

Red = 75.4534%
Green = 24.5466%
Residual Variance = 0.614468
Residual Standard = 0.783880
Residual Mean = 0.325845
Residual Max Value = 1.537690
Residual Min Value = -1.51769

Large Squares 75/25 Red/Green Mix (Rotated)
73 Data Points Used

Red = 73.1881%
Green = 24.2567%
Yellow = 2.55518%
Residual Variance = 0.249141
Residual Standard = 0.499140
Residual Mean = -0.00771091
Residual Max Value = 1.45873
Residual Min Value = -1.16877

TABLE 4. PERCENT CONCENTRATION RESULTS

Large Squares 50/50 Red/Green Mix (Repeated)
84 Data Points Used

Red = 51.1206%
Green = 48.8794%
Residual Variance = 0.769353
Residual Standard = 0.877128
Residual Mean = 0.241784
Residual Max Value = 2.036880
Residual Min Value = -2.04926

Large Squares 50/50 Red/Green Mix (Repeated)
70 Data Points Used

Red = 48.5735%
Green = 49.0389%
Yellow = 2.38761%
Residual Variance = 0.442796
Residual Standard = 0.665429
Residual Mean = 0.0265032
Residual Max Value = 1.792760
Residual Min Value = -1.73661

Large Squares 50/50 Red/Green Mix (Repeated Again)
70 Data Points Used

Red = 48.5496%
Green = 51.4504%
Residual Variance = 1.396780
Residual Standard = 1.181850
Residual Mean = 0.309275
Residual Max Value = 2.828240
Residual Min Value = -2.46116

Large Squares 50/50 Red/Green Mix (Repeated Again)
71 Data Points Used

Red = 47.2529%
Green = 48.6534%
Yellow = 4.09364%
Residual Variance = 0.821457
Residual Standard = 0.906343
Residual Mean = 0.0171588
Residual Max Value = 3.294860
Residual Min Value = -2.66248

TABLE 5. PERCENT CONCENTRATION RESULTS

Small Squares 50/50 Red/Green Mix
64 Data Points Used

Red = 47.728%
Green = 52.272%
Residual Variance = 2.07936
Residual Standard = 1.442
Residual Mean = 0.488669
Residual Max Value = 3.32402
Residual Min Value = -2.92235

Small Squares 50/50 Red/Green Mix
65 Data Points Used

Red = 45.3574%
Green = 49.5448%
Yellow = 5.09777%
Residual Variance = 0.697811
Residual Standard = 0.835351
Residual Mean = -0.0189529
Residual Max Value = 2.80651
Residual Min Value = -1.70586

Small Squares 50/50 Red/Green Mix (Rotated)
63 Data Points Used

Red = 46.4724%
Green = 53.5276%
Residual Variance = 1.60674
Residual Standard = 1.26757
Residual Mean = 0.295009
Residual Max Value = 3.2525
Residual Min Value = -2.16634

Small Squares 50/50 Red/Green Mix (Rotated)
60 Data Points Used

Red = 45.399%
Green = 50.2944%
Yellow = 4.30659%
Residual Variance = 0.749072
Residual Standard = 0.86549
Residual Mean = 0.0065667
Residual Max Value = 2.94102
Residual Min Value = -1.56352

TABLE 6. PERCENT CONCENTRATION RESULTS

Small Squares 25/75 Red/Green Mix
63 Data Points Used

Red = 24.1692%
Green = 75.8308%
Residual Variance = 1.95059
Residual Standard = 1.39664
Residual Mean = 0.608475
Residual Max Value = 3.1749
Residual Min Value = -4.60226

Small Squares 25/75 Red/Green Mix
63 Data Points Used

Red = 19.8927%
Green = 74.9423%
Yellow = 5.16505%
Residual Variance = 0.80603
Residual Standard = 0.897791
Residual Mean = 0.0905302
Residual Max Value = 1.93587
Residual Min Value = -2.78372

Small Squares 25/75 Red/Green Mix (Rotated)
63 Data Points Used

Red = 24.724%
Green = 75.276%
Residual Variance = 1.93654
Residual Standard = 1.3916
Residual Mean = 0.523531
Residual Max Value = 3.11238
Residual Min Value = -3.996

