Extended report on CTD processing for ASCA0618

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1 Salinometer drift

Over the length of the cruise the measured double conductivity ratio (X2R) of standard seawaters drifted negatively by 0.00017, and this despite the apparent stability of the autosal salinometer (as indicated by the stability of the zero reference value and of the standby value). The X2R drift corresponds to a practical salinity drift of 0.003 PSU, larger than the required accuracy (0.002) and precision (0.001) for salinity for international standards. In addition, the mean of the X2R was 1.999738 rather than 1.99976, twice the K_{15} value of the standard seawater batch 159 used for standardizating the salinometer. As a consequence, regression analysis was used to derive a time-dependent linear correction for the linear drift and the offset (Figure 1). This correction is then applied to all X2R sample values.

Including duplicates, 136 sample values were corrected for the time-dependent salinometer drift. The histogram of all corrections for salinity values is shown in Figure 2.

2 Sample salinity calculation

For each sample, three salinometer readings were acquired. If any two readings of the three differed by more than 210^{-5} unit, additional readings were taken, up to a total of 6, until 3 consecutive readings did not differ by more than 210^{-5} pairwise. If such stability of the reading could not be achieved, the operator moved on to the next sample. Out of 149 samples run, this occurred for 13 samples which were eventually discarded for the final analyses. For each sample, the median value of the three X2R readings was taken as the final sample value. The impact of taking the mean value or the median value for each set of three readings is evaluated in Figure 3 for salinity values. Differences of practical salinity values are always less than 2×10^{-4} PSU.

Practical salinity values are computed from X2R values using a standard algorithm (`gsw SP salinometer` of the TEOS-10 Matlab toolbox), for a salinometer bath temperature of 24.5°C. The impact of calculating salinity for a bath temperature of 24°C or 25°C instead is evaluated in Figure 3. Differences of practical salinity values are always less than 2×10^{-4} PSU.

3 Salinometer precision

Duplicates samples is used to assess the replicability of salinometer measurements and hence the salinometer *precision*. Duplicates were taken for 9 CTD stations (1–5, 8–11) but the salinometer duplicate pair values for CTD stations 1 and 5 exhibited dubious values which had to be discarded. The six remaining useful pair values were examined as a function of pressure of the samples. Except for the samples taken near 1000 dbar, the differences of double conductivity ratio for the duplicates were at most 0.00004. This corresponds to salinity value differences less than 0.001 PSU, the required precision for salinity measurements (Figure 4). 1000 db corresponds to a level of fast changes for salinity and it is likely that vertical gradients within the Niskin bottle is responsible for the large difference of salinity between duplicates ($>$ 0.002 PSU).

4 Comparison and regression with CTD conductivity values

The salinity values of each sample are used to calculate the in-situ conductivity values of the samples using the `gsw C from SP` function of the GSW Matlab toolbox. Conductivity is a function of salinity, temperature and pressure. Two sets of values are computed, one using the temperature values from the first temperature sensor and a one using the temperature values from the second temperature sensor. The pressure values used are common to the two sets. The temperature and pressure values used for the calculation are derived from the 24 Hz CTD data, using averages of values acquired for two seconds (48 scan counts) from the initial scan count of each bottle closure. For 9 of the 113 calculated values the difference of conductivity is larger than 0.003 mS/cm, the expected initial accuracy of the CTD sensors (Figure 5). These sample values are discarded from the regression analyses used to correct the CTD conductivity. This exclusively occurs when the difference of temperature values between the two temperature sensors is larger than the expected initial accuracy of the CTD temperature sensor (0.001 K). For a number of values however, the temperature difference is larger than 0.001 K but the conductivity difference is smaller than 0.003 mS/cm.

Comparisons of salinometer and CTD conductivity values are examined as a function of conductivity values, pressure, time, and temperature (Figure 6). Linear regressions in each case indicate that the differences of conductivity value are significant function of conductivity, temperature, and pressure but not of time (or CTD station).

