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USE OF THEMATIC MAPPER FOR WATER QUALITY ASSESSMENT

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I. ABSTRACT

Simulated TM data were evaluated for discriminating levels of various water quality constituents. Temperature, suspended solids, turbidity, conductivity, pH, and depth were measured in situ concurrent with a TMS overflight at twenty-five predesignated sample sites. Highly significant regressions were developed for conductivity, turbidity, and suspended solids while statistical results for pH, temperature, and depth were not considered significant. For suspended solids, an equation was developed using a multiple regression with the seven TM bands. Logarithm conductivity was used in a multiple regression with TM bands 1,2,3,4, and 6. Principal components 1 through 4 were used in a multiple regression developed for turbidity mapping. Regression equations were assessed for high coefficient of determination (R^2) and statistical significance (F-ratio). To assess the robustness of the regressions used for mapping conductivity, turbidity, and suspended solids in this study, confidence intervals about the mean regression point were calculated. Also, cross validation was conducted by regressing random subsamples of sites and comparing the resultant range of R^2 .

II. INTRODUCTION

The present research involves water quality mapping with TM data and is part of a larger effort to develop and test analytical techniques for hazardous waste disposal impact assessment. One of the risks associated with hazardous waste disposal is the potential for contamination of nearby water bodies as a consequence of inadequate containment of

toxic wastes. Hazardous substances gaining access to a waterway may then be easily transported and the health concerns spread over a larger area. Therefore, detection of changes in water quality plays an important role in hazardous waste management and the protection of public health. The capability for assessing water quality with remotely sensed data may facilitate locating new pollutant sources, detecting leaks from known sites, assessing the extent of polluted water, or monitoring industrial activity.

The ability to efficiently assess water quality on a large scale and thereby detect water pollution has been the aim of many remote sensing studies. Remote sensing of turbidity has been conducted by Bartolucci et al. (1977, pp. 595-598), Schertz et al. (1975, pp. 320-343), Rogers et al. (1976, pp. 1-13), Khorram (1981, pp. 667-676), and Weisblatt et al. (1973, pp. 3A-42 -3A-59). Suspended solids investigations have been conducted by Klemas and Polis (1977, pp. 549-612), Khorram (1981, 667-676), Johnson (1977, pp. 25-31), and Holyer (1978, pp. 323-338). Khorram (1982, pp. 15-22) and Rogers et al (1976, pp. 1-13) have studied the ability to discriminate salinity levels using remotely sensed data. Thermal discharges were examined by Scarpace (1975, pp. 1223-1231) and Schott (1979, pp. 753-761). A summary of these investigations is given in Table 1.

The objective of this study was to evaluate Landsat-4 Thematic Mapper (TM) data for water quality mapping. Simulated TM data (TMS) obtained on an ER-2 aircraft was used due to the lack of TM data over the western U.S. It was anticipated that TM's increased spatial, spectral, and/or radiometric resolution with synoptic coverage would facilitate large scale water quality assessment.

III. DATA COLLECTION

A. Study Site Selection

The area selected for the study was the Carquinez Strait, an estuary in the northeastern extension of San Francisco Bay, California. The location was chosen because of the existence of numerous known abandoned waste sites and high degree of nearby industrial activity which were considered potential sources of water pollution. The historic location of industrial facilities along the Carquinez Strait, with the proximity to railroad lines and deep water ports, resulted in a high concentration of major industries and consequent waste disposal sites within the area. In addition to many existing waste disposal sites, the California Department of Health Services found approximately twelve abandoned waste sites in the area being used for the test site (Abandoned Sites Project, 1981). The Carquinez Strait area was also considered a good choice for remote sensing of water quality because, as a mixing zone where fresh and saline water meet, there is a large range in the levels of water quality constituents.

B. Water Quality Data

Twenty-five ground truth sites were selected and plotted on navigational charts prior to beginning the water sampling. Logistical constraints of time, equipment, and staffing required confinement of the sampling activity to Suisun Bay. The TMS overflight was timed to coincide with slack tide so that differences were minimized between the spectral data and the water quality conditions they represented. All sampling occurred within one hour of the ER-2 overflight. At each predesignated sampling site, a bucket was dropped overboard and filled with water from within one foot of the surface, within the light penetration zone. Sample bottles were filled from the bucket and put on ice to freeze for later laboratory analysis.

