Systematic Adjustments of Hydrographic Sections for Internal Consistency*

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ABSTRACT

A significant legacy of the World Ocean Circulation Experiment (WOCE) is the large number of high quality, high-resolution, full-depth, transoceanic hydrographic sections occupied starting in the mid-1980s. The section data provide an unprecedented survey of World Ocean water properties. Most stations sampled pressure, temperature, salinity, dissolved oxygen, and nutrients (nitrate, phosphate, and silicic acid) at up to 36 depths. While the WOCE Hydrographic Program (WHP) strenuously advocated employing standardized measurement techniques on all sections, small but significant systematic differences among cruise legs are found. A simple method for adjusting measurements to maximize internal consistency is presented and applied to available WOCE data in the Pacific Basin. First, the sections are broken into distinct cruise legs between port stops. Then, crossovers are identified where two different cruise legs cross or approach each other. Using hydrographic data from each cruise leg near each crossover, linear fits are made of properties on potential temperature surfaces against distance along cruise track. These fits are then used to evaluate property differences and their uncertainties at crossovers. A set of least squares models are used to generate sets of adjustments, with related uncertainties, for all the properties of each cruise leg. These adjustments minimize differences of water properties among cruise legs at the crossovers in a least squares sense. The adjustments can be weighted by difference uncertainties, and damped by a priori estimates of the expected differences. Initial standard deviations of crossover differences are 0.0028 for salinity, 2.1% for oxygen, 2.8% for nitrate, 1.6% for phosphate, and 2.1% for silicic acid. The adjustments roughly halve these values, bringing cruise legs into agreement within WHP target accuracies.

1. Introduction

In the Pacific Ocean, scientists involved in the World Ocean Circulation Experiment (WOCE) Hydrographic Program (WHP) one-time survey occupied a large number of high quality, high-resolution, full-depth, transoceanic hydrographic sections from 1985 through 1996 (Fig. 1). We set out to use all of these sections in an inverse model incorporating the basic hydrographic properties (temperature, salinity, dissolved oxygen, nitrate, phosphate, and silicic acid). The inclusion of both zonal and meridional sections in the model resulted in at least one novel feature. We were dividing the Pacific Ocean into a large number of small boxes, some of which had no coastal boundaries at all. Property anomalies on dense neutral surfaces (Jackett and McDougall 1997) around the edges of these boxes sometimes showed large jumps at box corners where sections crossed. These jumps suggested that on the relatively small scales of individual boxes, cruise-to-cruise measurement biases might be overwhelming the true property gradients in the deep water. This situation was troublesome, so we decided to adjust the measurements for internal consistency, as detailed below.

An example of the problem and its amelioration is shown here for motivation. Unadjusted oxygen values (Fig. 2, ☆'s) interpolated to $\theta = 2°C$ around a small box of stations from different cruise legs on each side in the subtropical South Pacific (Fig. 1, stations immediately surrounding the ☆) exhibit large jumps at three out of four box corners (Fig. 2, vertical dotted

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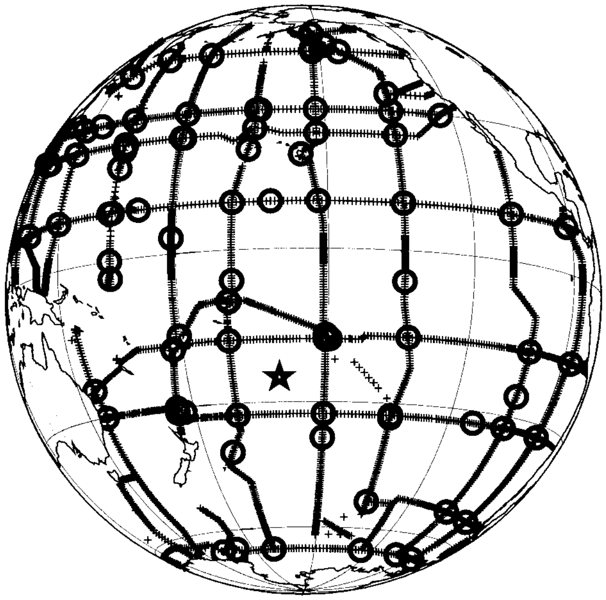

FIG. 1. Pacific WOCE Hydrographic Program one-time survey station locations (+'s) with crossover locations (thick ○'s), and Fig. 2 analysis location (☆).

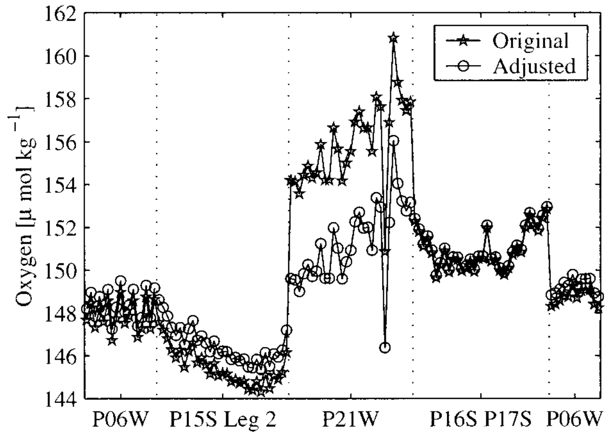

FIG. 2. Select station oxygens interpolated to $\theta = 2°C$, both original (☆'s) and with WLSQ adjustments from section 4 applied (○'s). Values plotted from left to right correspond to a clockwise procession around the box of stations immediately surrounding the ☆ in Fig. 1, starting from the bottom center of that box. Box corners (dashed vertical lines) separate cruise legs (designated at plot base) along the box edges.

lines) where one cruise leg meets another. Applying weighted least squares (WLSQs) adjustments from section 4 to the data from each cruise leg (Fig. 2, ○'s) greatly reduces the magnitude of the larger jumps. Of course, the jumps are not entirely eliminated locally because they have been minimized basin-wide in an overdetermined system.

There have been many attempts to adjust water properties when combining data from different sources. A review of the various adjustment methods is found in a paper describing a South Pacific hydrographic climatology produced by combining WOCE and high quality historical hydrographic data (Gouretski and Janke 1999). Adjustment schemes range from ''allowances were made in contouring'' (Wyrtki 1971) to more recent work using least squares techniques (Gouretski and Janke 1999, 2001; Gouretski 1999). The work described here takes this least squares approach the next logical steps. It incorporates uncertainties for each crossover difference as well as initial estimates of probable magnitudes of cruise-to-cruise bias. The robust estimates for the uncertainties of the adjusted fields available from the technique are also presented.