Following established methods, we decide to derive regression coefficients for the following correction model

$$C_c = \alpha C + \beta P + \gamma$$

with C conductivity and P pressure. The parameters α, β, and γ are derived for each of the two conductivity sensors by the least squares method, regressing CTD data against sample conductivity. After analyzing various models, based on adjusted R^2 and mean squared errors statistics, we find that a better model for both set of sensors is one for which $\gamma = 0$. A first calculation was conducted to obtain model parameters by least squares estimation. After analysis of the results, a number of data points for which the residuals were larger than or equal to two standard deviations were discarded before conducting a second calculation to obtain the final model parameters (Table 1). Graphical representations of the results are shown for conductivity values in Figure 7 and for salinity values in in Figure 7.

An estimate of the final error or uncertainty for conductivity is given by the square root of the mean square error ($\widehat{\sigma}$, Table 1). For both sensors this error is acceptable as it is less than 3×10^{-3} mS/cm, the nominal accuracy from the CTD specifications. We further estimate the final error, or uncertainty, for salinity by calculating the root mean square differences between sample salinity and in situ salinity. For both set of sensors this error is 0.003 PSU when rounded to 3 digits after the decimal point. This is unfortunately 50% larger than the required accuracy for salinity for international standards (0.002). However, for data points at pressure levels deeper than 2000db, the rounded error is 0.002 PSU, hence is acceptable. On average and most often (Figure 9) the uncertainty appears to be less for the first set of sensor which is therefore chosen to produce the final dataset.

	Sensor set #1	Sensor set #2
α	1.00004590384064	1.00001015838234
β	-4.82017943662524e-07	-6.44091892442368e-07
$\widehat{\sigma}$ Conductivity (mS/cm)	0.00251	0.00253
$\widehat{\sigma}$ Salinity (PSU)	0.00273	0.00280
$\widehat{\sigma}$ Salinity (PSU) P>2000 dbar	0.00246	0.00247
$\widehat{\sigma}$ Salinity (PSU) P<2000 dabr	0.00300	0.00313

Table 1: Results from second regression for conductivity and salinity.

5 Influence of salinity bottle type

A comprehensive analysis of the influence of the salinity bottle type will be conducted once the data from the DEA bottles are obtained.