Six water variables were chosen for assessment of water quality. These were conductivity, pH, suspended solids, turbidity, temperature, and depth. Within Suisun Bay, sampling stations were chosen to encompass a wide range of water quality types. Approximately eighteen of the sites were located along two transects to measure overall water quality. The remaining six were placed near known or suspected sources of chemical or thermal pollution.

Suspended Solids. Water quality variables may affect the electromagnetic energy measured by the scanner either

directly or indirectly. Solid particles held in suspension in the water column influence spectral reflectance directly as a result of light backscattering. The suspended solids measurement represents all solid material held in suspension in the water column. High concentrations of suspended solids return a strong energy signal to the spectral scanner (Moore, 1978, pp. 445-462). Suspended materials may be phytoplankton, zooplankton, clay, fine sand, silt, or other inorganic particles. The amount of total suspended solids was determined in the laboratory and found to range from 13 to 88 mg/l.

Turbidity. Water turbidity is a function of materials present in the water and is augmented by stirring forces such as wind or current. Turbidity and suspended solids are closely related although turbidity influences water quality in a somewhat different manner. Stirring action brings materials into the water column which then reduces the transmission of light through the water. The reduced light transmission prevents eutrophication while the aeration and stirring promotes phytoplankton growth. Turbidity is therefore directly and indirectly detected by the scanner. Water samples collected for this study were measured in the laboratory and ranged from 16 to 65 nephelometer turbidity units (NTUs).

Temperature. Water temperature was measured in the water collecting bucket at each of the 25 sites. The low temperature was 17.0 C, the high was 18.9 C. Temperature is a variable that is directly sensed by the scanner because the temperature of the water represents its thermal energy which can be sensed by a scanner sensitive to thermal infrared portions of the spectrum. TM band 6 senses thermal energy in the 10.4 to 12.5 um region.

Conductivity. Water conductivity is not a variable that affects electromagnetic energy, although it may influence other parameters such as suspended solids which may be spectrally sensed. The salinity of the water is represented by the conductivity measurement. Fresh river water meets saline ocean or bay water in the Carquinez Strait estuary. When the conductive salt water mixes with sediment-laden fresh water from the delta, flocculation of sediment particles occurs and a suspended solids gradient is apparent in the area called the mixing zone. Phytoplankton distribution may also be salinity-related, and chlorophyll does reflect light in the visible and near infrared wavelengths. For this study, conductivity was measured in situ and ranged from 117 to 406

micromhos/centimeter (umhos/cm).

pH. Water pH is another variable that is not directly sensed by the scanner but may have spectral expression through other water constituents, such as phytoplankton. pH can be an important property of water quality in that it drives oxidation-reduction of toxic heavy metal compounds, taking them in or out of solution and determining their dispersion. This in turn may influence other factors, such as suspended solids, which can be detected by the scanner. Laboratory analysis of pH in the stored samples showed that pH ranged between 7.2 and 8.1, from neutral to slightly alkaline.

Depth. Although depth is not a water quality property, depth sounder readings were recorded at each sampling station to enable later determination, if necessary, of whether the bay floor was being detected by the scanner. Water most easily transmits light in the blue and green wavelengths and at shallow depths, bottom reflection may be detected by the spectral scanner if the water is not too turbid. Whitlock et al. (1978, pp. 1405-1410) investigated apparent remote sensing penetration depth at 520 nm wavelength and found that at suspended solids levels of between 10 and 100 ppm [mg/l], penetration depth varied generally from about 0.4 to 1.8 m. Bartolucci et al. (1977, pp. 595-598) reported that at depths greater than 30 cm, bottom reflectance in turbid water (> 100 mg/l) did not influence Landsat MSS spectral response. At one sampling site in Suisun Bay, the water depth was 6 feet (1.8 m), but all other depths were 10 to 64 feet (3.0 - 19.5 m).

C. Thematic Mapper Simulator (TMS)

TMS data were acquired May 13, 1982 from 3:05 to 3:12 pm on ER-2 flight 82-078. The TMS data were collected by the Daedalus DEI-1260 multispectral scanner configured to simulate the characteristics of the TM sensor aboard Landsat-4. Ground resolution was 28 meters at an altitude of 70,000 feet and the spectral channels were identical to the Landsat TM channels. A subsection of flightline C-D provided almost entirely cloud-free coverage of the study site. The overflight was flown east to west to reduce sun glint reflection on the water.

