
Methodology for Flow and Salinity Estimates in the Sacramento-San Joaquin Delta and Suisun Marsh

**23rd Annual Progress Report
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Chapter 6: Calibrating DSM2-QUAL Dispersion Factors to Practical Salinity

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6 Calibrating DSM2-QUAL Dispersion Factors to Practical Salinity

6.1 Introduction

DSM2-QUAL's current set of dispersion factors that are used in simulating the transport of salinity in the Delta were calibrated to measured electrical conductivity (EC). Concerns have been raised about using EC for this purpose due to its failure to behave as a truly conservative indicator of salinity. This chapter briefly discusses this problem and presents practical salinity, as derived from EC, as an alternative water quality parameter for calibrating dispersion factors.

6.2 Background

In past development of Delta water quality simulation models, DWR has used both total dissolved solids (TDS) and EC to calibrate and validate models for the transport of conservative mass. Both approaches have advantages and disadvantages and are briefly summarized below.

6.2.1 Calibrating QUAL to EC

The IEP DSM2 Project Work Team established the set of dispersion factors currently used by DSM2-QUAL (QUAL) in 2000 as part of the most recent calibration and validation of DSM2 (Nader-Tehrani, 2001). EC was chosen for calibrating the dispersion factors for conservative mass transport primarily because of its availability at DSM2 boundaries and at important interior Delta locations. EC is recorded every 15 minutes or hourly at multiple sites within the Delta and data extend back to the 1980s or earlier, depending upon the site. Other potential constituents for calibration, such as chloride and TDS, are far less available in the Delta and would have to be inferred from relationships to EC.

An important drawback to using EC to calibrate dispersion factors is its acknowledged failure to behave as a truly conservative constituent of salinity. As salinity and ionic concentration increases, electrical conductance increases. For high concentrations, however, the proximity of ions to each other depresses their activity and consequently their ability to transmit electrical current. As a result, EC increasingly underestimates true salinity at higher concentrations, a trend manifest in a nonlinear relationship between EC and any conservative constituent. This behavior is described by Hem (1985) as typical for all salts. As an example, Hem presents the case of KCl at a concentration of 7,460 mg/L which displays a conductance of 12,880 $\mu\text{S}/\text{cm}$ instead of the expected 14,000 $\mu\text{S}/\text{cm}$, an under measurement of 8%. It was also explicitly presented in an equation developed by Poisson (1980) relating EC to salinity for diluted standard seawater and simplified by Schemel (2000) for surface data taken at 25 $^{\circ}\text{C}$ (Figure 6.1):

$$EC = \left(\frac{S}{S_{Seawater}} \right) (EC_{Seawater}) + S(S - S_{Seawater}) (J_1 + J_2 S^{1/2} + J_3 S + J_4 S^{3/4}) \quad [\text{Eqn. 6-1}]$$

where S is practical salinity (dimensionless) or salinity in parts per thousand (ppt), and:

$$\begin{aligned} S_{seawater} &= 35 \\ EC_{seawater} &= 53,087 \text{ } \mu\text{S/cm} \\ J_1 &= -16.072 \\ J_2 &= 4.1495 \\ J_3 &= -0.5345 \\ J_4 &= 0.0261 \end{aligned}$$

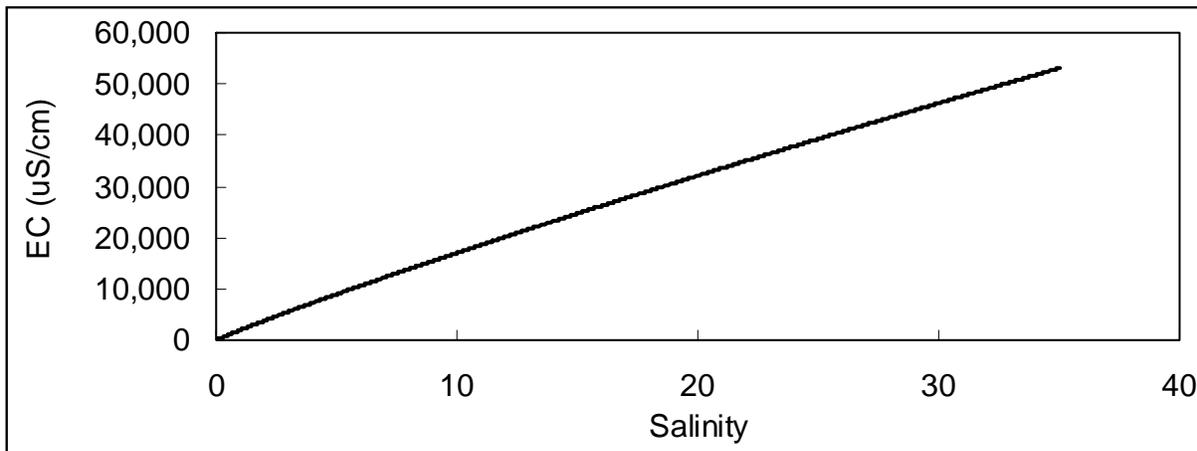


Figure 6.1: EC as a Function of Salinity per Equation 6-1 (Schemel, 2000).

EC's non-conservative behavior is also evident when viewing the nonlinear relationship between Delta EC and TDS and Delta EC and chloride, considering that TDS and chloride are generally considered conservative (Figures 6.2 and 6.3). These figures are consistent with the relationship of EC to TDS and chloride from the Gila River in Arizona presented by Hem (1985). In contrast to EC, Figure 6.4 shows that Delta TDS and chloride are linearly related. The data for these figures and much of the analysis in this chapter come from grab samples collected by DWR over the past 30 years for various programs, primarily the Municipal Water Quality Investigations Program and D-1485 Water Quality Monitoring Program. TDS and chloride have been converted from mg/l to parts per thousand (ppt) by dividing values by sample density, ρ , estimated by:

$$\rho = 1 + \left[\frac{X_s}{X_{sw}} \right] (\rho_{sw} - 1) \quad [\text{Eqn. 6-2}]$$

where:

$$\begin{aligned} X_s &\text{ is sample concentration (either TDS or chloride) in mg/l,} \\ X_{sw} &\text{ is concentration of seawater (19,370 mg/l chloride or 35,000 mg/l TDS), and} \\ \rho_{sw} &\text{ is the density of seawater, assumed to be 1.0243.} \end{aligned}$$

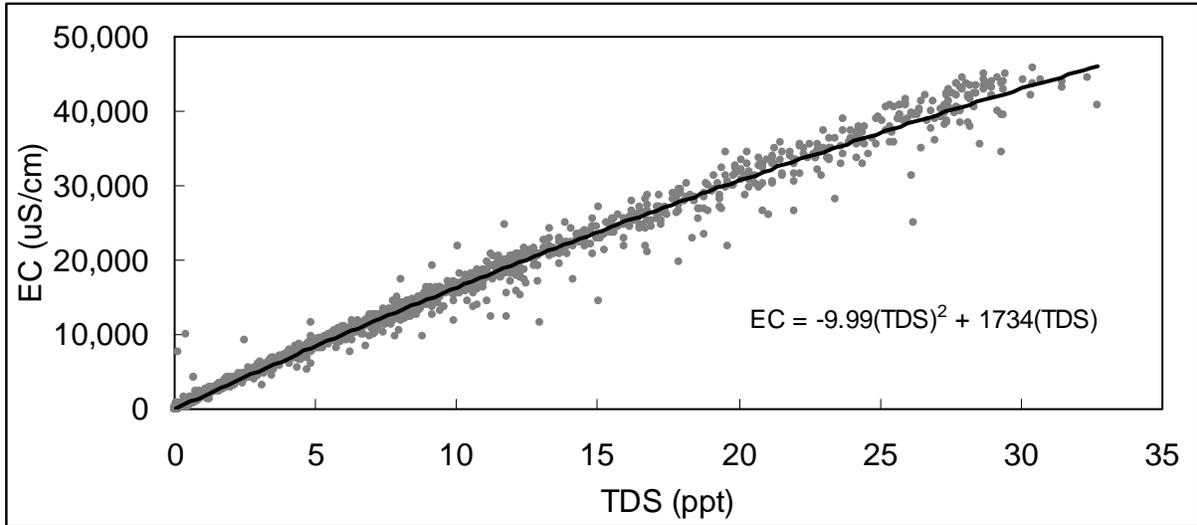


Figure 6.2: Nonlinear Relationship between EC and TDS from Delta Grab Samples.