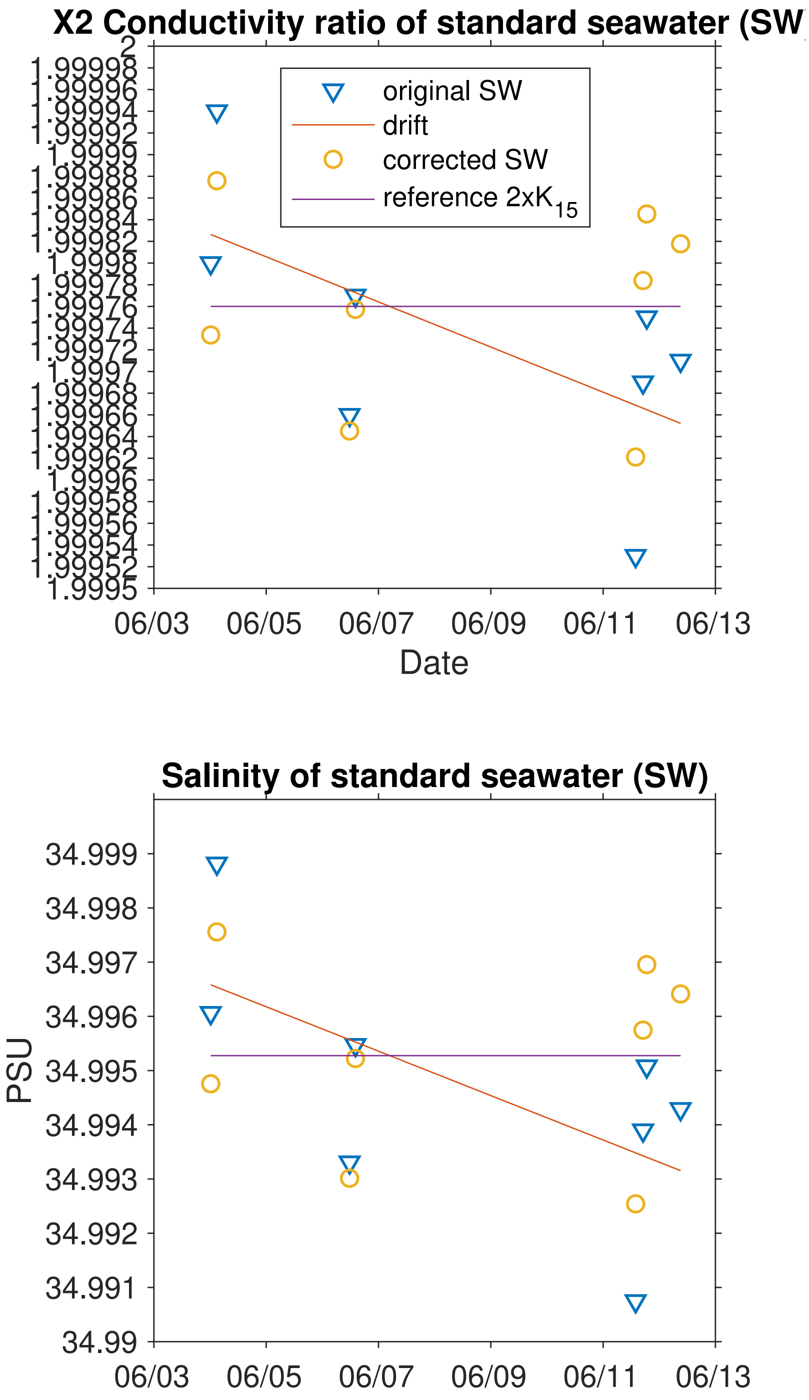

Figure 1: top: double conductivity ratio for standard seawaters showing original values, the drift estimate, the corrected values, and the reference $2 \times K_{15}$ value. bottom: after conversion to practical salinity values.

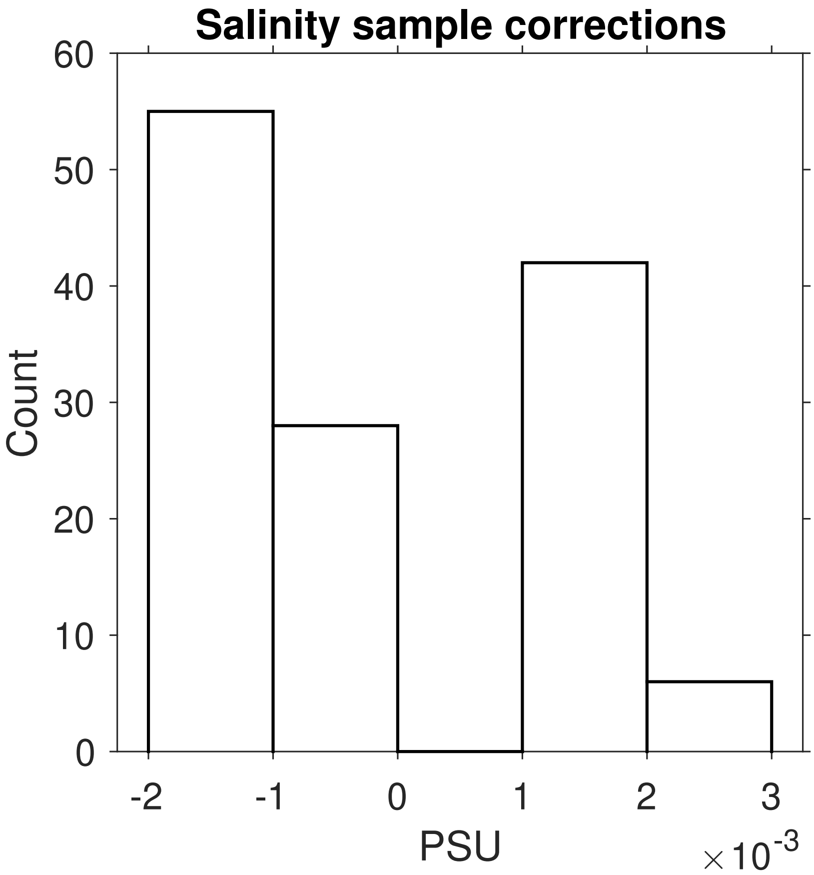

Figure 2: Histogram of salinity corrections for drift and offset. Histogram bins are of 0.001 width but the actual corrections can be smaller.