To determine the spectral values of the water sites, the sites were located on the aerial photographs by triangulation and transferred to USGS maps. Registration of a small window encompassing the sampling locale was used to develop a second-degree nearest neighbor transformation. The transformation equation was used to

convert the latitude-longitude coordinates of the sampling sites to row-column coordinates in the TMS scene. To compensate for possible inaccuracies in location of the sample sites, a nine pixel (3 by 3) area was centered on the calculated site locations and the mean spectral reflectance of the nine pixels was used in subsequent statistical analyses. The variance of the spectral radiances within the nine-pixel sites was calculated to indicate how well the spectral means represented the sample site. For example, high spectral variance might suggest that the site was located on a gradient or at a boundary between distinctive water quality levels. For any particular poorly placed site, a high variance would be expected in most of the bands. Sites 3, 7, 8, and 19 were the sites that had large variances in most channels.

IV. DATA ANALYSIS

Multiple, stepwise, and polynomial regressions were run for each of the water parameters, using spectral values as the independent variables and the water values as dependent variables. Whitlock et al. (1982, pp. 151-164) describes in detail recommended criteria for conducting regression analyses specifically for water quality remote sensing studies. His environmental criteria were followed as much as possible over the sampling area. Specifically, changes in atmospheric transmission over the scene were assumed to be small because the water sampling area was confined to a limited region. As recommended, water depth was greater than the scanner penetration depth where samples were collected. Also, a near-constant vertical water constituent gradient within the remote sensing penetration depth was assumed since the turbidity of the water indicated vertical mixing action.

The suggested ground truth conditions were also complied with to the extent possible. Therefore, a single remote sensing scene was used and contained large differences in radiance. Multiple sampling points were located in suspected thermal plumes and water masses. The samples were collected at constant depths and they were handled and analyzed in a consistent manner. And finally, the total number of sample points, twenty-five, was greater than the number of TM bands used as independent variables in the regression equations.

Criteria for significant regressions were high R^2 , high significance, and evenly distributed residuals. By

examining the plots of residuals, the suitability of a higher or lower order dependent variable could be determined. For example, if instead of an even distribution of residuals, there was a trend to increasing residuals with increasing water quality, a square root and/or log of the water variable was input to the regression. Similarly, a polynomial regression was applied to the data using a third degree polynomial equation to describe the relationship between the water parameters and spectral values. F-ratios were calculated for all regressions to indicate significance of the regression equation.

The noise within the spectral data was not quantified because it was assumed to be constant over the data set, but two steps were taken in an effort to reduce it. Noisy bands 5 and 7 were eliminated from the set of independent variables and the regressions were repeated. Also, a principal components transformation of the 7 TM bands was conducted and the first four components input to the analysis as independent variables. Land was masked from water via thresholding of TM4 so that spectral data for only the water would be used in the principal components analysis. Components one through four accounted for 97 percent of the scene variance. The bands contributing most to principal components transformation were 2, 4, 5, and 6.

In many studies, volume reflectance has been separated from surface reflectance so that the actual water column is being measured [(Holyer, (1978, pp. 323-338), Schertz (1975, pp. 320-343)]. Assessment of volume reflectance was not attempted in this study since no clear or shadowed water bodies were present in the scene to enable calibration. This was not of major concern in this study because the results were not intended for application to multiple data sets, and the surface reflectance component was assumed to be constant over the data set used.

V. RESULTS

The regression results were interpreted according to the following statistical criteria in order to select the best ones for generating water quality maps. An R^2 approaching 1.0 was desired as it represents the percentage of variance in the water quality constituent that is explained by the spectral information. A ratio of F to the tabled F greater than or equal to 4.0 was recommended by Whitlock et al. (1982, pp. 151-168) for indication of statistical

significance of the regression equation. A significance level P approaching 0.0 was optimal; any regression below the .05 level was not considered. The polynomial regressions were rejected on the basis of low R^2 and F, and high P. The best regression and best single band for each water quality variable were determined and are listed in Table 2.