Small Squares 25/75 Red/Green Mix (Rotated)
63 Data Points Used

Red = 21.0989%
Green = 74.4886%
Yellow = 4.41252%
Residual Variance = 1.08177
Residual Standard = 1.04008
Residual Mean = 0.0763604
Residual Max Value = 2.05594
Residual Min Value = -2.42596

TABLE 7. PERCENT CONCENTRATION RESULTS

Small Squares 75/25 Red/Green Mix
63 Data Points Used

Red = 75.964%
Green = 24.036%
Residual Variance = 1.90755
Residual Standard = 1.38114
Residual Mean = 0.399542
Residual Max Value = 3.64191
Residual Min Value = -3.37843

Small Squares 75/25 Red/Green Mix
63 Data Points Used

Red = 75.126%
Green = 21.1961%
Yellow = 3.67788%
Residual Variance = 1.31538
Residual Standard = 1.1469
Residual Mean = 0.0340338
Residual Max Value = 3.92794
Residual Min Value = -2.0951

Small Squares 75/25 Red/Green Mix (Rotated)
63 Data Points Used

Red = 77.5492%
Green = 22.4508%
Residual Variance = 1.98097
Residual Standard = 1.40747
Residual Mean = 0.450635
Residual Max Value = 3.61223
Residual Min Value = -3.88359

Small Squares 75/25 Red/Green Mix (Rotated)
63 Data Points Used

Red = 76.6859%
Green = 19.1925%
Yellow = 4.12161%
Residual Variance = 1.28975
Residual Standard = 1.13567
Residual Mean = 0.0522504
Residual Max Value = 3.92398
Residual Min Value = -2.48484