Here we estimate differences of basic hydrographic properties (nitrate, phosphate, silicic acid, dissolved oxygen, and salinity) among the WOCE cruise legs in the Pacific Ocean. We apply a hierarchy of least squares models to obtain adjustments to these properties for each cruise leg so as to minimize these differences in a least squares sense. These models can incorporate weighting by the uncertainties of differences at crossovers. In addition, the models can be damped by a priori expectations of the size of the differences. The models return uncertainties associated with these cruise adjustments. Data reduction is documented in the next section, then the models are outlined, then the results are presented. The paper ends with a short conclusion.

2. Data reduction

Hydrographic data from each cruise were separated into cruise legs, which were defined as stations occupied by a single ship between port stops. Subdivision by cruise legs allows for any changes in analysts, equipment, or standards during port stops. There were 47 cruise legs in the Pacific Ocean for which data were available and a crossover was present. These legs are designated hereafter by the index *n*. It was assumed that there was negligible variability in both measurement accuracy and precision during each cruise leg, but that there might be significant differences in either accuracy or precision among cruise legs. In other words, the models assumed that a single adjustment and associated uncertainty for each property on each cruise leg was appropriate.

The next step was to identify where cruise legs crossed or approached one another within 200 km. Every such pair of adjacent cruise legs was designated a crossover. The crossover points were located at the intersections of the cruise legs. The station groups for each cruise within 350 km of each crossover point were examined. A few stations with obvious outlying data were rejected. A few more stations were rejected as not representative of deep hydrographic conditions at their respective crossover points (for instance when they were in a different deep basin from their crossover point). After this process any crossover group with less than three stations from either cruise was eliminated from the analysis. The remaining 111 crossovers (Fig. 1) had between 3 and 38 stations (a mean of 10) for each cruise leg. Crossovers are represented by the index *o*.

This 350-km distance from crossover points strikes a balance between including enough stations in groups for good statistics and keeping within regions of relatively uniform deep water properties. There are three factors to keep in mind. First, the length-scale chosen is suited to the deep Pacific Ocean, with its relatively large basins and homogenous water property distributions. Second, the groups were screened for data not representative of deep hydrographic conditions at crossover points. Third, the linear fits to the data versus distance, as described below, accounted for regional trends in water properties. Finally, at crossover points where the deep water properties were variable over this distance, the fits had an appropriately large uncertainty. Hence these crossover differences had a reduced weighing in the more sophisticated models used.

Water properties at these stations were interpolated on a grid of potential temperature θ surfaces by a local shape-preserving spline (Akima 1970). A rather large set of 98 θ surfaces, designated by the index *p*, were chosen to span the full oceanographic temperature range and to ensure that there were surfaces between every water sample. The analysis was carried out on θ surfaces, rather than potential or neutral density surfaces, for three reasons. First, θ is the most accurately measured hydrographic quantity in terms of signal-to-noise ratios. The assumption was made that the pressures and temperatures were so accurate that they could be assumed to be correct for our purposes. Second, θ is the natural coordinate for evaluating salinity, *S*, differences since θ and *S* are the two components in the equation of state. Third, this choice keeps the evaluations of all fields independent of errors in S, which would result in density errors. Finally, while water flow more closely follows potential density than θ, over the relatively small groups of stations within 350 km of the crossover points the deep θ–*S* relation is relatively constant, meaning that there is little practical difference between using θ and potential density at depth.

Following the interpolation in θ, each property for the crossover station group *o* from each cruise leg *n* was subject to a linear fit versus distance along the cruise track from the crossover location on each θ surface *p*. These fits, $P(n, o, p)$, were then evaluated at the crossover locations, along with their uncertainties, $\sigma(n, o, p)$. Crossover locations and distances along cruise tracks were chosen so that the fits were evaluated in the middle of their station groups whenever possible. The result was a set of concentrations and associated uncertainties for each cruise leg pair at the 111 crossovers on as many as 98 θ surfaces for the five hydrographic properties analyzed.

At this point, the analysis diverged for salinity versus all the other properties. A decision was made to correct salinity by means of additive offsets for each cruise leg. This decision was made because it seemed most likely that systematic salinity errors, including batch differences among standard sea water, would appear mostly as offsets. At each crossover *o* and θ surface *p*, the salinity differences, $d(o, p) = P(n_1, o, p) - P(n_2, o, p)$, and their uncertainties, $\sigma(o, p) = [\sigma(n_1, o, p)^2 + \sigma(n_2, o, p)^2]^{0.5}$, were calculated, where the subscripts refer to the two cruise legs at the crossover. This last equation reflects the assumption made that uncertainties of the salinity fits for each cruise at a crossover were uncorrelated when calculating the uncertainties for their differences.

The other property adjustments, for oxygen and nutrients, were made using multiplicative scale factors applied to each cruise leg. The reasoning for this decision was severalfold. First, multiplicative factors help avoid the potential problem of negative values in the nutrient-poor surface layers and anoxic regions after adjustments are applied. Second, the dominance of multiplicative corrections is at least plausible, presuming that standardization errors are the main problem in accuracy, although this assumption may not always hold (Ross et al. 1999). Finally, in deep regions of tight property–θ relations where oxygen and nutrient concentrations are often relatively high and uniform, additive and multiplicative adjustments are nearly indistinguishable. Proceeding for the other properties at each crossover *o* and θ surface *p*, differences were calculated as deviations of ratios from unity, $f(o, p) = P(n_1, o, p)/P(n_2, o, p) - 1$, and their uncertainties as $\sigma(o, p) = \{[\sigma(n_1, o, p)/P(n_1, o, p)]^2 + [\sigma(n_2, o, o)/P(n_2, o, p)]^2\}^{0.5}$. The latter equation states that the uncertainties were normalized by property concentrations. These simple transformations allowed application of the same least squares method used to adjust salinity for internal consistency to all of the other properties.