The most significant regression equations were applied to the TMS data and

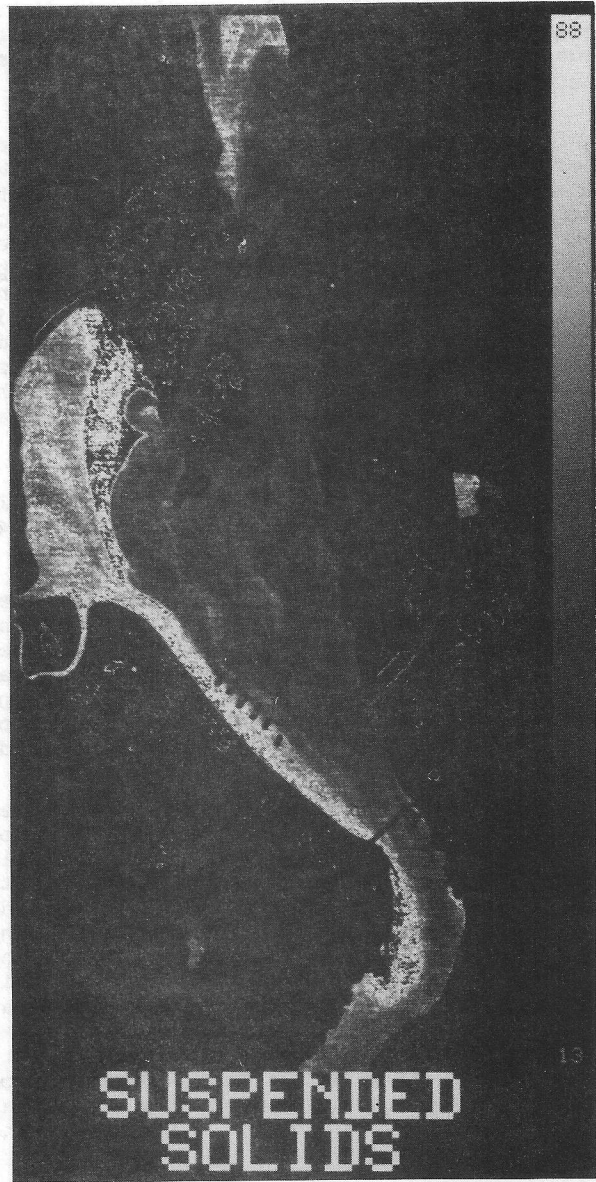


Figure 1. Suspended Solids gradient, mg/l.

water quality maps were produced. The resultant maps appeared noisy and levels of the water quality constituents were not spatially continuous. Therefore, a 3-by-3 averaging filter was passed over the raw data and the regressions were reapplied. The output maps showed much better contouring of the water quality constituents and much less noise. Although the maps produced with non-averaged data may have shown greater detail, location of a single pixel of certain water quality is not possible in a moving body of water, nor was it the intended use of such mapping. Water quality maps were thus made for conductivity, suspended solids, and turbidity.

Using the seven TM channels in a multiple regression with suspended solids levels, a high R^2 of .92 was achieved. No transformation was necessary, although the principal components, log and square root of suspended solids also yielded good results. The suspended solids map, presented as a black and white gradient map between 13 and 88 mg/l, is shown in Figure 1. Land and suspended solids values beyond the sampling range are mapped to black background. The regression equation that provided the map is:

$$\begin{aligned} \text{suspended solids} &= -179.51 - 18.79(\text{TM1}) \\ &+ 100.41(\text{TM2}) - 2.32(\text{TM3}) - 2.94(\text{TM4}) \\ &- 6.00(\text{TM5}) + .508(\text{TM6}) + .675(\text{TM7}) . \end{aligned}$$

The best single band for mapping suspended solids was TM3, with $R^2 = .7129$. As can be seen by referring to Table 1, Klemas and Polis (1977, pp. 599-612), Khorram (1981, pp. 667-676), and Holyer (1978, pp. 323-338) also utilized the red portion of the spectrum (TM3) for suspended solids mapping.

The second highest R^2 of the water quality constituents was .77 for conductivity. In this case, a multiple regression between logarithm conductivity and TM bands 1,2,3,4, and 6 was developed. Khorram (1982, pp. 15-22) used the equivalent MSS bands, excluding TM 6, for mapping salinity (see Table 1). In this study, the logarithm of conductivity was used to reduce the tendency for plotted residuals to increase as conductivity increased. To a lesser extent square root conductivity also improved the residual plot and increased the R^2 . The resultant regression equation is:

$$\begin{aligned} \log \text{ conductivity} &= 6.55 - .289(\text{TM1}) \\ &+ .100(\text{TM2}) - .027(\text{TM3}) + .019(\text{TM4}) \\ &- .008(\text{TM6}) . \end{aligned}$$