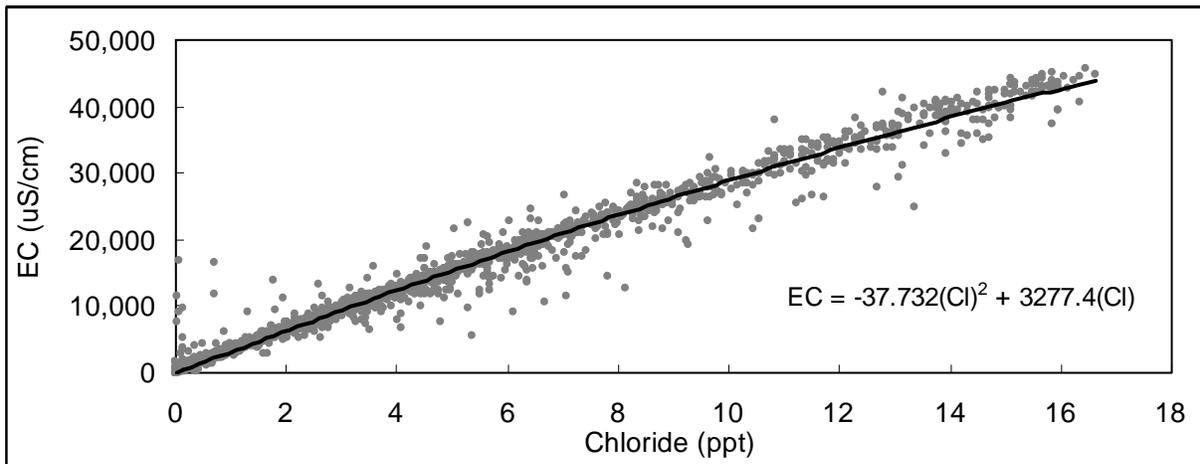


Figure 6.3: Nonlinear Relationship between EC and Chloride from Delta Grab Samples.

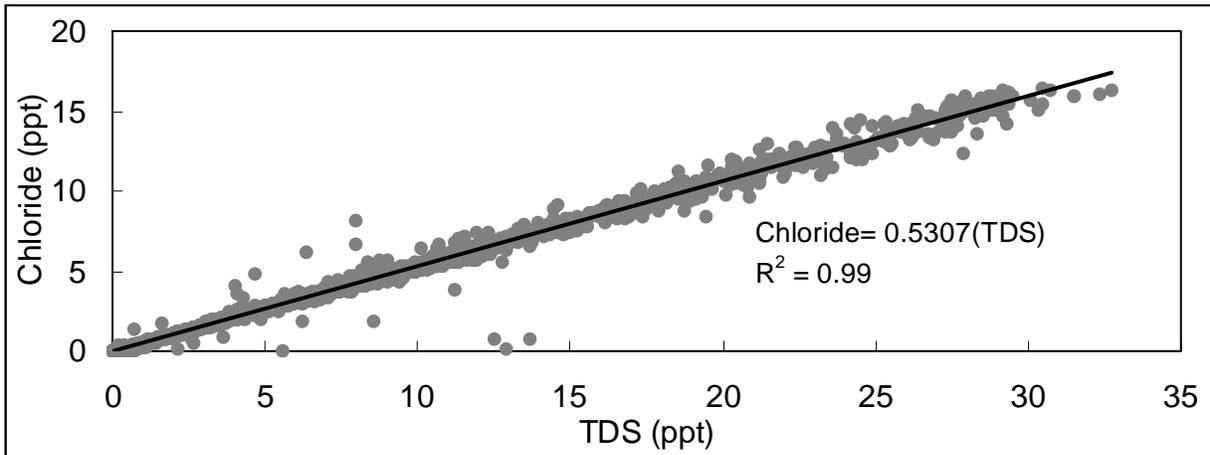


Figure 6.4: Linear Relationship between Chloride and TDS from Delta Grab Samples.

Delta values go up to 17 ppt for chloride, 33.5 ppt for TDS, and 45,800 uS/cm for EC. These ranges relate to the location and tidal and hydrologic conditions at the time the sample is taken. However, samples with higher salinity tend to have been collected in the Suisun Bay, nearer to DSM2's downstream boundary. The non-conservative property of EC may be insignificant for relatively fresh water, but in Suisun Bay EC can exceed 30,000 $\mu\text{S}/\text{cm}$. Using EC as an indicator of relative salinity may be problematic and has implications for the calibration of dispersion factors. Higher measured EC in Suisun Bay and DSM2's downstream boundary of Carquinez Strait at Martinez, will tend to be too low relative to true salinity while lower EC values at interior Delta locations will more accurately reflect actual salinity. As a result, calibrating DSM2 for salinity transport with measured EC will cause dispersion factors in Suisun Bay to be set artificially high in order to transport sufficient EC into the Delta to match more accurate interior EC values.

The current dispersion factors in DSM2 are therefore probably higher in Suisun Bay than would be calculated if a truly conservative transport constituent was used for calibration. However, as long as EC is simulated in QUAL, model results are probably valid, although a bias for overestimating EC during wetter conditions is possible. Total organic carbon (TOC) simulations are also probably valid since downstream boundary contribution is trivial. In calibrating QUAL, dispersion factors are typically adjusted until annual peak salinity at upstream locations is reproduced in the late summer or fall. Thus, calibration naturally focuses on periods when boundary EC will be highest. Wetter conditions when EC in Suisun Bay is much lower, and thus a more accurate representation of salinity, will still use the same dispersion factors and too much inland transport of mass could conceivably occur. However, such a bias of over predicting interior EC in wetter periods is not readily apparent in the current validation of DSM2 (<http://iepdsm2pwt/dsm2pwt.html>).

6.2.2 Calibrating QUAL to TDS

TDS is another water quality constituent that is used to calibrate dispersion factors in mass transport models. TDS has been collected in the Delta, along with many other constituents, in monthly or semi-monthly grab samples. While this data is insufficient to use directly as boundary input for simulating a historic period for calibrating or validating DSM2, sufficient samples exist to establish relationships between EC and TDS at the boundaries (Figure 6.5). Boundary conditions for any calibration period that are based on such relationships will introduce additional error to the simulated values. In addition, historical EC field measurements from internal Delta channels would need to be converted to TDS in order to compare modeled results while calibrating and validating the model. Such modification of historically measured data in order to document model validation is viewed as undesirable.