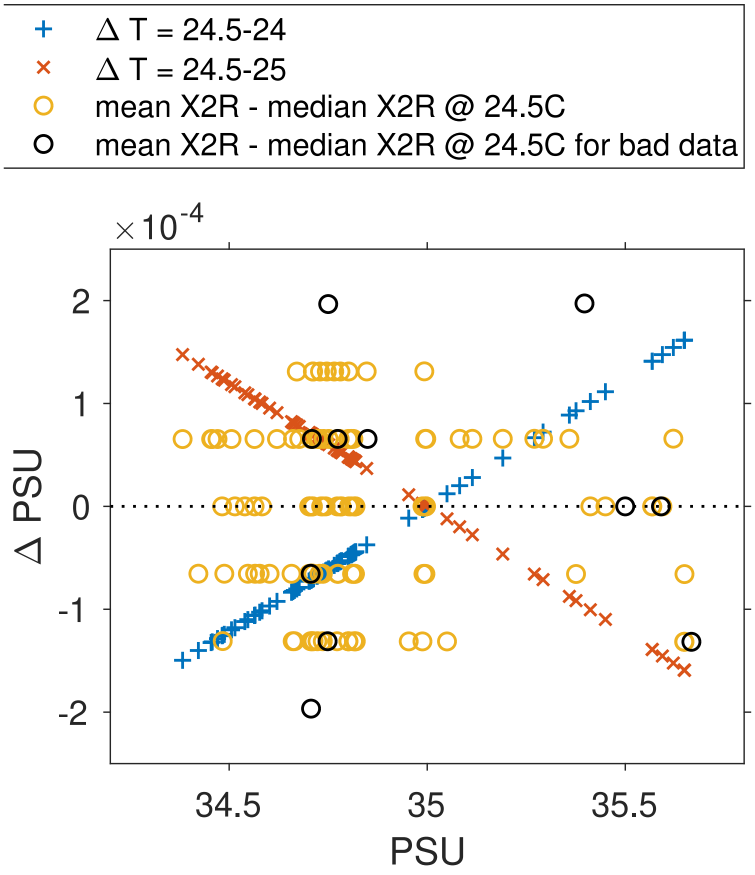

Figure 3: Salinity differences by varying the set temperature of salinometer bath and the method to compute X2R.