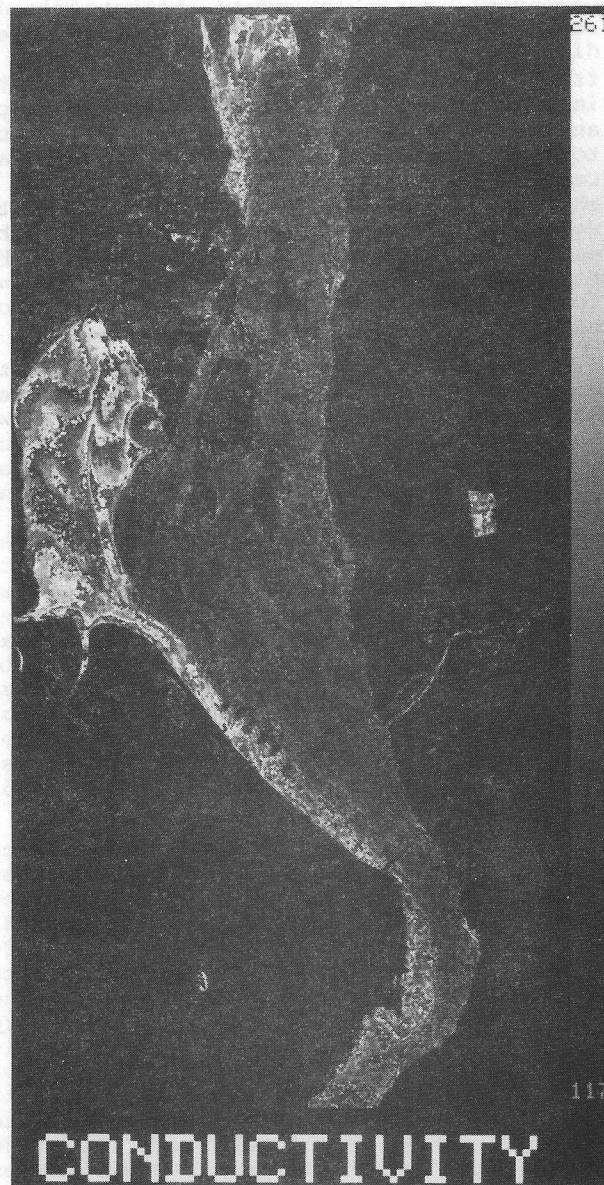


Figure 2. Conductivity gradient, umhos/cm.

Application of the equation to the "averaged" TMS data set resulted in an output image depicted in black and white gradient in Figure 2. The best single band for conductivity was TM 4, at $R^2 = .66$.

Turbidity was also mapped using the TMS data (see Figure 3). The first four principal components (PC1,...,PC4) derived from the TM bands were used in a multiple regression and an $R^2 = .75$ was achieved. The first four components accounted for 97

percent of the data set variance. The TM bands contributing the most information to the principal components transformation were bands 2,4,5, and 6. The single TM band found to yield the highest R^2 was TM 4 ($R^2 = .70$). Other investigators also found the TM4 wavelength useful for mapping turbidity (see Table 1), although the TM3 wavelength was more commonly used.

$$\text{turbidity} = -5.82 + .249 (\text{PC1}) + .155 (\text{PC2}) - .200 (\text{PC3}) + .123 (\text{PC4}) .$$

The remaining water quality constituents did not meet the regression criteria for water quality mapping used in this project. Depth had a moderate R^2 and F-ratio, but these parameters were statistically insignificant for pH and temperature. Therefore, water quality maps were not produced for these variables. A good correlation between temperature and TM6 radiance was initially anticipated since the TM6 wavelength is in the thermal infrared portion of the spectrum, however, this relationship was not found. It is possible that atmospheric moisture interfered with the TM 6 radiance. A low range in data values may also have been the reason for the poor correlation; 88 percent of the sites were between 17 and 18 degrees C. The minimum thermal resolution of the scanner was .35 degrees C, so there may not have been a wide enough range in temperature for thermal mapping. The spectral data for TM6 ranged between DN's 111 and 118, similarly a small range. The moderate results for depth, when none were expected, may be explained by the presence of some factor, such as suspended solids, which is probably depth related.