For each crossover *o* the salinity differences and associated uncertainties on all *p* θ surfaces were used to estimate a single weighted difference $d(o)$ as follows:

$$d(o) = \frac{\sum_{p=1}^{98} d(o, p)/(\sigma(o, p))^2}{\sum_{p=1}^{98} 1/(\sigma(o, p))^2}. \qquad (1)$$

The use of the inverse of standard deviations squared is standard practice in weighted least squares estimations (Beers 1957). Similarly, a weighted uncertainty $\sigma(o)$ was calculated substituting $\sigma(o, p)$ for $d(o, p)$ and $\sigma(o)$ for $d(o)$ in (1). For all the other properties, the deviations of ratios from unity, $f(o, p)$, and their uncertainties, $\sigma(o, p)$, on all *p* θ surfaces were similarly used to estimate a single weighted deviation of ratio from unity, $f(o)$, and associated uncertainty, $\sigma(o)$, at each crossover, using equations analogous to (1). (From here on crossover ''differences'' will refer to arithmetic biases for salinity and deviations of ratios from unity for the other water properties.) The weights allowed the θ surfaces with larger signal-to-noise ratio to dominate the differences. This dominance generally meant that while differences and associated errors were estimated using information over

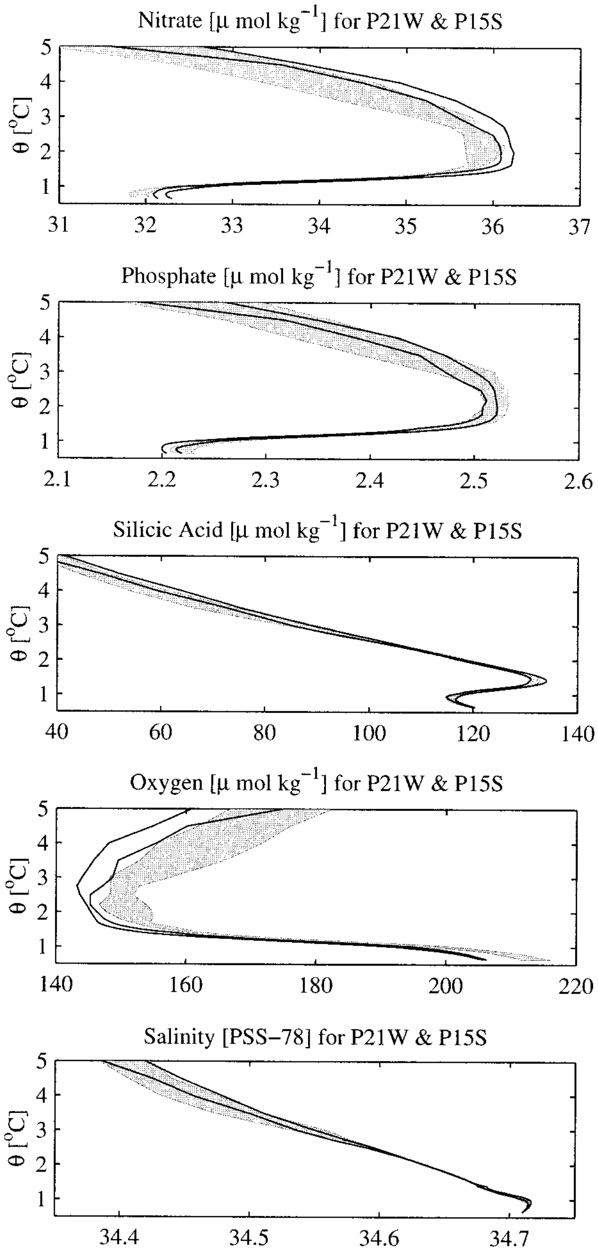

FIG. 3. Property envelopes as a function of potential temperature at the crossover of P21W and P15S Leg 2 (located at 17.5°S, 170°W) from linear fits and their uncertainties (shaded regions for P21W and regions between the two thicker lines for P15S Leg 2).

the entire water column, the deeper parts of the water column where the signal-to-noise ratio was highest were most influential in determining the crossover differences and associated uncertainties.

The crossover of P21W and P15S Leg 2 (located at 17.5°S, 170°W) is illustrative. Property envelopes for the two cruises (based on uncertainties about the means at the crossover point from the linear fits) as a function of potential temperature below 5°C show the influences of several water masses (Fig. 3). The relatively cold, salty, oxygen-rich, nitrate and phosphate-poor, and silicic acid-rich northward spreading Circumpolar Deep Water (CDW) is found near the bottom. Within this water mass the subtle differences between slightly more nutrient-rich Antarctic Bottom Water (AABW) found below 1°C and the saltier North Atlantic Deep Water (NADW) just above can be discerned. Farther up in the water column, between 1.5° and 3°C are the nutrient maxima and oxygen minimum that characterize the southward spreading Pacific Deep Water (PDW). By 5°C the predominant influence is of the relatively fresh, nutrient-poor, and oxygen-rich Antarctic Intermediate Water (AAIW).

The property ratios and salinity differences with associated uncertainties at the crossover (Fig. 4) further highlight some important points. The property difference uncertainties (dominated by lateral oceanographic variability) generally increased with temperature. These uncertainties became so large higher in the water column that crossover differences there made no real contributions to the weighted crossover mean differences and their associated uncertainties. Above 2.5°C the differences (lower nutrients, higher oxygens, and lower salinities) all suggested a stronger AAIW signature in P21W compared to P15S leg 2. However, all the properties had relatively constant differences between the two cruise legs and small uncertainties from the bottom up to about 2.5°C. That these differences were relatively constant across the contrasting property signatures of AABW, NADW, and PDW suggests that the method is reliably estimating the cruise-to-cruise differences at crossovers. For nitrate the derived ratio of 0.992 was further away from unity than its uncertainty, indicating that the P21W nitrates were significantly lower than the P15S nitrates at this crossover point. For phosphate and silicic acid the ratios were indistinguishable from unity. The mean oxygen ratio of 1.038 was larger than the uncertainty, suggesting P21 oxygens were significantly higher than those from P15S. Salinity differences were not distinguishable from zero. (Salinity values are unitless and reported on the 1978 Practical Salinity Scale, PSS-78. Here the salinity differences are quoted at 1000 times PSS-78, that is, roughly in parts-per-million, or ppm.) Interestingly, the silicic acid and salinity uncertainties both had a local maximum near 1.2°C. This crossover location exhibited a strong contrast of NADW and PDW influences, owing to the nearby deep western boundary current flowing northward along the Tonga Ridge, hence high natural variability at this level.