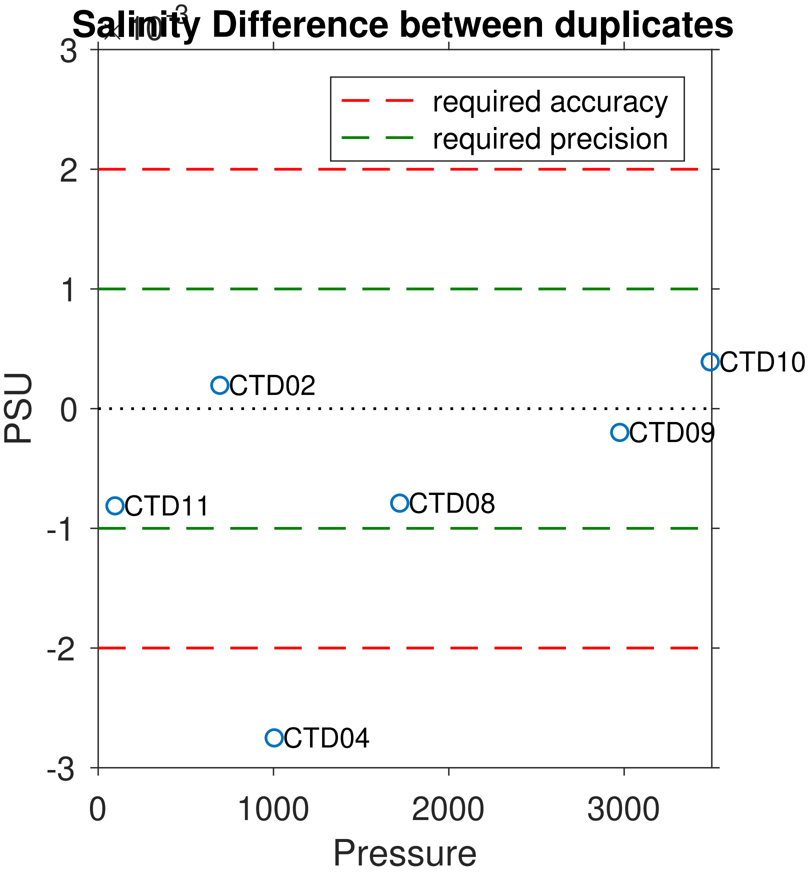

Figure 4: Salinity duplicates differences as a function of pressure.

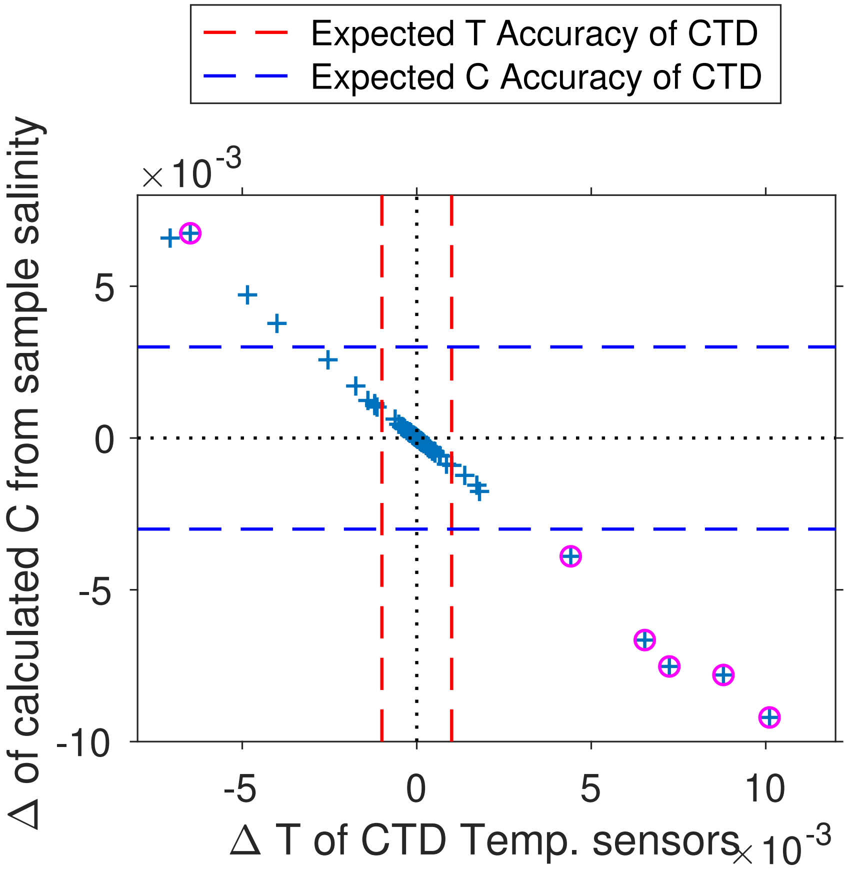

Figure 5: Differences of calculated conductivity of samples as a function of temperature differences between the sensors.

