

# **REFERENCE-QUALITY WATER SAMPLE DATA**

## **Notes on Acquisition, Record Keeping, and Evaluation**

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### **1. OVERVIEW**

Generating reference-quality water sample data involves procedures learned over years of experience. Some simple-to-implement aspects of practice do, however, lead to improved reliability and documentation of water sample data. These include:

- For water sample data
  - verification of the collection depth and unambiguous association of that depth with a unique sample identifier,
  - understanding the degree to which the water which issued from the sampling spigot matched the characteristics of the ambient water from the collection level,
  - verification that all data values associated with a water sample are correctly matched to the water sample identifier, and
  - determination if the values for each parameter are correct.
- Data evaluation must begin at sea. This is usually the only time all involved personnel and all records are together. Also, it is possible then to correct repetitive problems before they can further degrade the data.
- The care of the data analyst and access to complete records are in general more important than the specific scheme of data evaluation.
- The analyst must determine if the appropriate standards were met by the bulk of the data. Emphasis should be placed on adherence to proven, documented methodology over agreement with historical data. Quality standards should be applied consistently.
- The analyst determines which data values are suspect, partly by identifying outliers and assessing their severity and cause, or finding that the anomalies are likely genuine. Suspicion of a data problem based on a data value alone, without probable cause for an erroneous value, should normally not of itself be cause to demote the quality of a value.
- Apparent problems should be corrected if possible.
- The analyst's report and a report of subsequent actions must be archived. These should be added to a data report which also contains ancillary information about the cruise, a summary of data acquisition and processing methodology, data quality information, and a complete list of contacts for further information regarding the cruise, methodology, and the data.

## 2. INTRODUCTION

The common laboratory practices which sum to a quality assurance program are well known and widely disseminated (e.g., cf. Dux, 1990). However, it must be deficiencies in methodology which underlie the occasional startling cruise-to-cruise differences in seawater property data between laboratories or within one laboratory. (Here referring to offsets in data values outside the natural ranges of variation thought to obtain for the water masses in question.)

From Wikipedia, 2008:

**"Data Quality** refers to the quality of data. Data are of high quality 'if they are fit for their intended uses in operations, decision making and planning' (J.M. Juran). Alternatively, the data are deemed of high quality if they correctly represent the real-world construct to which they refer. These two views can often be in disagreement, even about the same set of data used for the same purpose.

"Definitions

- "1. Data Quality refers to the degree of excellence exhibited by the data in relation to the portrayal of the actual phenomena. [GIS Glossary](#)
- "2. The state of completeness, validity, consistency, timeliness and accuracy that makes data appropriate for a specific use. [Government of British Columbia](#)
- "3. The totality of features and characteristics of data that bears on their ability to satisfy a given purpose; the sum of the degrees of excellence for factors related to data. [Glossary of Quality Assurance Terms](#)"

Such concepts come to mind when one applies the term "reference-quality data" to measurements of seawater properties from research vessels ("hydrographic measurements", in the context of physical/chemical oceanography). Sufficient information accompanies reference-quality data so that data users having no prior association with their collection and reporting will judge that their inherent quality - their absolute accuracy and various aspects of their precision - is excellent for studies of the large scale ocean circulation and the regional and temporal variations in ocean water properties at all levels.

The most common hydrographic measurements are vertical profiles of temperature and salinity, and sometimes other properties, generated with an electronic profiling CTD (Conductivity, Temperature, Depth) device. A CTD device commonly used in reference-quality measurements is the Sea-Bird SBE 911*plus* CTD. A configuration of the 911*plus* used for such measurements may include the central underwater unit with a Paroscientific Digiquartz pressure sensor, two pairs of ducted flow conductivity and temperature sensors, an SBE-43 dissolved oxygen sensor, and sometimes a SBE-35 reference thermometer. Other instruments - for example an altimeter, fluorometer, and/or transmissometer - may be included as part of the CTD instrument package.

A CTD device can be used on its own, deployed from a armored conducting cable (or, if self-powered and internally-recording, from some other type of cable or platform). Indeed, the typical accuracy, precision, and temporal stability of the 911*plus* pressure sensor is such that its pre- and post-cruise laboratory calibrations, plus application of appropriate acquisition,

calibration, and correction algorithms, can suffice to produce CTD pressure values of reference quality, when the work is carried out by well-trained, experienced persons. And much the same holds for data from the 911*plus* temperature sensor, though one reason these are commonly used in pairs is that occasional drifts or sudden offsets are observed in output from the temperature sensors. A change in the difference between the pair alerts the observant seagoing team to the importance of at least a careful examination of pre-cruise versus post-cruise laboratory temperature calibrations. [Use of the Sea-Bird SBE-35 reference thermometer to collect an independent observation of temperature during stops for bottle closures can also provide useful ancillary data to chase down the timing and source of an apparent drift or sudden offset in a CTD temperature sensor.] But it is generally not feasible to collect reference-quality ocean salinity data via the 911*plus* conductivity sensors unless corrections based on water samples are applied, and the parallel caveat certainly applies to dissolved oxygen data from the SBE-43 oxygen sensor.