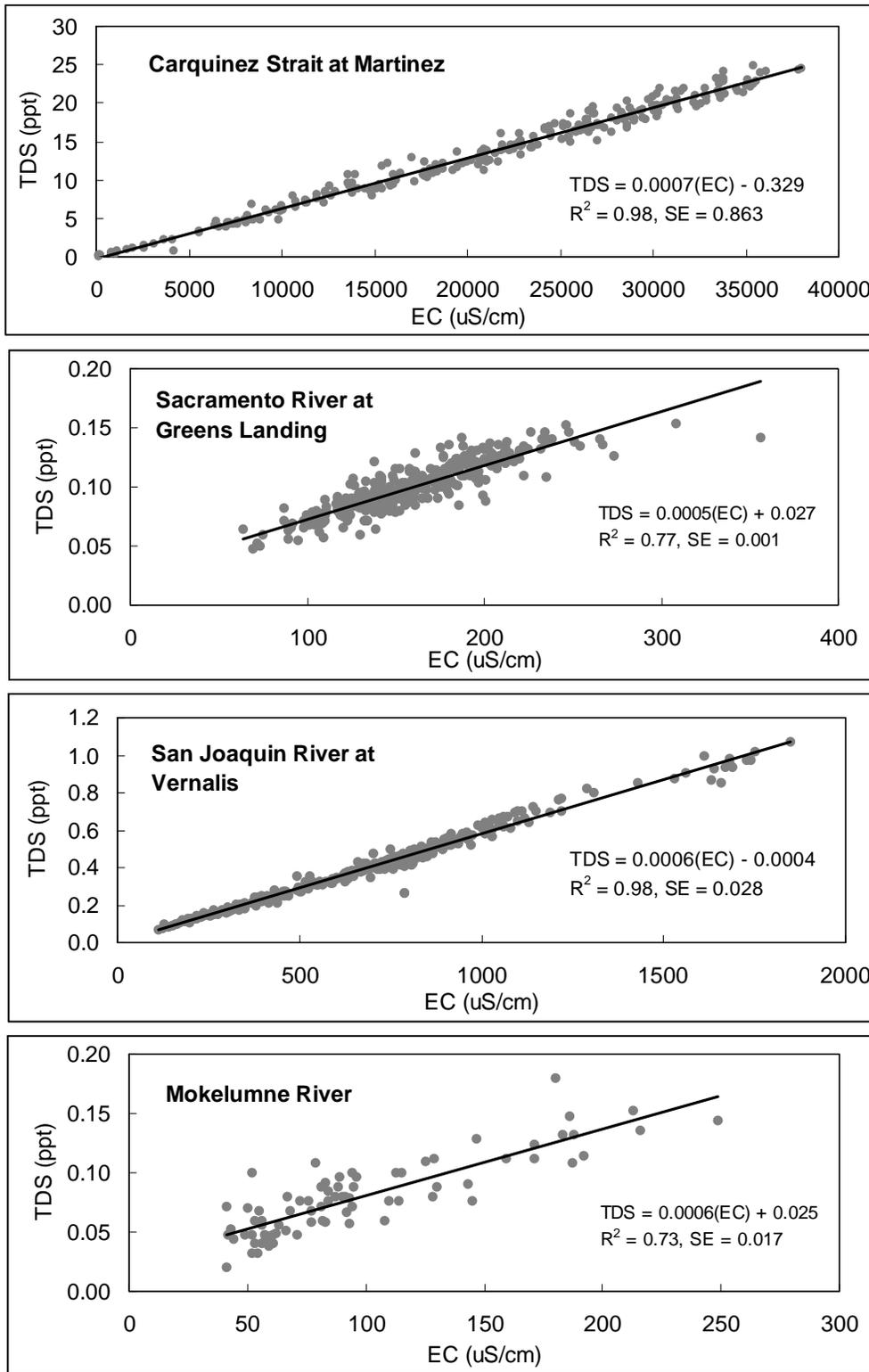


Figure 6.5: Relationship between TDS and EC at Delta Boundaries.

6.3 Calibrating QUAL to Practical Salinity

An alternative approach to using EC or TDS to calibrate QUAL was sought that would both correct for the non-conservative behavior of EC at high salinity concentrations and allow for field EC data to be used unaltered for validation. Using practical salinity to calibrate QUAL is now presented as an alternative.

6.3.1 Practical Salinity Background

A standard expression of salinity is the Practical Salinity Scale 1978, first proposed by Lewis (1980). This scale converts *in situ* electrical conductivity readings into salinity. Practical salinity is defined as a function of electrical conductivity and temperature (and assuming any pressure component to be negligible):

$$S = a_0 + a_1 R_T^{1/2} + a_2 R_T + a_3 R_T^{3/2} + a_4 R_T^2 + a_5 R_T^{5/2} + \frac{(T - 15)}{1 + k(T - 15)} \{ b_0 + b_1 R_T^{1/2} + b_2 R_T + b_3 R_T^{3/2} + b_4 R_T^2 + b_5 R_T^{5/2} \} \quad [\text{Eqn. 6-3}]$$

where:

$a_0 = 0.0080$	$b_0 = 0.0005$	$k = 0.0162$
$a_1 = -0.1692$	$b_1 = -0.0056$	
$a_2 = 25.3851$	$b_2 = -0.0066$	
$a_3 = 14.0941$	$b_3 = -0.0375$	
$a_4 = -7.0261$	$b_4 = 0.0636$	
$a_5 = 2.7081$	$b_5 = -0.0144$	

$$\sum a_i = 35.0000; \quad \sum b_i = 0.0000$$

$$R_T = \left(\frac{EC_{sample}}{EC_{seawater}} \right)_{Temperature T}; \quad -2^\circ\text{C} \leq T \leq 35^\circ\text{C}$$

Practical salinity is commonly expressed as dimensionless or as parts per thousand.

Equation 6-3 is based upon analysis of data obtained by diluting standard seawater with distilled water or evaporating by weight. As formulated above, the Practical Salinity Scale 1978 is valid over the range of 2 - 42, which roughly corresponds to EC values in the Delta in excess of 4,000 $\mu\text{mhos/cm}$.

Electrical conductivity data recorded at various monitoring stations within the Delta are typically collected at shallow depths and are normalized to a standard temperature of 25 °C. Schemel (2000) provided a simplified equation for calculating practical salinity from EC data. Assuming $T = 25^\circ\text{C}$ and atmospheric pressure,

$$S = K_0 + K_1 R_T^{1/2} + K_2 R_T + K_3 R_T^{3/2} + K_4 R_T^2 + K_5 R_T^{5/2} \quad [\text{Eqn. 6-4}]$$

where:

$$\begin{aligned} K_0 &= 0.0120 \\ K_1 &= -0.2174 \\ K_2 &= 25.3283 \\ K_3 &= 13.7714 \\ K_4 &= -6.4788 \\ K_5 &= 2.5842 \end{aligned}$$

R_T is as defined in Equation 6-3. Schemel (2000) assumed EC_{seawater} to be 53,097 $\mu\text{S/cm}$.

As previously mentioned, the Practical Salinity Scale 1978 as originally formulated was valid for the range from 2 to 42, with seawater at 35. Hill et al. (1986) developed a standard correction to Equation 6.3 to extend the Practical Salinity Scale 1978 to salinity below 2. This correction is expressed by:

$$\text{Standard Correction} = -\frac{a_0}{1 + 1.5x + x^2} - \frac{b_0 f(T)}{1 + y^{1/2} + y + y^{3/2}} \quad [\text{Eqn. 6-5}]$$

where:

$$\begin{aligned} f(T) &= \frac{(T - 15)}{1 + k(T - 15)} \\ x &= 400R_T \\ y &= 100R_T \\ a_0 &= 0.008 \\ b_0 &= 0.0005 \\ k &= 0.0162 \end{aligned}$$

This correction approaches 0 at a practical salinity of 2, leaving the original equation, Equation 6-3, intact while forcing the practical salinity to equal 0 when the conductivity is equal to the value for pure water (Figure 6.6). The standard correction to practical salinity below 2 is based on dilutions of standard seawater and is only strictly applicable to waters that have the major ions in the same proportions as standard seawater. This correction does not necessarily apply to coastal waters diluted by land drainage such as occurs in the Delta (Hill, 1986). The American Public Health Association et al. (1995) state that the standard correction can be used, with some limitations, with estuarine water. Buchanan et al. (2001) apply the standard correction to Practical Salinity Scale 1978 as derived from *in situ* EC collected from the San Francisco Bay-Delta as part of USGS's standard methodology. In contrast, Kimmerer et al. (1998) makes no mention of a correction but suggests limiting use of the Practical Salinity Scale 1978 in the San Francisco Bay-Delta to salinity values above 2. Still others state that Practical Salinity Scale 1978 values calculated from fresh water EC need no correction if EC values have already been corrected to 25 °C (Schemel, 2000; Seabird, 2001). Other literature on estuarine salinity where practical salinity values below 2 are presented are mute on this issue

(Blanton et al. 2001; Schoellhamer, 2001). The issue of applying a correction to the Standard Salinity Scale 1978 for low salinity Delta water is further explored below.