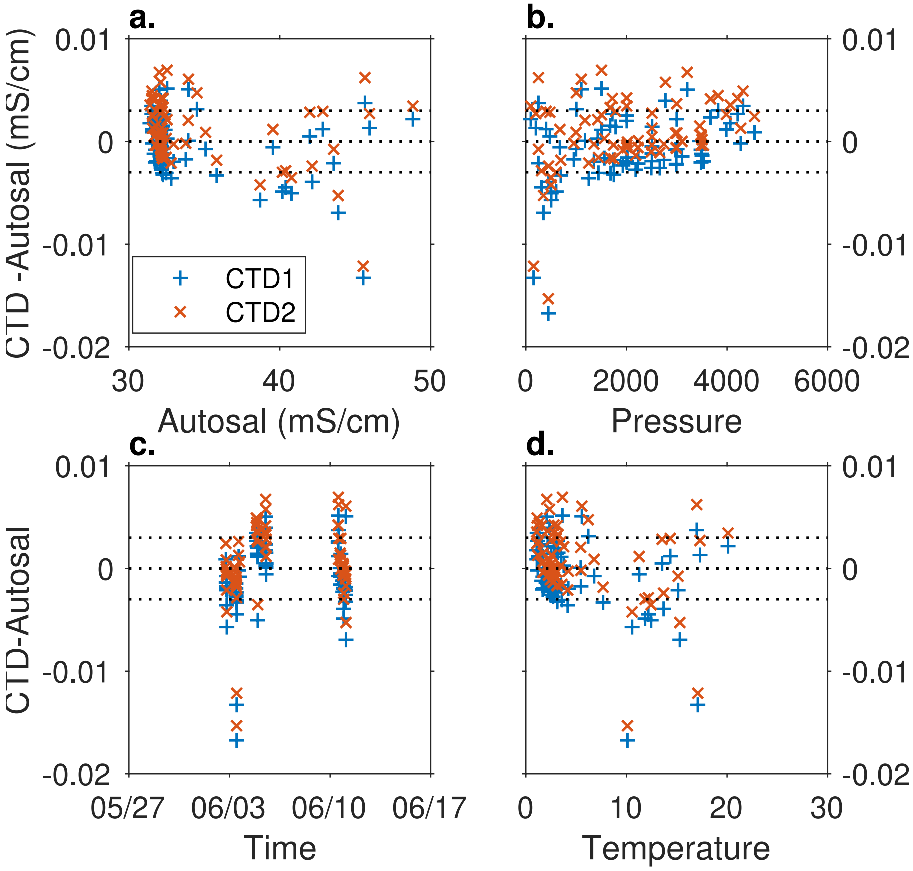

Figure 6: Conductivity differences between salinometer values and CTD values as a function of conductivity values (a), pressure (b), time (c), and temperature (d).