Accuracy assessment of water quality maps can be difficult to incorporate into studies. It is necessary to conduct water sampling as closely as possible to the time that the spectral data is recorded due to the highly dynamic nature of water bodies. Therefore, the number of sites sampled is often be limited by logistical and economic resources. Moreover, all samples must often be used for the development of the best regression model possible, leaving no sites remaining for assessment of the results. Steps were taken in this study to assess the robustness of the regressions used for mapping conductivity, turbidity, and suspended solids. Confidence intervals about the mean regression were calculated, and cross validation of random subsamples was performed.

Confidence intervals were calculated for each water quality variable to indicate the actual range of predicted water quality represented by the

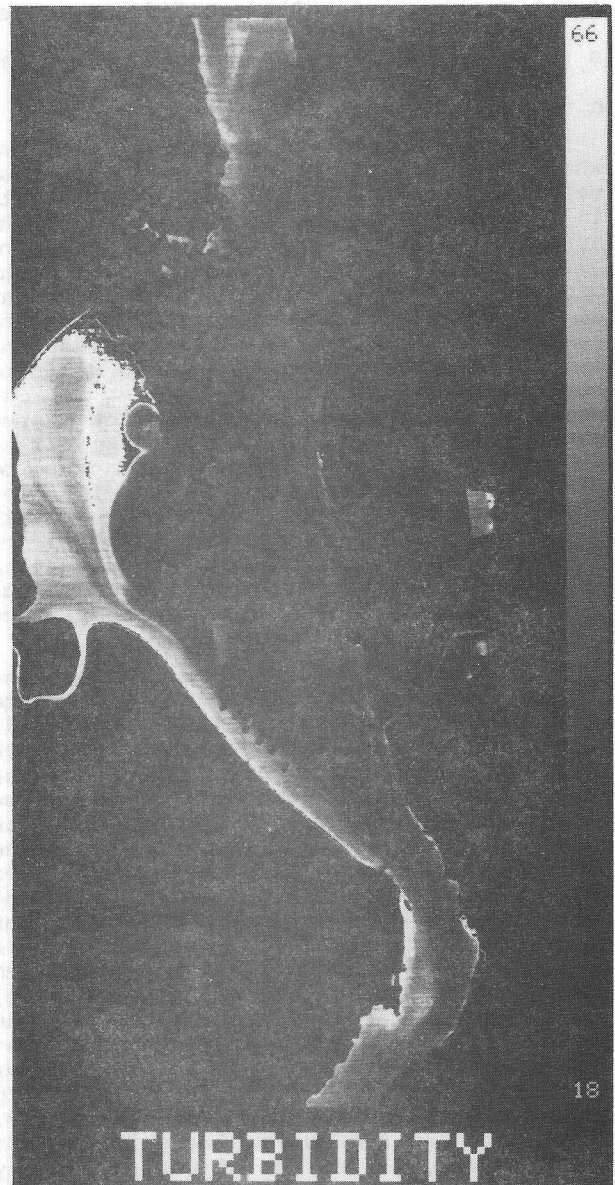


Figure 3. Turbidity gradient, NTUS

regression equations. The equation used for calculating the confidence interval at the mean spectral values is:

$$\bar{y} \pm (t_{.025; 22}) \frac{s}{\sqrt{n}}$$

where:

\bar{y} = predicted water quality value from the regression equation when mean values are used for the TM values
 t = t statistic for 95% confidence level and 22 degrees of freedom
 s = standard error of estimate for data (residual standard deviation)
 n = sample size

The confidence interval is smallest when calculated at the mean spectral values; away from the mean its length increases. Applying the equation to the suspended solids regression, a range of 49.15 to 56.01 mg/l suspended solids was derived. In other words, with 95 percent confidence in future sampling, using the same spectral values in the regression, the predicted suspended solids would be between 49.15 and 56.01 mg/l. So, in using a water quality map, the mapped water quality level could have been off by as much as 3.43 mg/l, which may be acceptable for many uses. Applying the same technique to the conductivity regression, a 95 percent confidence interval for conductivity at the mean spectral values was 2.14 to 2.20 umhos/cm. The turbidity 95 percent confidence interval was 29.19 - 35.89.