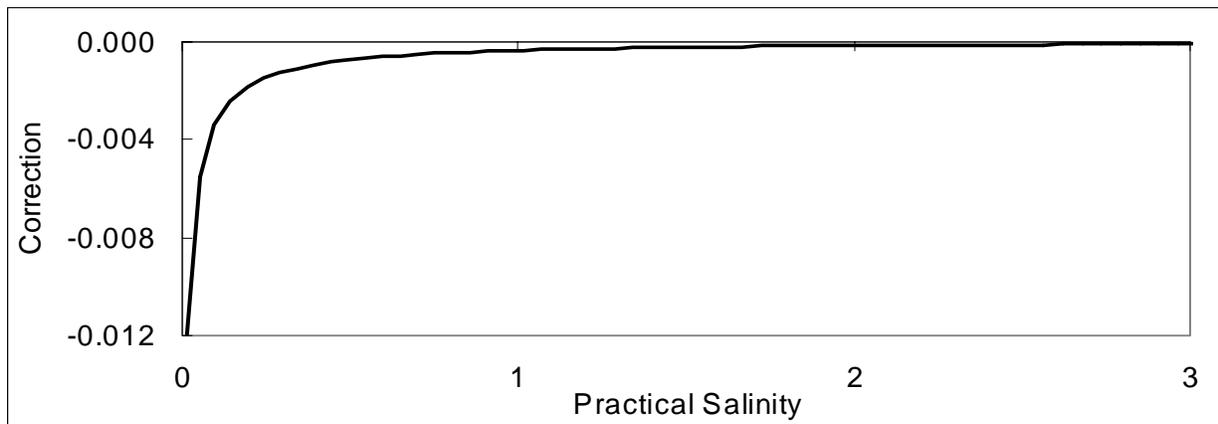


Figure 6.6: Standard Correction to Practical Salinity Scale 1978 (Hill et al., 1986).

6.3.2 Practical Salinity in the Sacramento-San Joaquin Delta

EC from DWR grab samples throughout the Delta collected the past 30 years was converted to practical salinity by the Practical Salinity Scale 1978 (Equation 6.4) and plotted against the chloride that was simultaneously measured (Figure 6.7). When extreme outliers are removed, the resulting relationship, practical salinity / chloride, is found to be 1.78. This is consistent with a published relationship of 1.81 between salinity and chlorinity (Lewis, 1980; Cox et al., 1967).

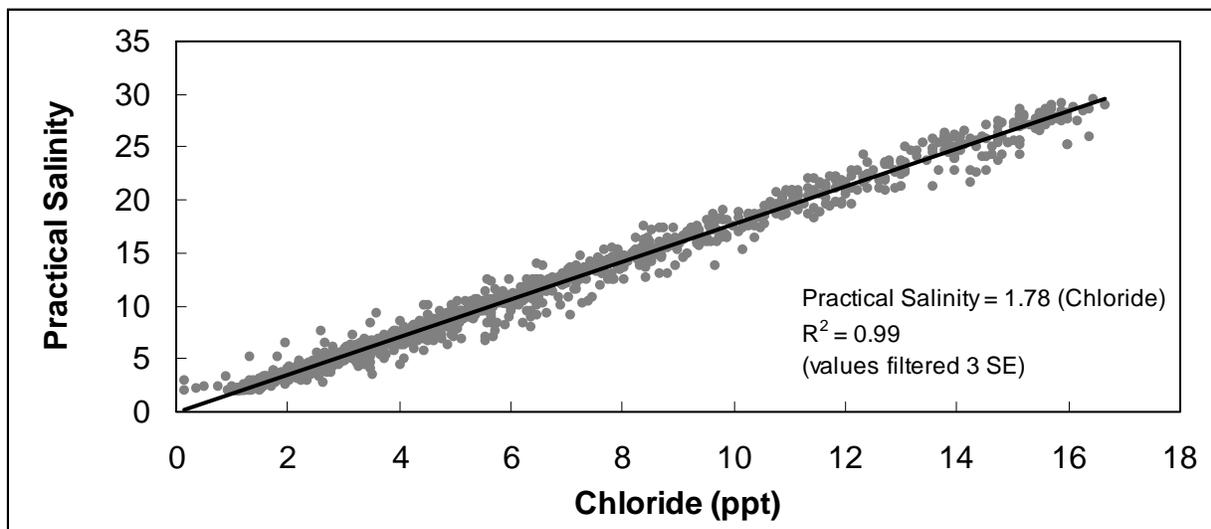


Figure 6.7: Relationship between Delta Practical Salinity Scale 1978 and Observed Chloride.

Practical salinity was also plotted against TDS, again collected from grab samples (Figure 6.8). As Figure 6.8 shows, the overall relationship between practical salinity and TDS is linear, correcting EC's non-conservative behavior. However, examination of practical salinity at low salinity (TDS < 1.2 ppt) shows that the validity of calculating practical salinity in the range of 0

to 2 remains an issue (Figure 6.9). If the Practical Salinity Scale 1978 is valid for all the data, practical salinity in the range of 0 to 2 will fall along the extended regression for the practical salinity range of 2 to 42. However, Figure 6.9 shows that the uncorrected practical salinity data calculated from Delta EC, in fact, deviates from this regression. The linear relationship between practical salinity and TDS actually holds down to a TDS of 1 ppt (Figure 6.10), but below this level, the influence of the Sacramento and San Joaquin rivers and perhaps agricultural drainage apparently causes the Practical Salinity Scale 1978 to err. The Delta water quality samples seem to display behavior inferred by Hill et al. (1986) who cautioned that the assumption of constancy with seawater of relative composition does not apply to coastal waters diluted by land drainage.

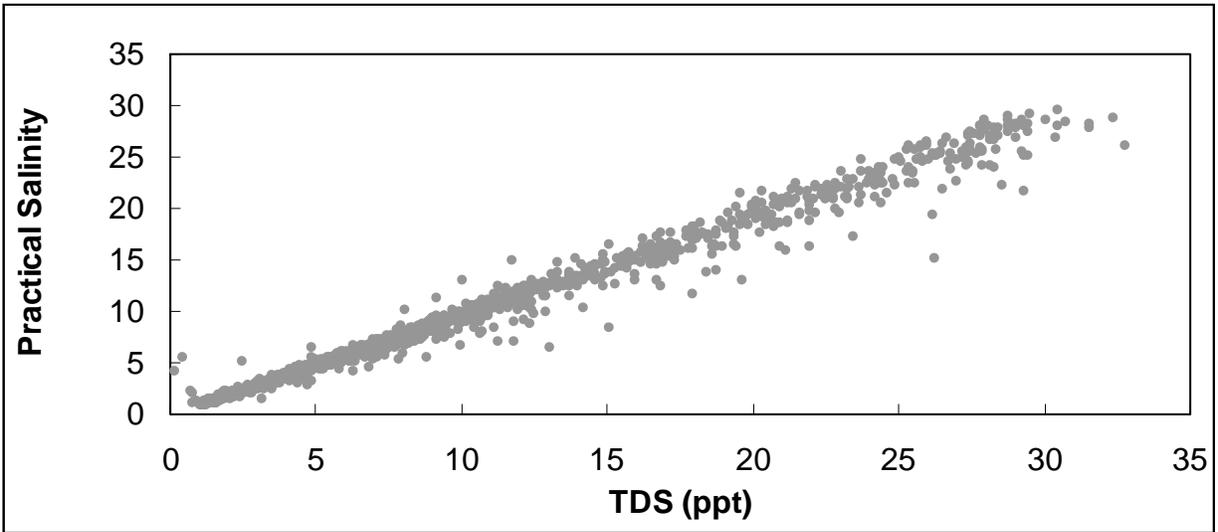


Figure 6.8: Relationship between Delta Practical Salinity Scale 1978 and Observed TDS.