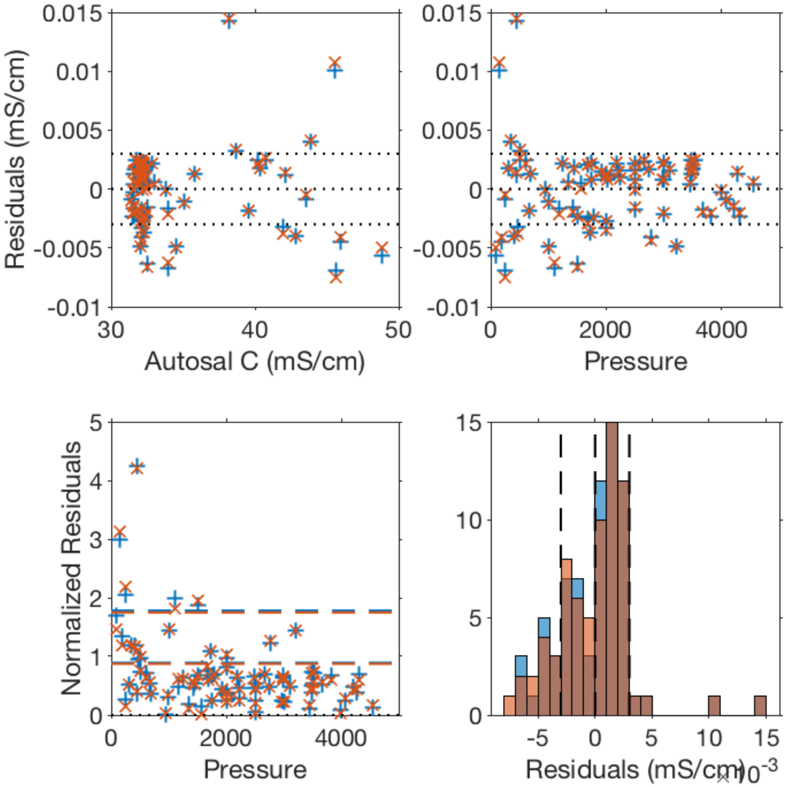

Figure 7: Results of regressions for conductivity

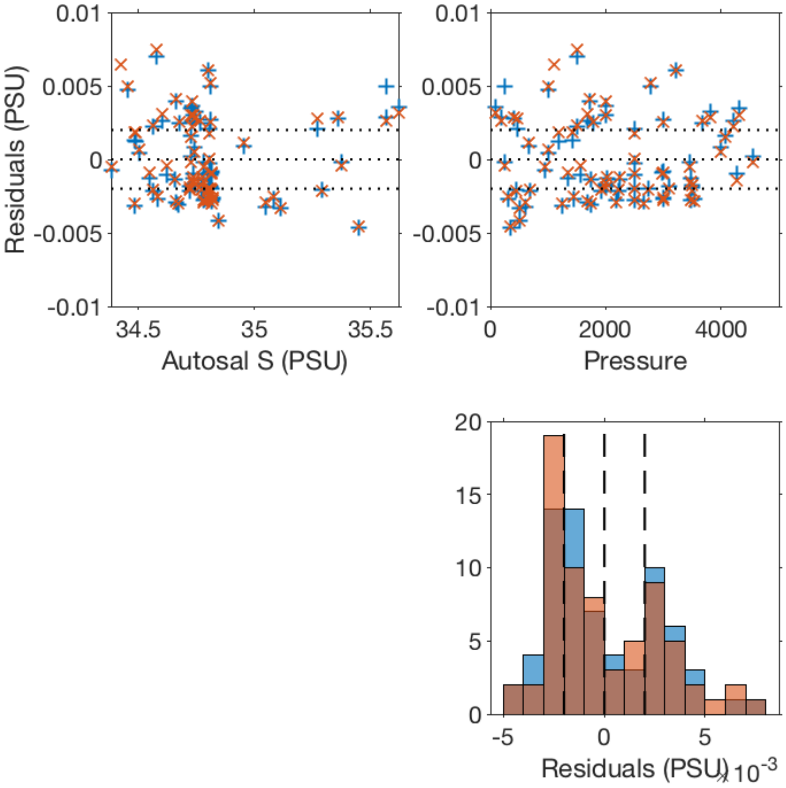

Figure 8: Results of regression for salinity

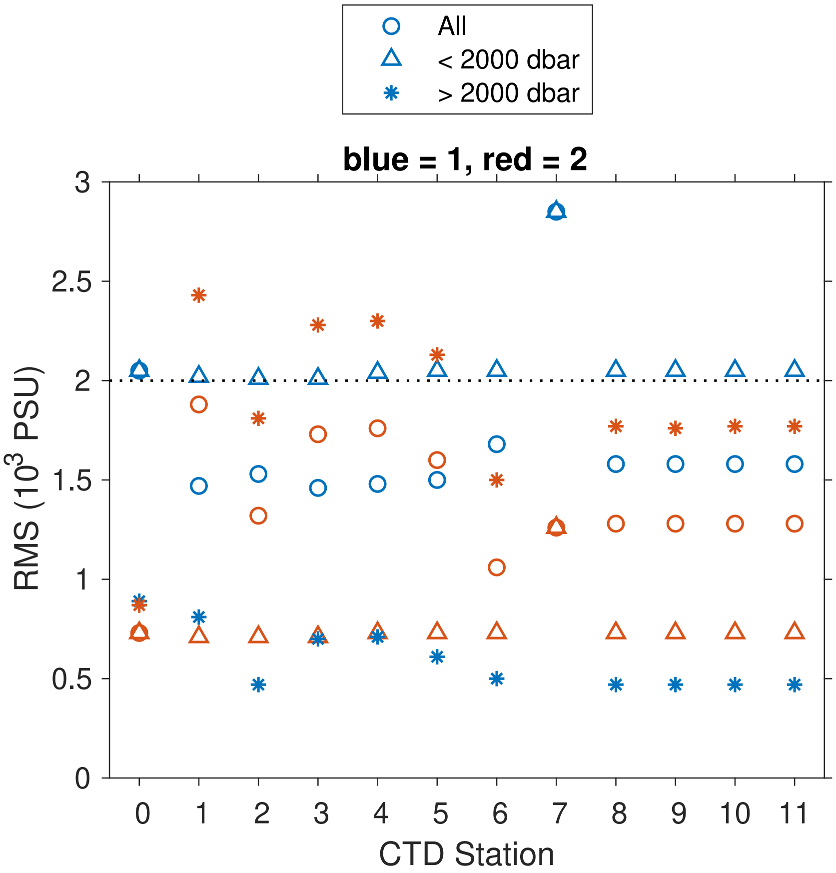

Figure 9: RMS of Salinity errors per on CTD station for first set of sensors (1) and second set of sensors (2).