3. Least squares adjustments

The next step was to use these crossover differences and associated uncertainties for each property to determine property adjustments for each cruise leg that would maximize consistency among the cruise legs at crossovers. These adjustments were determined by a hierarchy of least squares models (Menke 1984; Wunsch 1996). The models were formulated to determine the

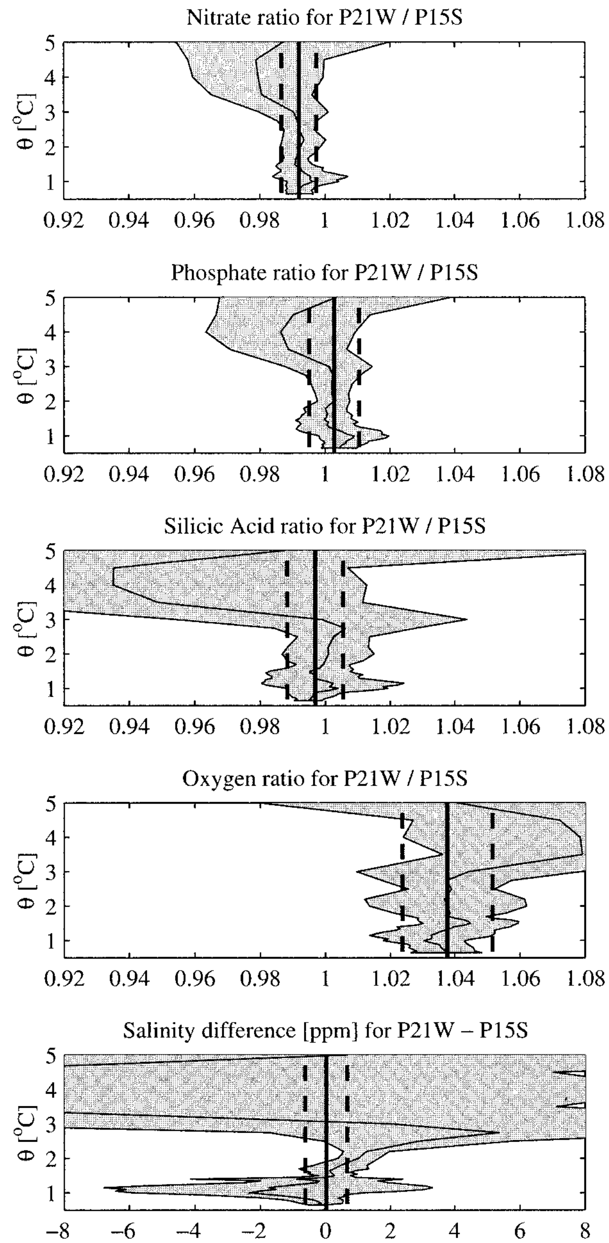

FIG. 4. Property ratios and salinity differences (thin solid lines horizontally centered in shaded regions) for the crossover of P21W and P15S Leg 2 (located at 17.5°S, 170°W) plotted with uncertainties (shaded regions) as a function of potential temperature below 5°C. Mean uncertainty-weighted ratios or differences (thick solid vertical lines) and their associated uncertainties (thick dashed vertical lines) mostly reflect the deeper values with smaller uncertainties.

adjustments for that property to apply to each cruise leg that would minimize the crossover differences in a least squares sense.

The model matrix, **G**, was $o = 111$ by $n = 47$, with the 111 rows being crossovers and the 47 columns cruise legs. Since there were more constraints (111) than unknowns (47), the system was overdetermined. In each row of **G** there were zeroes except for a single $+1$ located in the column of the first cruise leg at that crossover and a single -1 in the column of the second cruise leg at that crossover. The data vectors, $\mathbf{d}(o)$ or $\mathbf{f}(o)$, were columns o elements long which consisted of the property crossover differences. The model solution vectors, $\mathbf{m}$, were n elements long, and represented the cruise leg additive corrections (for salinity after a sign change) or multiplicative corrections (for the other properties after subtraction from unity). That is to say, for salinity, corrections would be applied as $P_{\mathrm{corr}}(n) = P_{\mathrm{orig}}(n) + [-\mathbf{m}(n)]$ and for the other properties, as $P_{\mathrm{corr}}(n) = P_{\mathrm{orig}}(n)[1 - \mathbf{m}(n)]$. Here the subscript orig denotes the original property values for a given cruise leg n, the subscript corr denotes the corrected values for that cruise leg, $\mathbf{m}(n)$ the appropriate term of the solution vector, and the terms in square brackets are the additive or multiplicative corrections reported in the next section.

The system and its solution are given by

$$\mathbf{G} \cdot \mathbf{m} = \mathbf{d}, \quad \text{so} \quad \mathbf{m} = \mathbf{G}^{\mathrm{T}} \cdot (\mathbf{G} \cdot \mathbf{G}^{\mathrm{T}})^{-1} \cdot \mathbf{d}. \qquad (2)$$

This model has also been used for cruise adjustments by Gouretski and Janke (1999, 2000). A model of this form estimates cruise leg adjustments regardless of how well the crossover differences were determined or any a priori expectations of what these adjustments should be. This model will be referred to a simple least squares (SLSQ).

One aspect of SLSQ not used in previous work on cruise adjustments is the model solution covariance matrix,

$$\mathrm{cov}\mathbf{m} = \sigma_d^2(\mathbf{G}^{\mathrm{T}} \cdot \mathbf{G})^{-1}. \qquad (3)$$

Here σ_d^2 is the variance of the crossover difference residual. The model solution covariance matrix reflects how many crossovers influence the adjustment for a cruise leg, and is scaled by the residual variance. The square root of the diagonal elements of the model solution covariance matrix give the model solution uncertainties. We calculated these solutions and their associated uncertainties for purposes of comparison with the other more sophisticated models outlined below.

A second model incorporates information on how well individual crossover differences were determined and weights the solution by these factors. This model will be referred to as weighted least squares (WLSQ). For this model the appropriate uncertainties $\sigma(o)$ for each crossover difference are used for the weighing, or data covariance matrix, **W**. This **W** matrix is a diagonal o by o matrix with the inverse of each crossover uncertainty, $\sigma(o)$, in the appropriate location: $\mathbf{W}_{ii} = \sigma_i^{-1}$. The solution for this problem is

$$\mathbf{m} = (\mathbf{G}^{\mathrm{T}} \cdot \mathbf{W} \cdot \mathbf{G})^{-1} \cdot \mathbf{G}^{\mathrm{T}} \cdot \mathbf{W} \cdot \mathbf{d}, \qquad (4)$$

and the model solution covariance matrix is

$$\mathrm{cov}\mathbf{m} = (\mathbf{G}^{\mathrm{T}} \cdot \mathbf{W}^2 \cdot \mathbf{G})^{-1}. \qquad (5)$$

Again the square root of the diagonals of the model solution covariance matrix gives the solution uncertainty. This time, the adjustment uncertainties for a given cruise are influenced by crossover locations and how well the differences are determined at each crossover. Crossover differences with smaller uncertainty (owing to more data or less local oceanographic variability) are allowed greater weight in influencing the adjustments. With the crossover difference uncertainties incorporated into the model, the overall crossover residual variance is no longer needed to scale the model covariance matrix.