FIGURE 8. RESIDUAL PLOTS

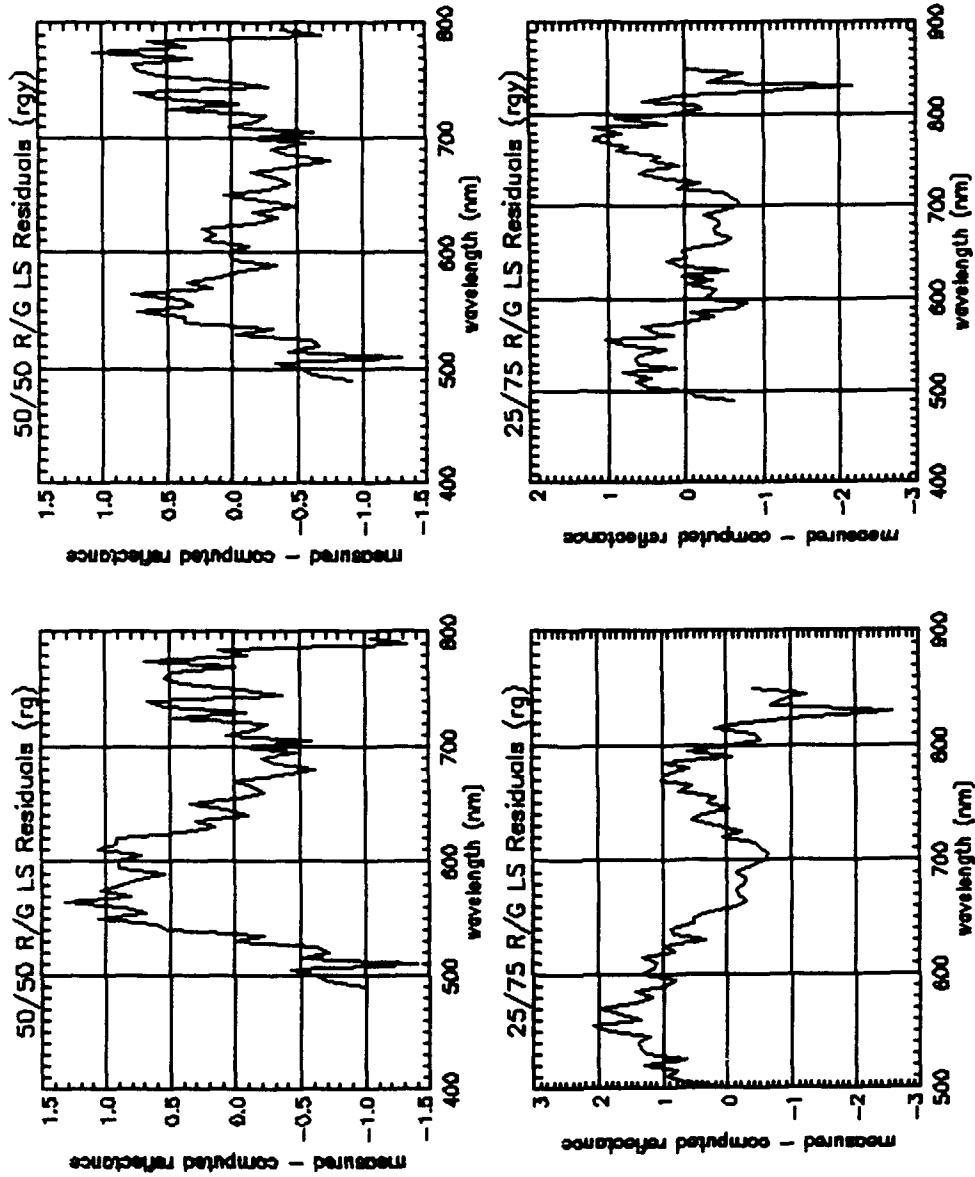


FIGURE 9. RESIDUAL PLOTS

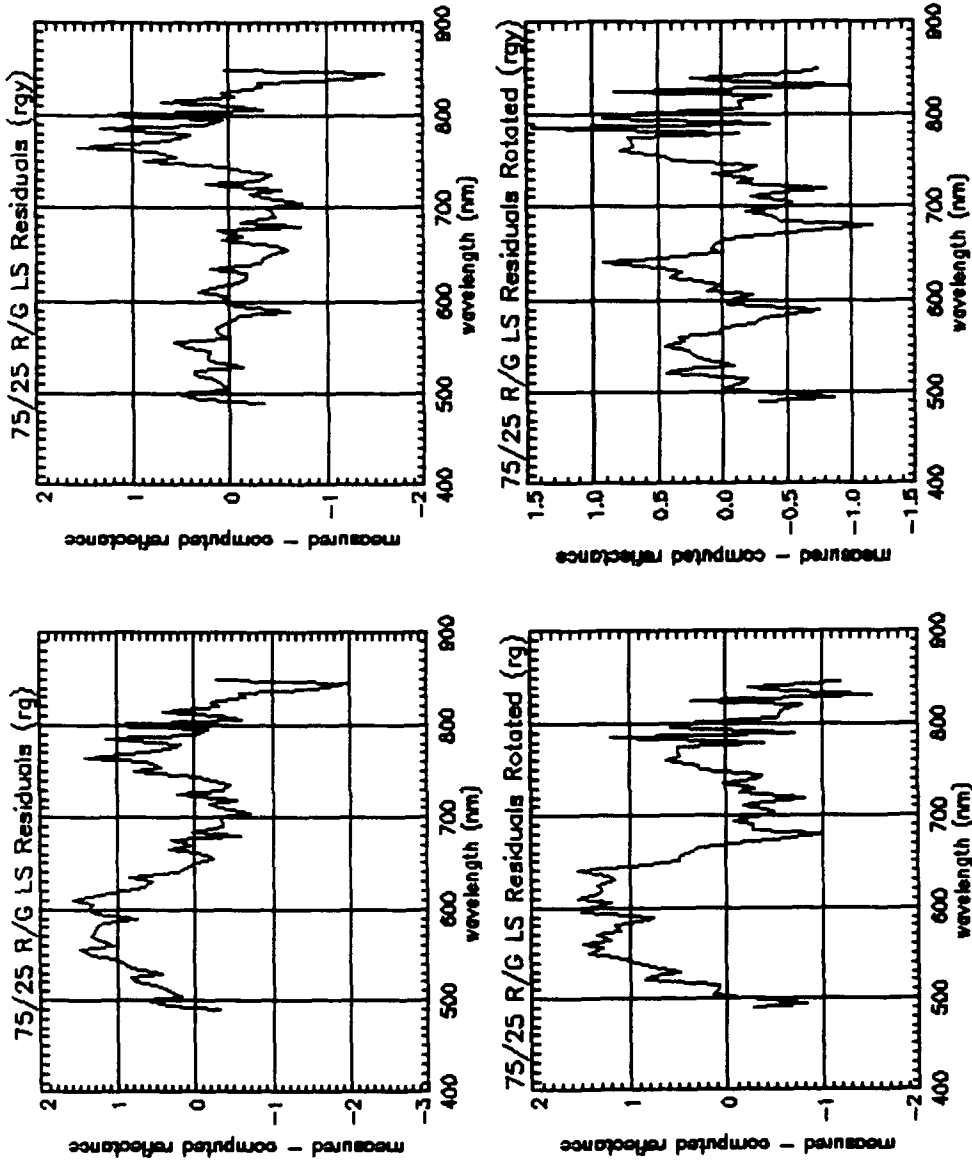


FIGURE 10. RESIDUAL PLOTS

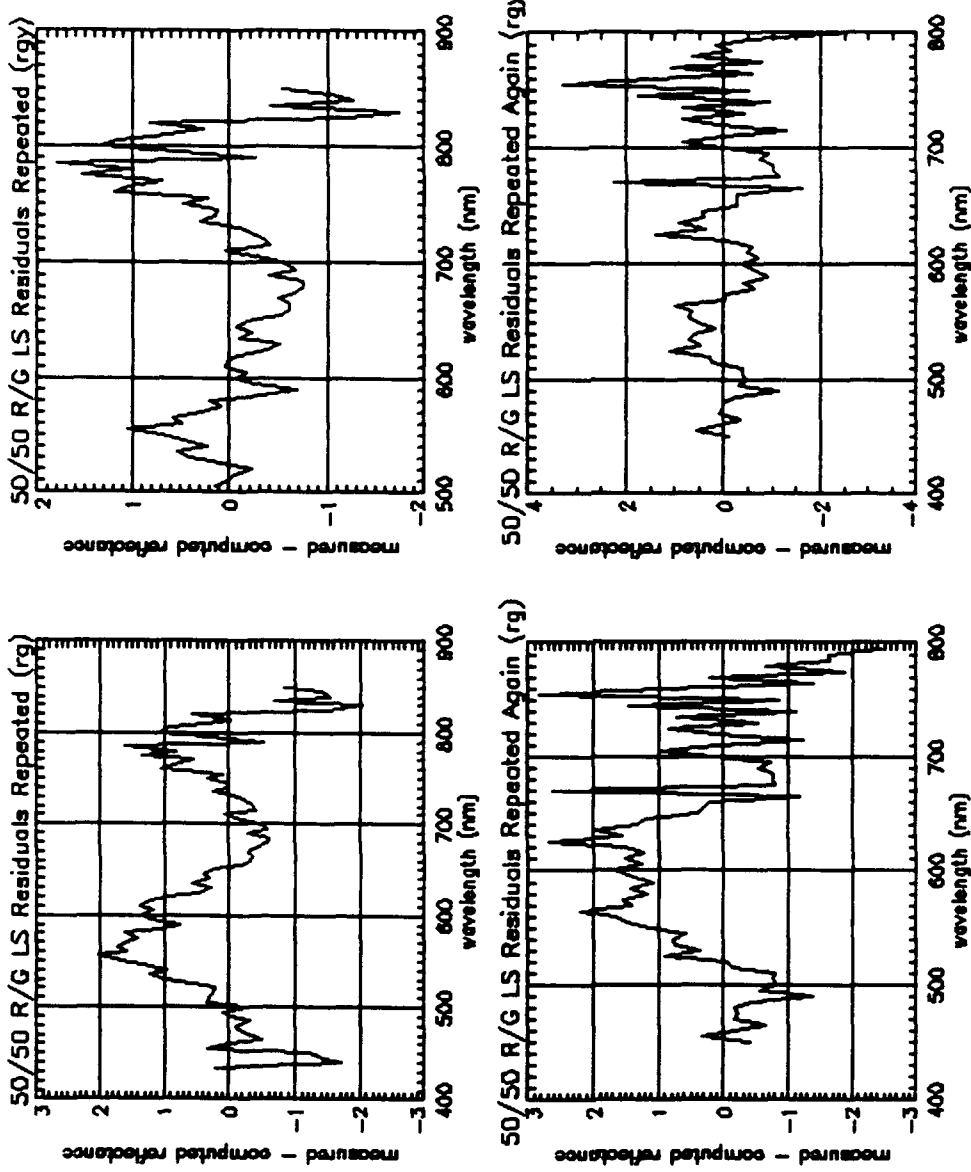


FIGURE 11. RESIDUAL PLOTS

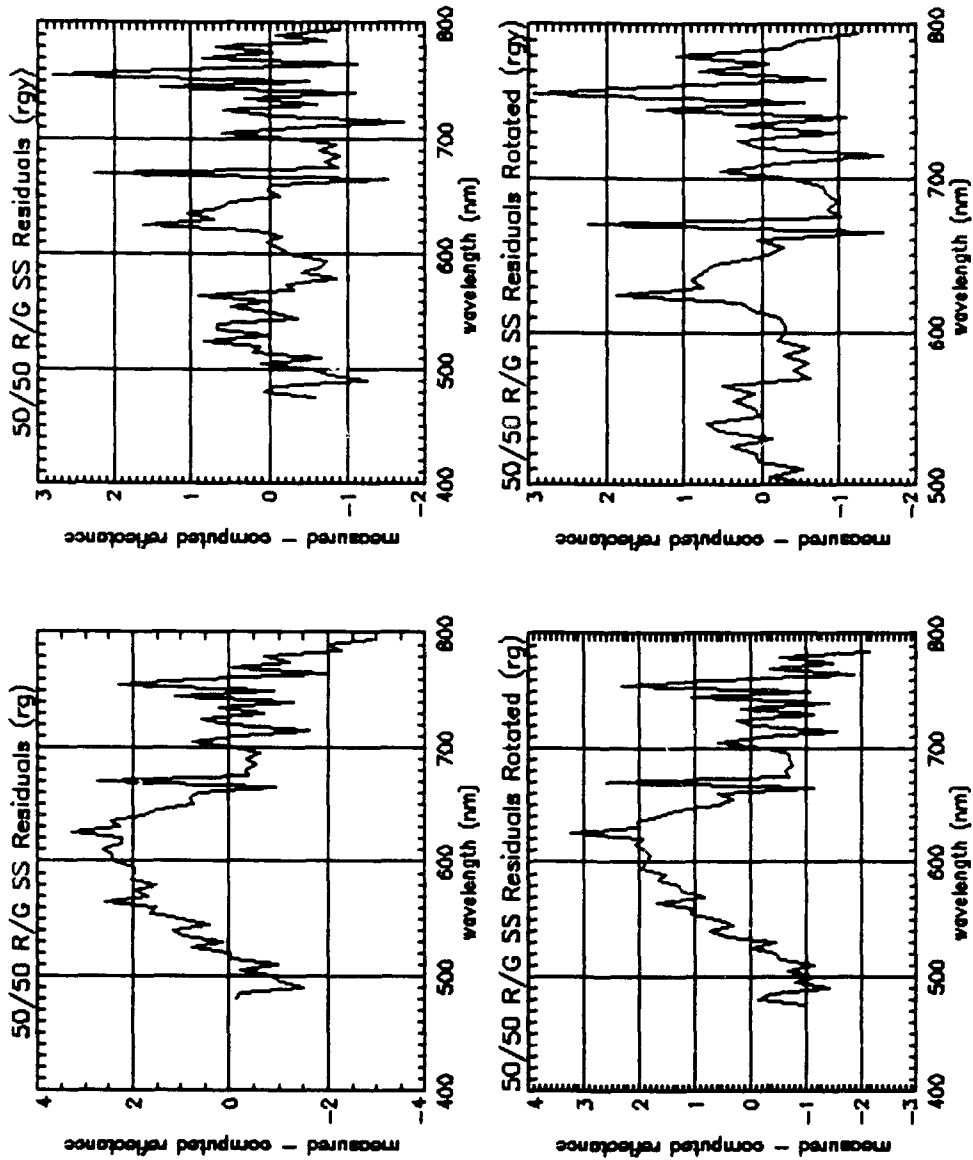


FIGURE 12. RESIDUAL PLOTS

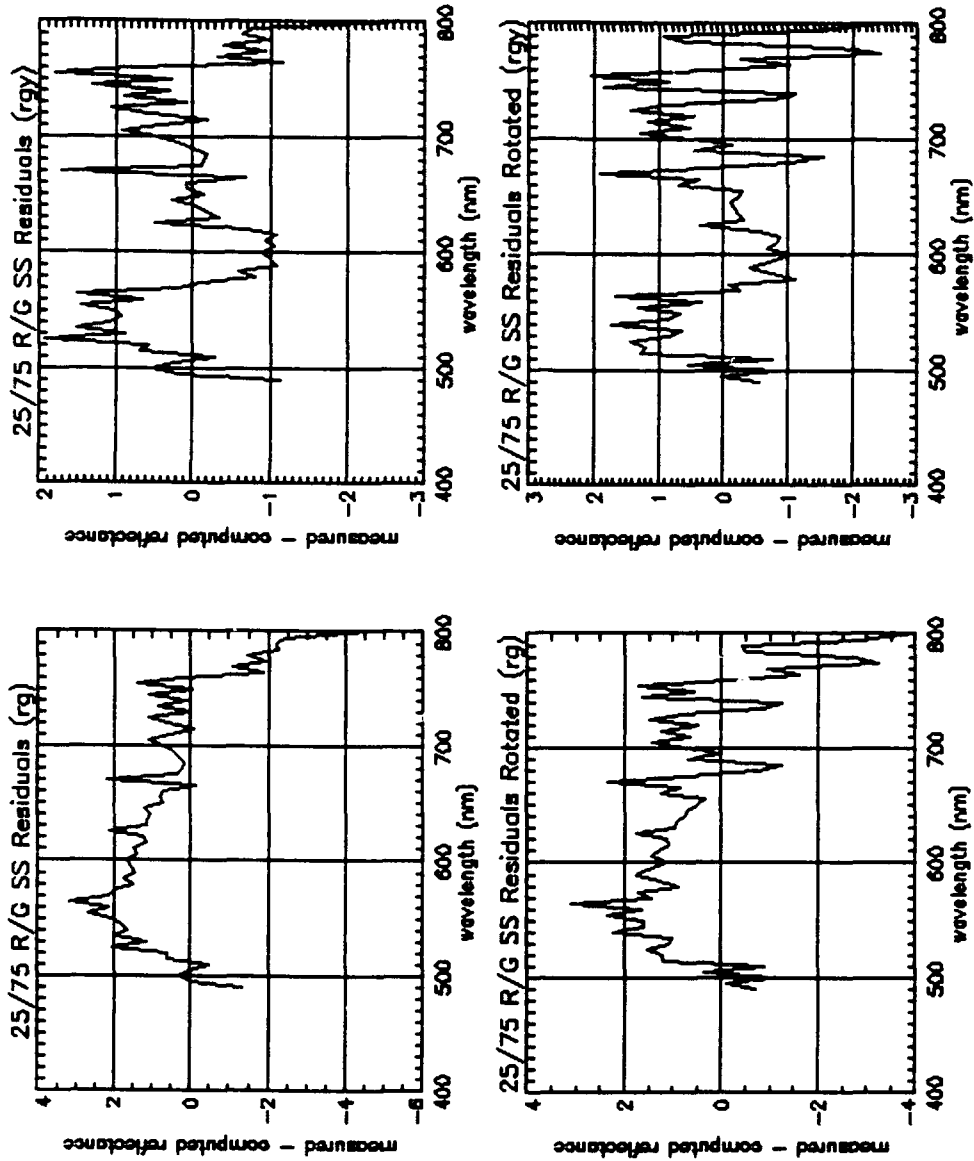


FIGURE 13. RESIDUAL PLOTS