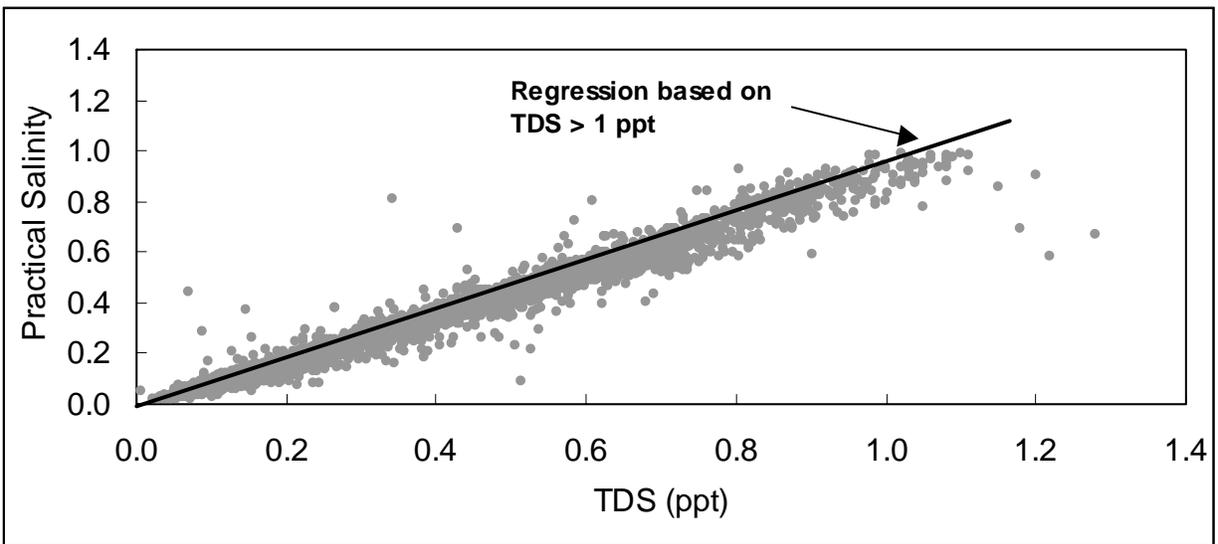


Figure 6.9: Deviation of Low Delta Practical Salinity from Valid Regression.

Applying the standard correction to the Practical Salinity Scale 1978 presented in Equation 6-5 had essentially no effect upon the results. As Schemel (2000) points out, the standard correction

is very small with respect to the generated values. An alternative correction, specific to the conditions in the Sacramento-San Joaquin Delta and the sources of fresh water, is needed.

6.3.3 An Alternative Correction to Extend Practical Salinity Scale 1978 Below 1 PPT TDS in the Delta

Examination of Delta grab sample data shows that practical salinity derived from Delta EC holds a linear relationship with TDS down to a value of approximately 1 ppt TDS (practical salinity of about 0.92). As Figure 6.10 shows, when outliers are removed, this relationship is expressed by:

$$\text{practical salinity} = 0.9528 (\text{TDS}) \quad [\text{Eqn. 6-6}]$$

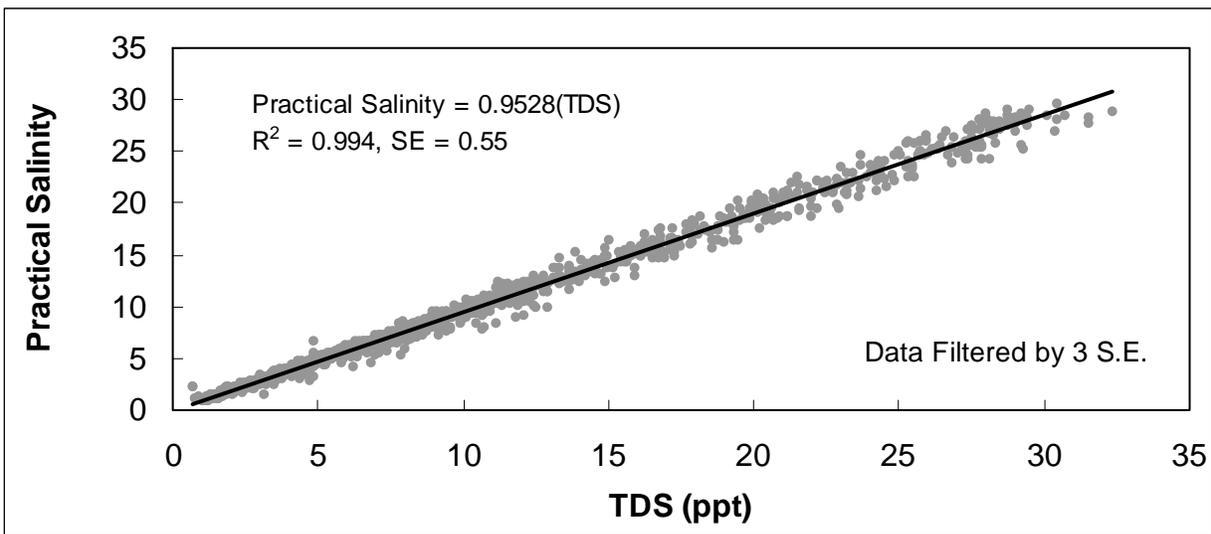


Figure 6.10: Relationship between Delta Practical Salinity and TDS for TDS > 1 ppt.

This regression is assumed to be the valid relationship between practical salinity and TDS in the Delta. Lower practical salinity values would fall along this regression if Equations 6-3 or 6-4 held for all values below 1 ppt TDS. The deviation from this regression is thus assumed to be the needed correction to Delta practical salinity. Figure 6.11 shows how this correction can be approximated by partitioning the range of 0 to 1 ppt TDS (0 to 0.92 practical salinity) into three intervals. The correction to practical salinity will then vary linearly over each interval (Table 6.1) and apply Deltawide since the data in Figure 6.11 come from locations throughout the Delta.

Table 6.1: Desired Correction to Delta Practical Salinity.

TDS (ppt)	EC (uS/cm)	Practical Salinity	Practical Salinity Correction
0	0	0	0
0.175	302	0.145	0.027
0.750	1346	0.671	0.052
1	1824	0.923	0

This correction can then be incorporated directly into the simplified Practical Salinity Scale 1978 for surface water at 25 °C:

$$S = M_0 + M_1 \left(K_0 + K_1 R_T^{1/2} + K_2 R_T + K_3 R_T^{3/2} + K_4 R_T^2 + K_5 R_T^{5/2} \right) \quad [\text{Eqn. 6-7}]$$

where,

$K_0, K_1, K_2, K_3, K_4,$ and K_5 defined as in Equation 6-4, R_T as defined earlier, and M_0, M_1 as specified in Table 6.2.