The final model uses weighted damped least squares (WDLSQ). It uses the same data covariance matrix, $\mathbf{W}$, as WLSQ. However, it also incorporates a model covariance matrix, $\mathbf{E}$. The model covariance matrix is a square n by n matrix which incorporates a priori information regarding the expected magnitude of adjustments among cruises. This knowledge reflects the expected reproduceability of measurement accuracy for different analysts using different laboratory equipment. We used the squares of the expected root mean square accuracies for each given property measurement as the diagonal elements of this matrix. We could have assigned a different model error for each cruise leg and each property; however, such an assignment would have been quite subjective. The WHP one-time survey standards were 1% for nitrate, 1%–2% for phosphate, 1%–3% for silicic acid, 0.5% for oxygen, and 2 ppm (or 0.002 PSS-78) for salinity (WHPO 1994). We asked two experts for their guesses at accuracies of the final WOCE data set and they gave similar answers (A. Mantyla and B. Warren 1999, personal communications). The values used here (squared before insertion along the diagonal) were 4 ppm for salinity and 2% for everything else. These somewhat pessimistic model error estimates reflect the fact that the WOCE Pacific one-time survey data originated from several different observational groups employing a variety of measurement techniques and instrumentation with a range of expertise.

With the matrices for the model $\mathbf{G}$, the data covariance $\mathbf{W}$, the model covariance $\mathbf{E}$, and the data vector $\mathbf{d}$ (or $\mathbf{f}$) all determined, the solution $\mathbf{m}$ for WDLSQ is given by

$$\mathbf{m} = \mathbf{E} \cdot \mathbf{G}^{T} \cdot (\mathbf{G} \cdot \mathbf{E} \cdot \mathbf{G}^{T} + \mathbf{W})^{-1} \cdot \mathbf{d}. \quad (6)$$

A comparison of (6), (4), and (2) shows that the solutions to these various models incorporate first only the model matrix, then the data covariance, and finally the model covariance. In addition to a solution vector, a solution covariance matrix can be determined from

$$\mathrm{cov}\mathbf{m} = \mathbf{E} - \mathbf{E} \cdot \mathbf{G}^{T} \cdot (\mathbf{G} \cdot \mathbf{E} \cdot \mathbf{G}^{T} + \mathbf{W})^{-1} \cdot \mathbf{G} \cdot \mathbf{E}. \quad (7)$$

WDLSQ incorporates the most information into the solution and solution covariance, and is thus arguably the best model (provided the a priori estimate of the model covariance matrix is close to reality).

4. Results

Differences at crossover locations can only be robust measures of actual cruise-to-cruise biases if they exceed the uncertainties of the estimates. The uncertainties of differences determined at each of the crossovers were generally quite small. The median values for the uncertainties were about 0.9%, 1.2%, 1.2%, 1.2%, and 1.1 ppm for nitrate, phosphate, silicic acid, oxygen, and salinity, respectively. Mean values for the uncertainties were about 1.3 times the median values, which reflected the presence of greater uncertainties at a few crossovers for each water property. The uncertainty was a combination of measurement precision and sampling error. Some of the high uncertainties were due to a lack of data in the stable low-gradient deep waters, because some crossover points were located in shallow waters. Other instances of high uncertainties were the result of relatively poor precision in the measurements from station to station within a cruise. Median uncertainties were near the WHP one-time survey standards. This suggested that deviations from these standards could be detected using the crossover data. It turns out that these deviations could also be, for the most part, corrected with the same information.

Many of the initial differences at crossover locations were also within WHP one-time survey standards (Fig. 5, left column). This fact is reflected by the large number of differences within 2 ppm of the origin for salinity and ratios within 1% of unity for everything else. Except for salinity, the majority of the computed differences for the properties were indistinguishable from zero within their uncertainties. There were, however, some crossovers showing substantial disagreement. The initial crossover residuals have standard deviations ranging from 2.80% for nitrate to 1.56% for phosphate (Table 1). The salinity differences have an initial standard deviation of 2.77 ppm. When normalized by their uncertainties, initial residual variances ranged from 1.37 for phosphate to 4.96 for salinity.

Application of any of the models greatly increased the internal consistency of the WOCE dataset. SLSQ produced the smallest residual standard deviations (Table 1), getting the residuals closest to zero (Fig. 5, second column from left). In contrast, WLSQ produced the smallest normalized residual standard deviations (Table 1), getting the residuals closest to zero with respect to their error bars (Fig. 5, third column from left). WDLSQ had the largest residual standard deviations, but normalized residual standard deviations usually between SLSQ and WLSQ (Table 1). The damping in WDLSQ forced smaller adjustments for most of the cruises, leaving most residuals closer to their initial values than the other two models (Fig. 5, right column). These different results are all consistent with what one would expect given the model formulations.

While all the models work well to reduce the standard deviations at crossovers (Table 1), it is arguable which model is the most appropriate. SLSQ is clearly the least appropriate, since it incorporates none of the uncertainty in crossover differences. It is not discussed further. Whether WLSQ or WDLSQ provides the more appropriate adjustments is not clear. On the one hand, WLSQ achieves the greatest consistency between all the indi-