As a means of cross validating the regressions, random subsamples of the data were regressed and resultant R^2 's compared. Five sites, selected randomly, were eliminated from the sample data and the regression run again using the same regression parameters as used for the final mapping. That is, for suspended solids, all seven TM bands were used, for conductivity, log conductivity was used with TM bands 1, 2, 3, 4, and 6. For turbidity, principal components 1-4 were used. This procedure was repeated ten times for each water quality variable, using different random subsamples. As can be seen in Table 3, the range of R^2 for suspended solids was .88 to .97. For conductivity, the R^2 's varied from .67 to .84, and from .67 to .92 for turbidity. When the new regressions were applied to the TMS data, the series of water quality maps were mostly very similar, although in some cases substantially different water quality contours resulted. These assessments indicate that sample size limitations are an important factor in water quality mapping.

VI. CONCLUSIONS

TM data proved to be useful for mapping select water quality factors, specifically, suspended solids, turbidity, and conductivity. For suspended solids, TM bands 1-7 were used in a multiple regression wherein the coefficient of determination and significance were the highest and variability in cross validation was the lowest of the water quality variables. TM was also suitable for mapping turbidity and conductivity which were similar in R^2 and significance, although the confidence interval and range of results for random subsamples was largest for turbidity. TM bands 1-4, and 6 were used with log conductivity in a multiple regression. Turbidity was mapped using a multiple regression with the first four principal components of the TM data. In this study, water temperature was not reliably sensed with TM6, probably because the range of temperatures sampled was small and there may have been atmospheric moisture interference. The TM regression technique was deemed suitable for water quality mapping given known confidence intervals and depending upon the application in question.

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AUTHOR BIOGRAPHICAL DATA

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Table 1. Summary of Water Quality Remote Sensing Investigations

Water Constituent	Investigators	Scanner	Bands	TM Equivalent
suspended solids	Klemas & Polis (1977)	Landsat	MSS 5	TM 3
	Khorram (1981)	OCS	.494-.518 um	TM 1
				.667-.679 um
	Johnson (1977)	-	.380-.440 um	(<TM 1)
	Holyer (1978)			.700-.740 um
			.652 um	TM 3
			.782	TM 4
conductivity	Khorram (1982)	Landsat	MSS 4,6,7	TM 2,4
	Rogers et al (1976)	Landsat	MSS 4/5 ratio	TM 2/3
turbidity	Bartolucci et al (1977)	Landsat	MSS 5	TM 3
	Schertz et al (1975)	Landsat	MSS 4,5,6,7	TM 2,3,4
	Rogers et al (1976)	Landsat	MSS 5	TM 3
	Weisblatt et al (1973)	Landsat	MSS 5,6	TM 3,4
	Khorram (1981)	OCS	.494-.518 um	TM 1
			.778-.790 um	TM 4

Table 2. Most Significant Regressions for Each Water Quality Parameter

Water Constituent	R ²	Bands Used	Sites Removed	Regression Type	F-Ratio	D.F.	Sig. P	Transformation
conductivity	.77	1-4,6	23	mult	*12.032	5,18	<.001	log cond
	.66	4	23	step	*20.07	2,21	<.001	-
depth	.72	1-4,6	4,24	mult	8.730	5,17	<.001	log depth
	.38	6	4	step	13.34	1,22	<.005	log depth
temperature	.60	all	none	mult	3.605	7,17	<.025	log temp
	.33	PCA4	none	step	11.47	1,23	<.005	pca
pH	.47	all	none	mult	2.130	7,17	ns**	square root pH
	.28	1	23	step	8.67	1,22	<.01	log pH
turbidity	.75	all	19	mult	*14.18	4,19	<.001	PCA
	.70	4	19	step	*20.94	1,22	<.001	square root turb
suspended solids	.92	all	2	mult	*27.513	7,16	<.001	-
	.83	3,6	2	step	*49.89	2,21	<.001	square root s.s.

* met Whitlock's criteria for F

**ns - not significant at the .05 level

Table 3. Cross Validation Regressions

Suspended Solids*			Conductivity**			Turbidity***					
1	.97	6	.90	1	.80	6	.69	1	.68	6	.67
2	.94	7	.93	2	.80	7	.83	2	.80	7	.73
3	.95	8	.94	3	.67	8	.72	3	.76	8	.80
4	.95	9	.88	4	.67	9	.84	4	.79	9	.79
5	.94	10	.93	5	.67	10	.83	5	.92	10	.81

* Range of F-ratios was 58.0 - 14.9 at <.001 level of significance

** Range of F-ratios was 13.7 - 5.2 at <.005 level of significance

*** Range of F-ratios was 7.14 - 41.1 at <.005 level of significance