Table 6.2: Coefficients M_0 and M_1 to Correct Low Practical Salinity in Delta Channels.

TDS Range (ppt)	EC Range uS/cm	Practical Salinity Range	M_0	M_1	Corrected Practical Salinity Range
< 0.175	< 302	< 0.145	0	1.1880	< 0.172
0.175 - 0.75	302 - 1346	0.145 - 0.671	0.0205	1.0470	0.172 - 0.723
0.75 - 1.0	1346 - 1824	0.671 - 0.923	0.1903	0.7939	0.723 - 0.923
> 1.0	> 1824	> 0.923	0	1	> 0.923

Practical Salinity from Delta-wide EC data was recalculated according to Equation 6-4 or Equation 6-7 and again compared to TDS. As shown in Figure 6.12, the corrected practical salinity over the range of 0 to 1 ppt TDS essentially falls along the desired regression of practical salinity = 0.9528(TDS), validating Equation 6-7.

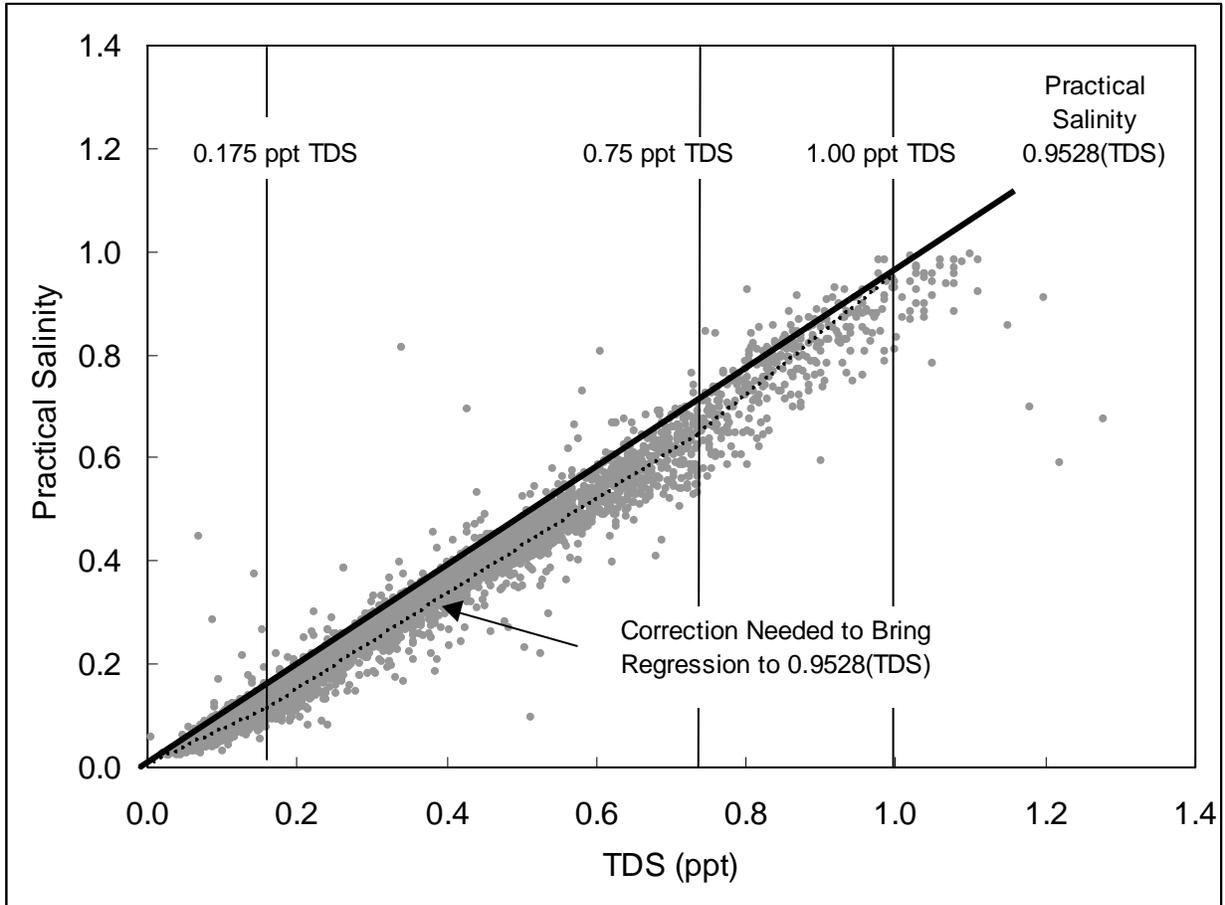


Figure 6.11: Needed Correction to Delta Practical Salinity for Values with TDS < 1 ppt.

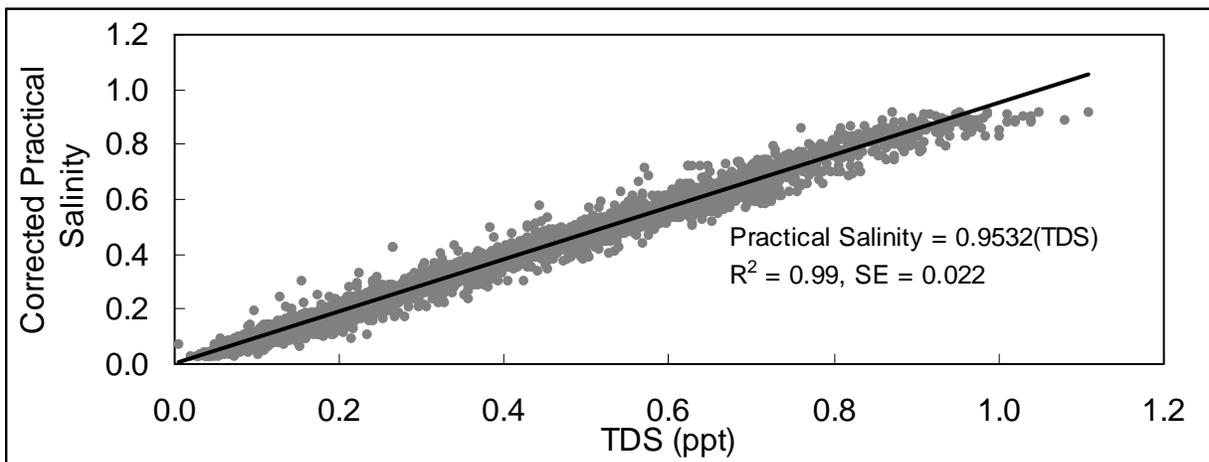


Figure 6.12: Corrected Delta Practical Salinity for Values with TDS < 1 ppt.

6.3.4 Practical Salinity at Delta Boundaries

TDS and EC field data from throughout the Delta were used to generate the correction coefficients in Table 6.2. The actual relationship between practical salinity and TDS that is used to calculate a correction may vary somewhat by location; however, this variability is hidden in Table 6.2. Equation 6-7 was applied separately to EC data at the Delta boundaries. As shown in Figure 6.13, Equation 6-7 holds well at the important boundaries of Carquinez Strait at Martinez and the Sacramento and San Joaquin rivers.