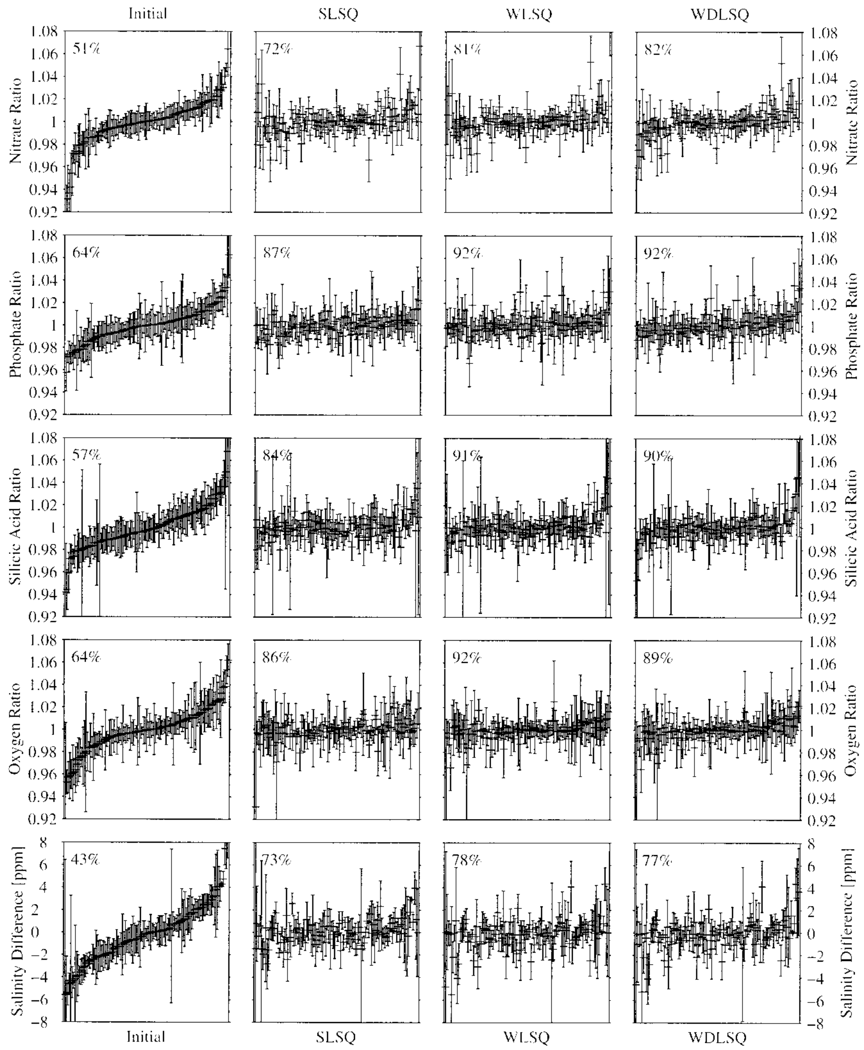

FIG. 5. Crossover residuals and their uncertainties. Rows correspond to properties and columns to models. The percentages in the upper-left corner of each panel are the numbers of crossovers indistinguishable from zero within their uncertainties. The crossovers for each property are sorted by their initial residual (left column). These sortings are retained for the various least squares models (all other columns).

vidual cruise legs in a manner that respects the accuracy of each crossover determination. It achieves this, however, at the cost of adjusting some properties from few cruises (e.g., P1W, P11A, P11S) by amounts which exceed the stated accuracy of the WOCE measurement program. If one is willing to accept that the true accuracy of these cruises is outside the goals of the WOCE project, the WLSQ estimates are preferable. On the other hand, all the adjustments are based on only a sampling of station data in the vicinity of the crossovers and one might expect that, for a large number of crossover realizations, there will be a few apparently large differences which arise solely from random errors. In this instance, one might prefer a compromise adjustment (WDLSQ) which balances the apparent need for a large correction with the assumption that no adjustment should exceed a certain bound (2% or 4 ppm for salinity in our analysis). Under these assumptions WDLSQ is preferred because it limits the magnitude of adjustments to a priori estimates of the absolute accuracy of the

TABLE 1. Crossover standard deviations reported in parts per million for salinity and percentages for the other properties. The values in parentheses were normalized by their uncertainties.

	Cross standard deviations (normalized)			
Model	Initial	SLSQ	WLSQ	WDLSQ
Nitrate	2.80 (2.25)	1.29 (1.04)	1.41 (0.85)	1.64 (0.88)
Phosphate	1.56 (1.37)	0.78 (0.77)	0.96 (0.58)	0.97 (0.63)
Oxygen	2.08 (1.48)	1.04 (0.65)	1.17 (0.49)	1.21 (0.51)
Silicic Acid	2.12 (1.50)	0.90 (0.68)	0.96 (0.60)	1.37 (0.63)
Salinity	2.77 (4.96)	1.06 (3.16)	1.37 (0.84)	1.42 (0.85)

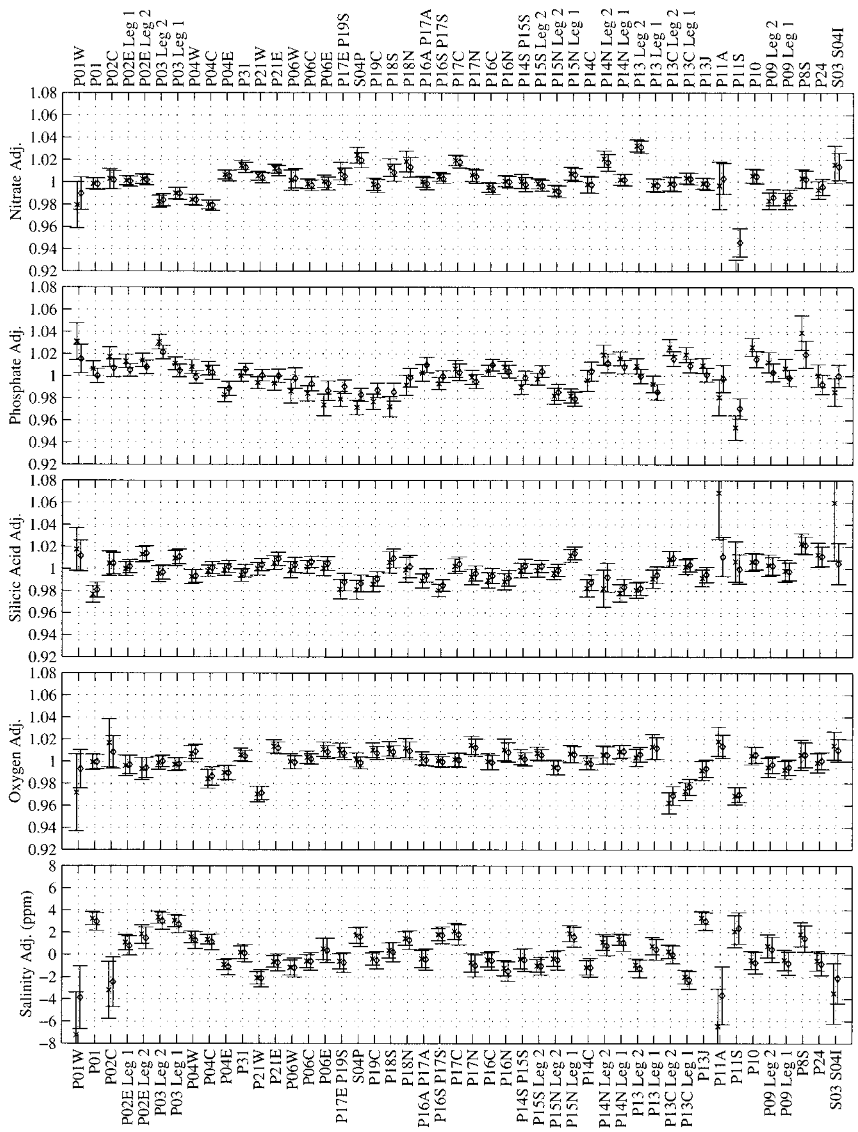

FIG. 6. Cruise adjustments and their uncertainties. From top to bottom the panels show multiplicative adjustments with uncertainties for nitrate, phosphate, silicic acid, oxygen, and additive adjustments for salinity. These values should multiply (or be added to for salinity) the original water properties for each cruise leg to obtain corrected water properties. Each property and each cruise leg has two adjustments, the WLSQ (crosses displaced left), and the WDLSQ (diamonds displaced right).

laboratory equipment but does so at the cost of allowing for larger crossover residuals to remain in the final adjusted dataset. The crossover adjustments for WLSQ and WDLSQ are compared next.