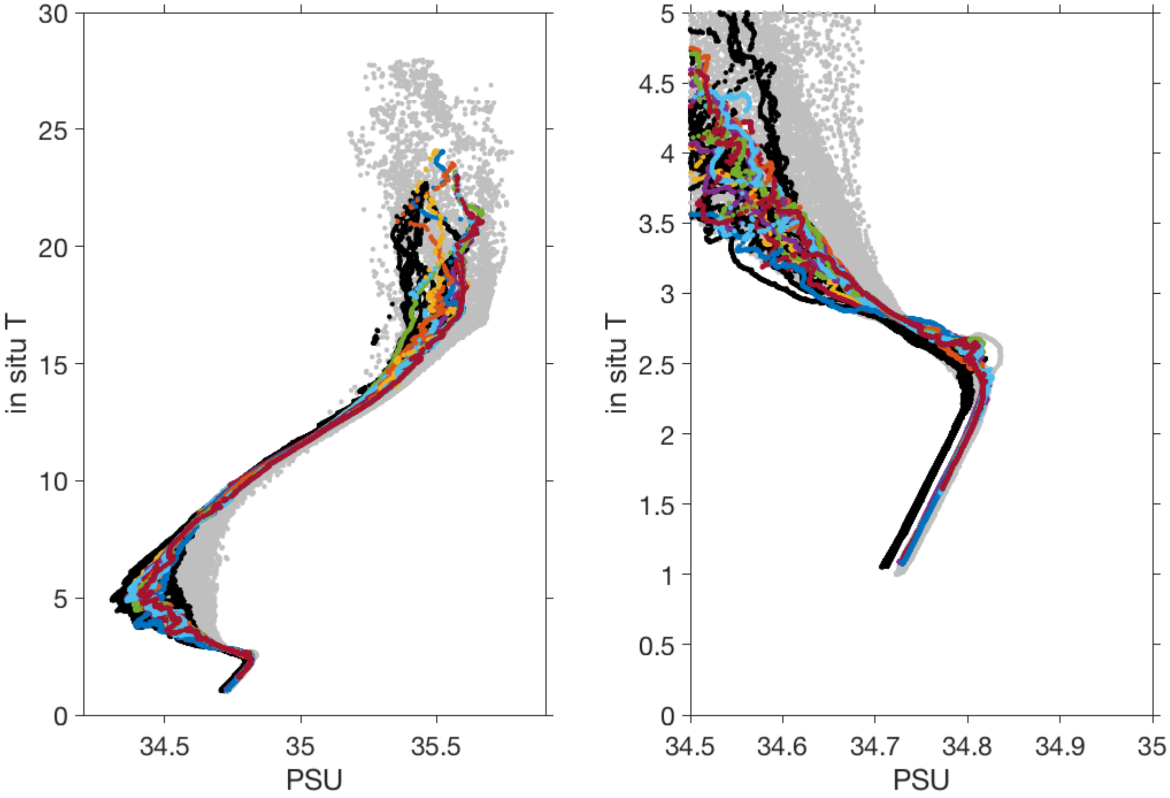

Figure 10: T-S diagram for the final ASCA0618 data (one color per CTD station). Theblack points correspond to the July 2016 ASCA data. The gray points correspond to historical AUCE and ACT CTD data. The right panel is a close-up for deep water masses.