6.3.5 Practical Salinity of Agricultural Drainage

Corrections to practical salinity for agricultural drainage were established separately from the global correction for Delta channel salinity. The relationship between EC and TDS for agricultural drainage appears substantially different from that seen from Delta channels, probably due to the exchange chemistry of soil-water interactions in drainage. In addition, there is no need to convert back from practical salinity to EC for agricultural drainage as there may be for salinity from Delta channels. Agricultural drainage water quality is grouped and evaluated according to the three regions shown in Figure 6.14. This grouping is the same as used in DWR's Delta Island Consumptive Use Model for describing the water quality of Delta agricultural drainage. Figure 6.15 compares uncorrected practical salinity to TDS in each region. The needed correction to practical salinity for agricultural drainage then is calculated as: $0.9528 / (\text{slope of regression of TDS-practical salinity relationship})$. Coefficients M_0 and M_1 for Equation 6-7 then can be expanded to include agricultural drainage (Table 6.3).

Table 6.3: Coefficients M_0 and M_1 to Correct Practical Salinity in Delta Agricultural Drainage.

	Delta Region		
	West	South-East	North
M_0	0	0	0
M_1	1.1665	1.1165	1.2687

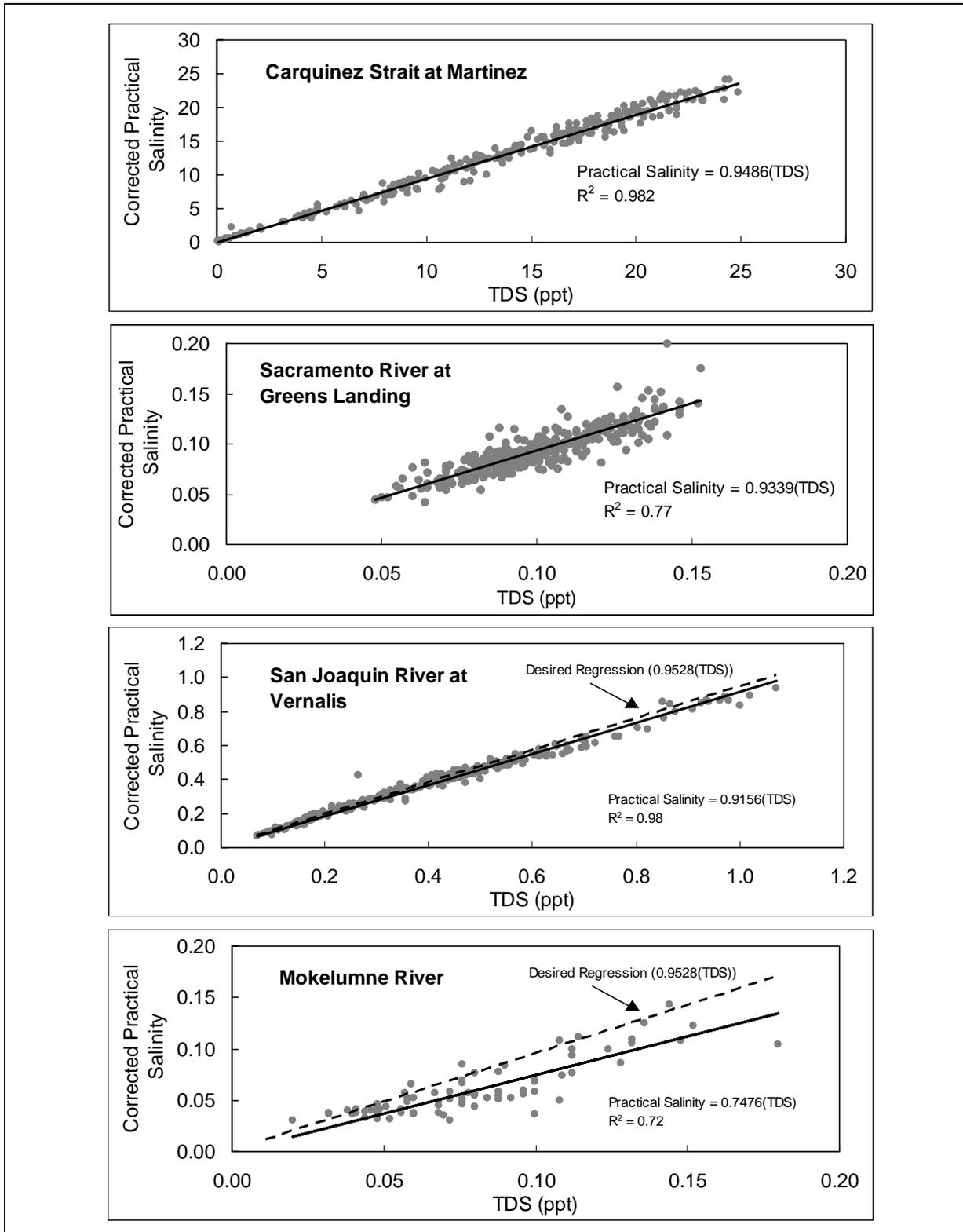


Figure 6.13: Corrected Delta Practical Salinity at Delta Boundaries.

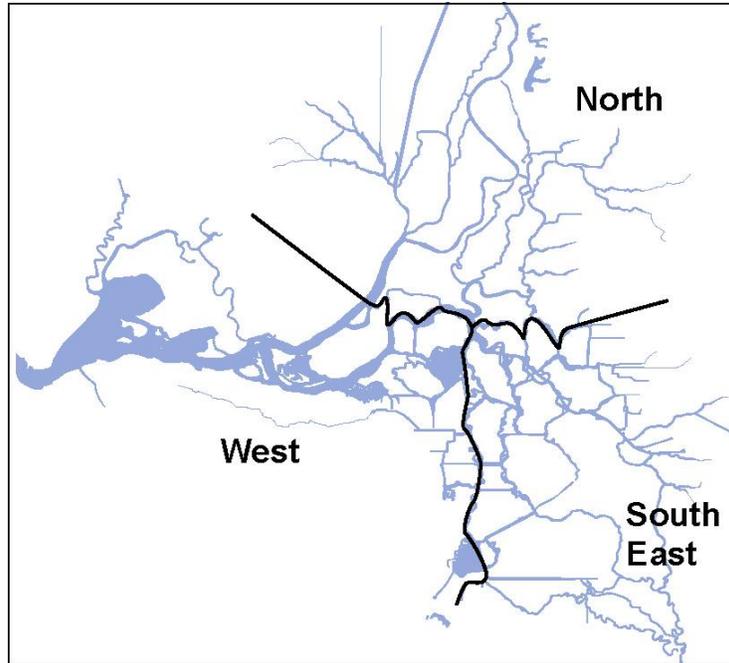


Figure 6.14: Regions for Different Corrections to the Practical Salinity of Agricultural Drainage.

6.3.6 Converting QUAL-Generated Practical Salinity to EC

Calibrating QUAL to practical salinity as calculated in Section 6.3.5 should result in dispersion factors appropriate for simulating transport of any conservative mass. However, Delta EC is still often needed for analysis and presentation of study results. Methods for converting from practical salinity back to EC were therefore explored. Expressing practical salinity in terms of EC requires two steps: removing the global correction to low practical salinity values that would be embedded in QUAL-generated values, then converting this practical salinity back to EC. Delta practical salinity with the correction removed is expressed by:

$$S_u = \frac{S - M_0}{M_1} \quad [\text{Eqn. 6-8}]$$

where S_u is uncorrected practical salinity, S is corrected practical salinity, M_0 and M_1 are as defined in Tables 6.2 and 6.3.