The cruise adjustments and their uncertainties are for the most part similar for WLSQ and WDLSQ (Fig. 6). As noted earlier, these values should multiply (or be added to for salinity) the original water properties for each cruise leg to obtain corrected water properties. As expected, the WDLSQ cruise adjustments were slightly smaller. This effect was largest for phosphate. Relative to the WLSQ uncertainties for the cruise adjustments the WDLSQ uncertainties were generally decreased by the damping, but were sometimes increased when very small. The large adjustments and uncertainties from WLSQ tended to be greatly reduced with WDLSQ.

While WDLSQ incorporates the most information, the a priori estimates of cruise accuracies used for the damping may not be accurate. There appear to be a few cruises that were well outside the WHP target accuracies where a large adjustment is warranted. The damping incorporates the information that the general magnitude of the adjustments should be near the size of the WHP target accuracies and thus tends to reduce large adjustments. Hence we recommend the WLSQ adjustments (Table 2).

These WLSQ adjustments were small, but generally

TABLE 2. Property adjustments for cruise legs estimated from the WLSQ model. The first column contains the WOCE Hydrographic Program one-time survey cruise designation followed by the expocode. The other columns contain multiplicative adjustments and uncertainties for all properties but salinity (which is additive in ppm). These values should multiply (or be added to for salinity) the original water properties for each cruise leg to obtain corrected water properties.

WHP cruise leg expocode	Nitrate	Phosphate	Silicic acid	Oxygen	Salinity
P01W RUBM9316/1	0.9795 ± 0.0207	1.0310 ± 0.0166	1.0175 ± 0.0193	0.9718 ± 0.0348	−7.24 ± 3.85
P01 31TTTPS47	0.9986 ± 0.0049	1.0065 ± 0.0069	0.9769 ± 0.0073	0.9993 ± 0.0070	3.26 ± 0.59
P02C 49EWBO9401/1	1.0029 ± 0.0090	1.0171 ± 0.0088	1.0048 ± 0.0112	1.0166 ± 0.0216	−3.20 ± 2.56
P02E Leg 1 492SSY9310/1	1.0014 ± 0.0042	1.0132 ± 0.0060	0.9998 ± 0.0063	0.9961 ± 0.0094	1.09 ± 0.69
P02E Leg 2 492SSY9310/2	1.0029 ± 0.0042	1.0142 ± 0.0062	1.0129 ± 0.0070	0.9932 ± 0.0100	1.83 ± 0.84
P03 Leg 2 31TTTPS24/2	0.9826 ± 0.0054	1.0306 ± 0.0066	0.9953 ± 0.0071	0.9985 ± 0.0058	3.34 ± 0.54
P03 Leg 1 31TTTPS24/1	0.9901 ± 0.0051	1.0112 ± 0.0058	1.0094 ± 0.0070	0.9971 ± 0.0058	3.05 ± 0.56
P04W 32MW893/1	0.9844 ± 0.0047	1.0081 ± 0.0061	0.9927 ± 0.0064	1.0067 ± 0.0075	1.57 ± 0.54
P04C 32MW893/2	0.9799 ± 0.0039	1.0068 ± 0.0062	0.9980 ± 0.0052	0.9840 ± 0.0085	1.35 ± 0.43
P04E 32MW893/3	1.0066 ± 0.0040	0.9829 ± 0.0063	0.9989 ± 0.0052	0.9899 ± 0.0063	−0.92 ± 0.44
P31 3250031/1	1.0150 ± 0.0040	1.0003 ± 0.0051	0.9941 ± 0.0057	1.0059 ± 0.0058	0.19 ± 0.57
P21W 318MWESTW/5	1.0055 ± 0.0039	0.9938 ± 0.0054	0.9999 ± 0.0058	0.9703 ± 0.0070	−2.10 ± 0.55
P21E 318MWESTW/4	1.0120 ± 0.0040	0.9934 ± 0.0062	1.0053 ± 0.0062	1.0136 ± 0.0059	−0.63 ± 0.53
P06W 316N138/5	1.0017 ± 0.0091	0.9861 ± 0.0106	0.9990 ± 0.0074	0.9999 ± 0.0068	−1.17 ± 0.67
P06C 316N138/4	0.9984 ± 0.0044	0.9842 ± 0.0068	1.0016 ± 0.0056	1.0036 ± 0.0056	−0.59 ± 0.57
P06E 316N138/3	1.0006 ± 0.0057	0.9737 ± 0.0098	1.0003 ± 0.0067	1.0109 ± 0.0064	0.50 ± 0.98
P17E P19S 316N138/10	1.0097 ± 0.0078	0.9790 ± 0.0067	0.9814 ± 0.0088	1.0100 ± 0.0064	−0.61 ± 0.68
S04P 90KDIOFFE6/1	1.0241 ± 0.0071	0.9715 ± 0.0066	0.9810 ± 0.0086	1.0013 ± 0.0064	1.72 ± 0.70
P19C 316N138/12	0.9980 ± 0.0056	0.9767 ± 0.0069	0.9860 ± 0.0068	1.0101 ± 0.0067	−0.39 ± 0.55
P18S 31DSCG94/2	1.0130 ± 0.0080	0.9722 ± 0.0091	1.0057 ± 0.0097	1.0114 ± 0.0065	0.37 ± 0.68
P18N 31DSCG94/3	1.0185 ± 0.0093	0.9916 ± 0.0090	0.9990 ± 0.0114	1.0119 ± 0.0087	1.46 ± 0.62
P16A P17A 316N138/9	1.0003 ± 0.0049	1.0028 ± 0.0074	0.9891 ± 0.0064	1.0027 ± 0.0059	−0.39 ± 0.79
P16S P17S 31WTTUNES/2	1.0049 ± 0.0039	0.9931 ± 0.0054	0.9803 ± 0.0055	1.0008 ± 0.0055	1.80 ± 0.53
P17C 31WTTUNES/1	1.0195 ± 0.0047	1.0064 ± 0.0077	1.0024 ± 0.0066	1.0017 ± 0.0060	2.10 ± 0.74
P17N 325021/1	1.0063 ± 0.0057	0.9988 ± 0.0065	0.9927 ± 0.0071	1.0147 ± 0.0083	−0.72 ± 0.85
P16C 31WTTUNES/3	0.9953 ± 0.0043	1.0047 ± 0.0051	0.9895 ± 0.0069	0.9998 ± 0.0071	−0.47 ± 0.65
P16N 31DSCGC91/2	1.0010 ± 0.0049	1.0078 ± 0.0055	0.9883 ± 0.0073	1.0105 ± 0.0098	−1.21 ± 0.68
P14S P15S 31DICG96/1	1.0009 ± 0.0063	0.9899 ± 0.0064	0.9985 ± 0.0066	1.0041 ± 0.0067	−0.40 ± 0.89
P15S Leg 2 31DICG96/2	0.9987 ± 0.0044	0.9973 ± 0.0054	0.9984 ± 0.0058	1.0072 ± 0.0058	−1.00 ± 0.56