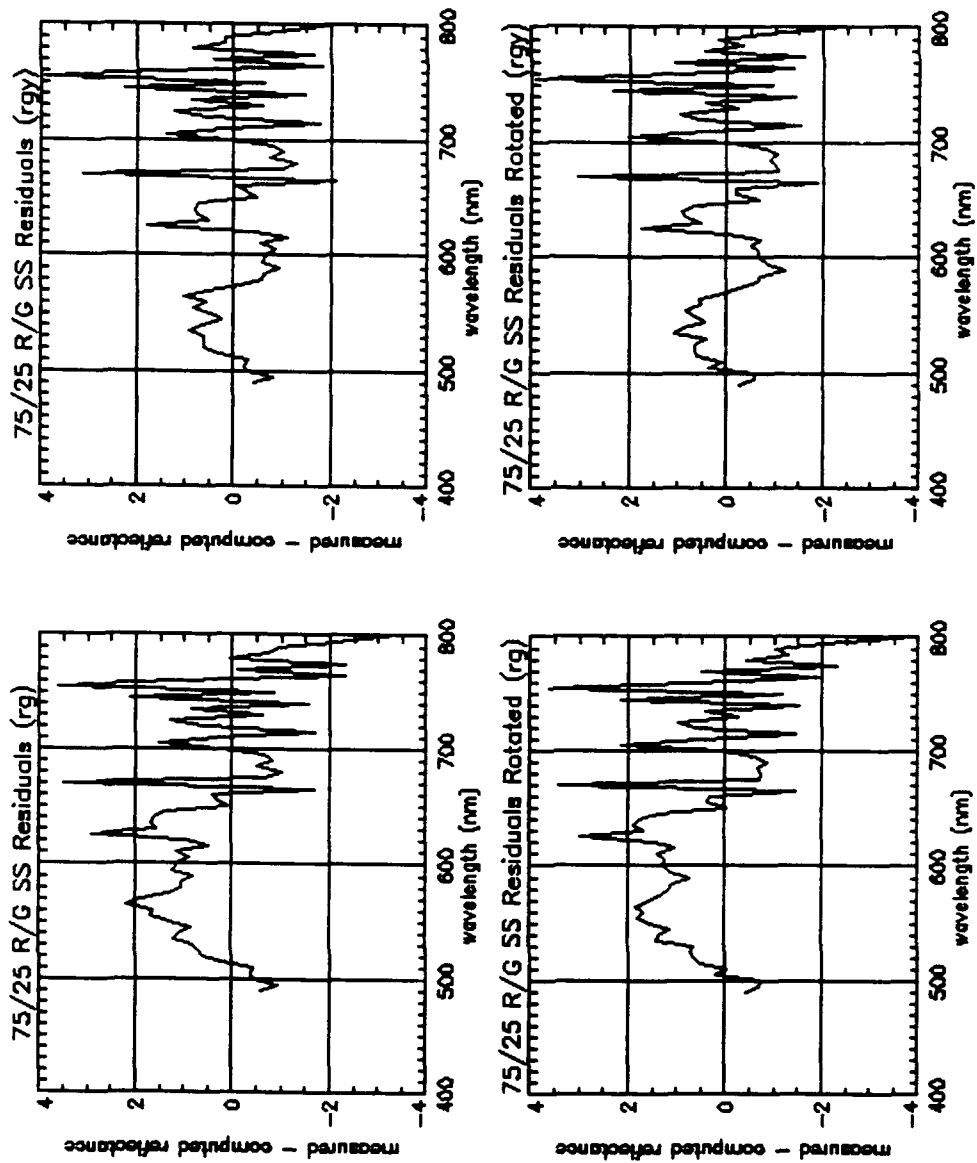


TABLE 8. PERCENT YELLOW IN TARGETS

Rank	Percent Yellow	Red/Green Combination	Size Square
1	5.15	25/75	Small
2	5.09	50/50	Small
3	4.09	50/50 (Repeated again)	Large
4	4.41	25/75 (Rotated)	Small
5	4.30	50/50 (Rotated)	Small
6	4.12	75/25 (Rotated)	Small
7	3.68	75/25	Small
8	2.56	75/25	Large
9	2.70	25/75	Large
10	2.39	50/50 (Repeated)	Large
11	2.25	75/25 (Rotated)	Large
12	1.56	50/50	Large

No effort was made to determine the various errors which may influence the results. Equation (4) above has an inherent error term, but was assumed to be zero for this effort. A misalignment, uneven dyes, uneven checkerboards and a number of other factors would cause errors, however in light of the analysis of the results and statistics, it appears that an error analysis at this point would not provide much information.

4. CONCLUSIONS

The results obtained show that a linear estimation model and a library of spectral prototypes are viable methods for de-mixing hyperspectral mixed pixel. The computed dye concentrations agree with the known concentrations to a small percent difference. The variance and standard deviation of the residuals are indicative of a valid model. The residuals themselves show no spectral bias. Fig. 8-13 show a plot of the residuals for the various tests. In the figures 'LS' means large squares, 'SS' small squares, 'rg' red/green vector, and 'rgy' red/green/yellow vector.

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