Poisson (1980) presents an equation for converting from practical salinity to EC (Equation 6-1). This equation is based on a set of samples diluted from standard seawater. A full-circle analysis can be done to validate the use of Equation 6-1: convert Delta EC to corrected practical salinity by Equation 6-7, convert to uncorrected practical salinity by Equation 6-8, and finally convert back to EC by Equation 6-1. Figure 6.16 shows the residuals of EC after performing this check. Errors in converting from practical salinity to EC range from 0 to 30 $\mu\text{S}/\text{cm}$. As mentioned before, Equation 6-1 was based on variations of standardized seawater. As an alternative approach, an equation was developed that directly relates EC from Delta samples and uncorrected practical salinity as calculated from the same EC data and Equation 6-5:

$$EC = h_0 + h_1 S_u^{1/2} + h_2 S_u + h_3 S_u^{3/2} + h_4 S_u^2 + h_5 S_u^{5/2} \quad [\text{Eqn. 6-9}]$$

where EC is electrical conductivity ($\mu\text{S/cm}$), S_u is uncorrected practical salinity, and:

$$\begin{aligned} h_0 &= -39.1632 \\ h_1 &= 170.6825 \\ h_2 &= 1953.7171 \\ h_3 &= -125.4956 \\ h_4 &= 11.5454 \\ h_5 &= -0.6103 \end{aligned}$$

A full-circle analysis with Equation 6-9 in shows that the equation reduces the maximum error to 2 $\mu\text{S/cm}$ (Figure 6.16). Combining Equations 6-8 and 6-9 then yields a method for converting QUAL-generated practical salinity in the Delta to EC:

$$EC = h_0 + h_1 \left(\frac{S - M_0}{M_1} \right)^{1/2} + h_2 \left(\frac{S - M_0}{M_1} \right) + h_3 \left(\frac{S - M_0}{M_1} \right)^{3/2} + h_4 \left(\frac{S - M_0}{M_1} \right)^2 + h_5 \left(\frac{S - M_0}{M_1} \right)^{5/2} \quad [\text{Eqn. 6-10}]$$

where S is QUAL-generated practical salinity, M_0 and M_1 are defined as in Table 6.2, and h_0 , h_1 , h_2 , h_3 , h_4 , and h_5 are defined as in Equation 6-9.

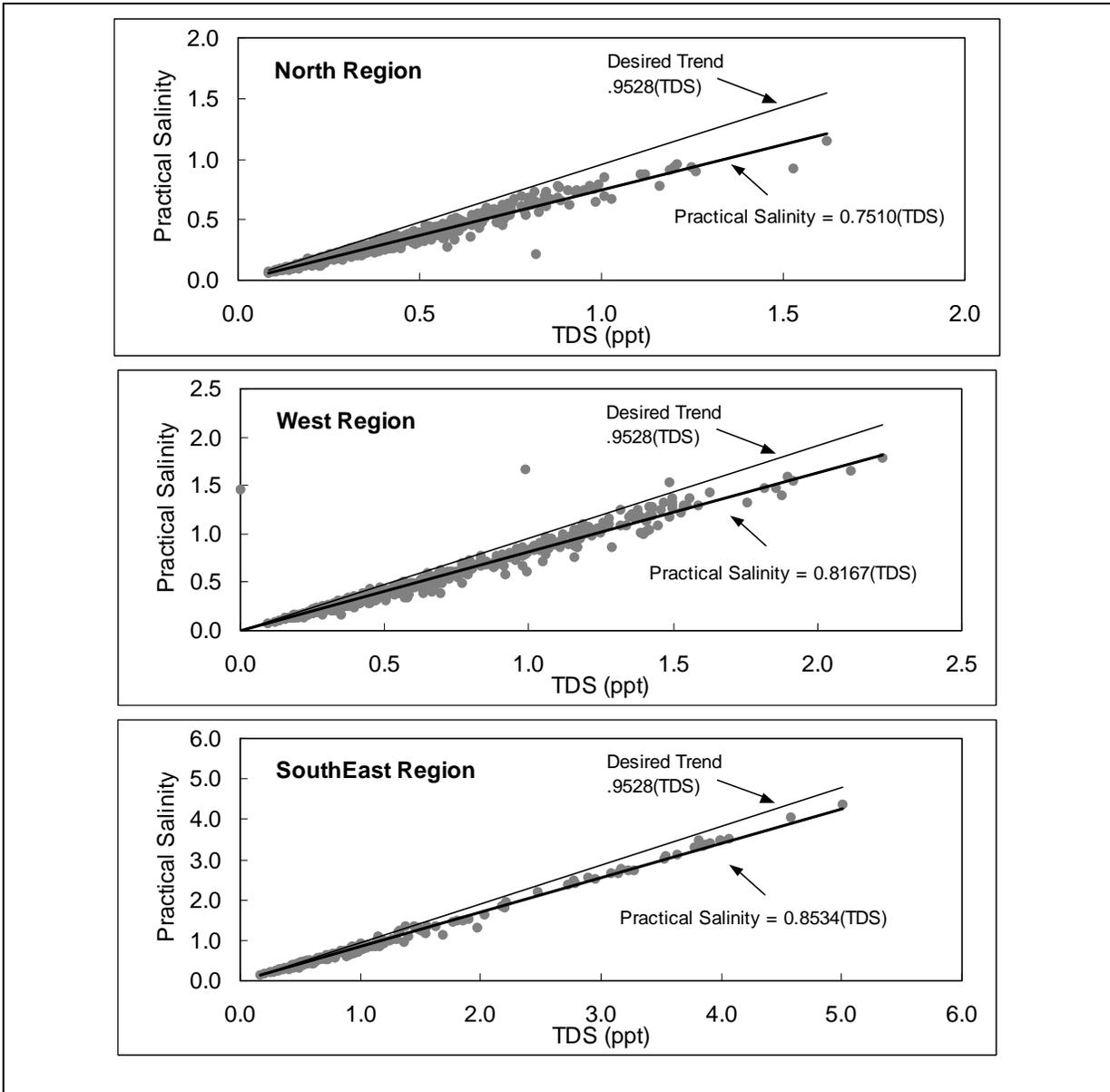


Figure 6.15: Needed Correction to Practical Salinity of Delta Agricultural Drainage.

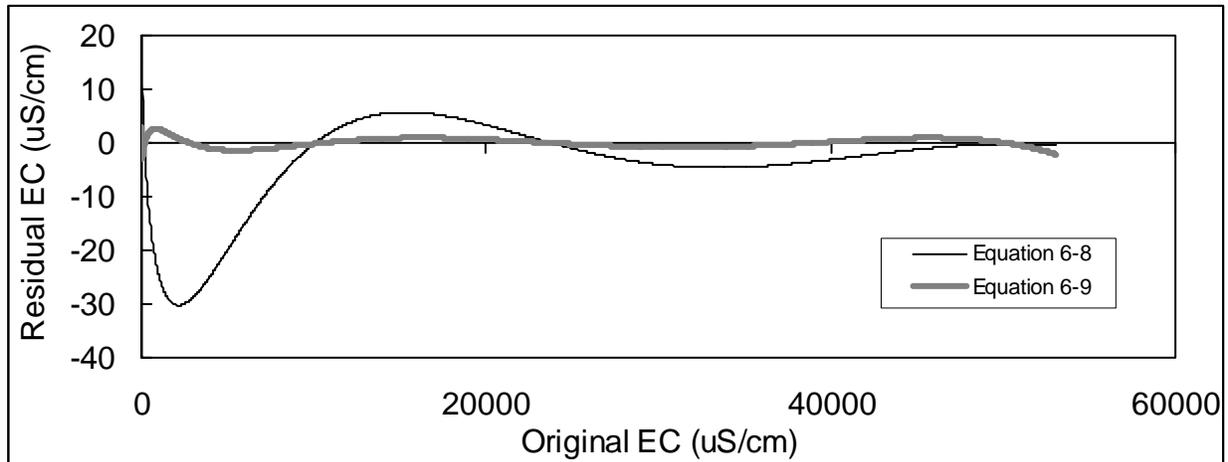


Figure 6.16: Residual in EC after EC - Corrected Practical Salinity - EC Analysis.

6.4 References

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