TABLE 2. (*Continued*)

WHP cruise leg expocode	Nitrate	Phosphate	Silicic acid	Oxygen	Salinity
P15N Leg 2 18DD9403/2	0.9925 ± 0.0048	0.9821 ± 0.0072	0.9959 ± 0.0054	0.9948 ± 0.0066	−0.37 ± 0.66
P15N Leg 1 18DD9403/1	1.0078 ± 0.0056	0.9821 ± 0.0064	1.0119 ± 0.0057	1.0068 ± 0.0079	1.91 ± 0.72
P14C 316N138/7	0.9980 ± 0.0074	0.9959 ± 0.0095	0.9823 ± 0.0078	0.9989 ± 0.0063	−1.16 ± 0.65
P14N Leg 2 325024/1	1.0209 ± 0.0073	1.0191 ± 0.0091	0.9821 ± 0.0168	1.0058 ± 0.0083	1.12 ± 0.70
P14N Leg 1 325023/1	1.0022 ± 0.0047	1.0157 ± 0.0062	0.9779 ± 0.0077	1.0087 ± 0.0061	1.37 ± 0.50
P13 Leg 2 3220CGC92/2	1.0327 ± 0.0054	1.0090 ± 0.0070	0.9804 ± 0.0068	1.0035 ± 0.0078	−0.94 ± 0.57
P13 Leg 1 3220CGC92/1	0.9974 ± 0.0058	0.9926 ± 0.0075	0.9909 ± 0.0083	1.0131 ± 0.0114	0.77 ± 0.77
P13C Leg 2 49HH915/2	0.9986 ± 0.0062	1.0258 ± 0.0072	1.0086 ± 0.0073	0.9624 ± 0.0097	0.27 ± 0.60
P13C Leg 1 49HH915/1	1.0037 ± 0.0049	1.0192 ± 0.0068	1.0017 ± 0.0068	0.9730 ± 0.0081	−2.01 ± 0.60
P13J 49HH932/1	0.9988 ± 0.0050	1.0094 ± 0.0067	0.9915 ± 0.0075	0.9918 ± 0.0086	3.32 ± 0.57
P11A 09AR9391/2	0.9970 ± 0.0214	0.9806 ± 0.0163	1.0687 ± 0.0421	1.0181 ± 0.0132	−6.46 ± 3.38
P11S 09FA693	0.9135 ± 0.0168	0.9533 ± 0.0111	1.0064 ± 0.0182	0.9688 ± 0.0080	2.08 ± 1.44
P10 3250TN026/1	1.0058 ± 0.0063	1.0260 ± 0.0081	1.0062 ± 0.0082	1.0052 ± 0.0081	−0.50 ± 0.82
P09 Leg 2 49RY9407/2	0.9832 ± 0.0074	1.0123 ± 0.0092	1.0032 ± 0.0097	0.9945 ± 0.0086	0.77 ± 1.04
P09 Leg 1 49RY9407/1	0.9830 ± 0.0073	1.0068 ± 0.0086	0.9981 ± 0.0099	0.9923 ± 0.0080	−0.50 ± 0.91
P8S 49XK9605	1.0034 ± 0.0083	1.0391 ± 0.0155	1.0229 ± 0.0090	1.0059 ± 0.0136	1.82 ± 1.09
P24 49RY9511/2	0.9931 ± 0.0078	1.0003 ± 0.0101	1.0126 ± 0.0108	0.9986 ± 0.0087	−0.56 ± 0.87
S03 S04I 09AR9404/1	1.0158 ± 0.0167	0.9856 ± 0.0124	1.0598 ± 0.0522	1.0143 ± 0.0127	−3.50 ± 2.72

distinguishable from zero if they exceeded 1% or 1 ppm for salinity. Adjustments were generally within 3% for the nutrients and oxygen, although a few cruise legs exceed 5% adjustments for one or another of the properties (Fig. 6). The adjustments for salinity were generally limited to 3 ppm, although again there were a few that exceed 5 ppm. The median uncertainties for the nutrient and oxygen adjustments were around 0.7%. The median uncertainty for the salinity adjustments was 0.7 ppm. The percentages of cruise leg adjustments greater than their uncertainties for WLSQ were 49%, 75%, 53%, 43%, and 66% for nitrate, phosphate, silicic acid, oxygen, and salinity, respectively.

5. Conclusions

We have presented a hierarchy of crossover-based least squares models to objectively determine nutrient, oxygen, and salinity adjustments. We used information throughout the water column to estimate crossover differences (favoring those portions where signal-to-noise was highest through weighting). We minimized these crossover differences with adjustments from these models, starting with the SLSQ model. The WLSQ model incorporated uncertainties of differences at crossovers. The WDLSQ model added a priori expectations of measurement accuracy as a damping. They all provided property adjustments and uncertainties for each cruise leg.

These models were successfully applied to the WOCE Pacific dataset. For all of the models, the adjustments greatly reduced crossover differences and generally brought cruises into agreement within WHP target accuracies. The WLSQ adjustments are recommended as the most appropriate. A majority of these adjustments were distinguishable from zero within their uncertainties. This system is applicable to other water properties such as the carbon system (Lamb et al. 2001).

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