Beyond that, many seawater characteristics of interest cannot be sampled, or sampled to high enough quality, by electronic sensors. For measurement of those, water samples must be collected from depth, brought into the laboratory, analyzed, and evaluated. This sampling from water sample bottles is a type of sampling which long predates CTD sampling. Today, nearly all reference-quality hydrographic water sample data are obtained from rosette water samplers which are teamed with a CTD and other instruments. The suite of measurements from the rosette water sampler on some recent cruises for the International Ocean Carbon Coordination Project has included salinity, dissolved oxygen, inorganic ‘nutrients’ [nitrate ( $\text{NO}_3$ ), nitrite ( $\text{NO}_2$ ), phosphate ( $\text{PO}_4$ ), silicate ( $\text{SiO}_3$ ; also  $\text{SiO}_4$  and  $\text{Si}(\text{OH})_4$  in some documents), and sometimes ammonium ( $\text{NH}_4$ )], various CFCs and related compounds (CFC-11, CFC-12, CFC-113,  $\text{CCL}_4$ ,  $\text{SF}_6$ ), helium, tritium, oxygen isotope ratio (labeled O18O16 or  $\delta^{18}\text{O}$ ) a suite of ocean carbon-related parameters [such as total dissolved inorganic carbon (TIC or DIC), the partial pressure or fugacity of  $\text{CO}_2$  ( $p\text{CO}_2$  or  $f\text{CO}_2$ , respectively), total alkalinity (labeled TALK or ALK), pH, dissolved organic carbon (DOC), dissolved organic nitrogen (DON),  $^{13}\text{C}$ ,  $^{14}\text{C}$ ], and sometimes other characteristics, such as phytoplankton pigments, trace metals (e.g., aluminum and iron compounds) or a suite of various dilute dissolved organic compounds that may together be termed Colored Dissolved Organic Matter (CDOM).

Methodologies appropriate to generating reference-quality CTD data are discussed in other documents. The primary consideration of CTD data in this document is use of the CTD data reported at the time of closure of a water sample bottle. Furthermore, regarding water sample data, the focus here is not so much on the laboratory techniques which attend to making reference quality hydrographic measurements, but more nearly on the various factors which together contribute to documenting and assessing the quality of the data values reported by the analysts for the various parameters. The procedures discussed here, when followed, add value to water sample data.

## 2.1 Selection of water sample depths

The water sample bottles on the rosette are usually closed on the up cast, and so the features seen on the down CTD trace can be used as a guide to sample important features with the bottles, recognizing that other features such as nutrient or  $^{14}\text{C}$  extrema may not be reflected in the CTD sensor data. Knowledge of near-by or historical data may help in sampling such features. Sometimes other criteria are important in choosing water sample levels. For example, if primary

productivity samples are to be collected, they are sampled from depths that are equivalent to the light levels that are in the on-deck incubators.

There are several goals underlying choice of water sample levels. One fundamental goal is to provide check samples for salinity and dissolved oxygen for adjustment of CTD salinity and dissolved oxygen data. To be most useful, these check samples must come from portions of the water column with small vertical gradients of salinity and/or dissolved oxygen. (It is not necessary that identical levels be sampled for both.) Sufficient vertical coverage is required to assist the CTDO data processor in assessing and making pressure-dependent corrections. Normally, only a small number of check samples are required per CTD cast. When water samples are being collected for other parameters - typically at 24-36 levels per cast in most reference-quality work - salinity and dissolved oxygen water samples from every rosette bottle should be collected and analyzed. The every-level CTD-versus-bottle salinity and dissolved oxygen comparisons help to verify the integrity and actual sampling level of the bottle samples.

Another goal of choosing water sample levels is to, in effect, define the overall concentrations, extrema, and first and second vertical derivatives for each of the parameters not sampled by the CTD. Although most water sample parameters are not visualized in the CTDO traces, the principal water masses can be discerned from the CTD trace by an oceanographer, and useful aspects of the vertical variation of the water sample parameters parallel the water masses in one way or another. Hence, as noted above, the features of the down CTD trace are indeed a useful guide to choice of water sample levels on the up cast.

All this said, those in charge of oceanographic sampling programs yearn for approaches to choice of water sample levels that are both effective and also easy to implement. The historical choice of many groups has been to issue a list of "standard levels" to be followed by the seagoing team. In all cases the sampling pressures are chosen to be appropriate for the region being sampled, usually more closely spaced in the high-gradient portions of the water column (the shallower waters in most cases) and further apart in the low-gradient deep waters, so as to resolve best all the features in the whole water column on each station, given the number of bottles (the number of discrete sampling levels) available. Such a scheme conceptually looks like this, with left-to-right indicating sampling at successive stations:

Station #->	D
.....	e
	p
.....	t
	h
.....	l
	v

Standard sampling levels are required in some time-series studies, where a major goal is to observe changes at given levels. But in some cases adherence to standard levels imposes limits in terms of incompletely-sampled extrema or improperly-registered curvature in the parameter values against pressure, for example in the less-intensely sampled deeper layers. For long transects, such as the recent reoccupations of key WOCE Hydrographic Program One-Time Survey sections, use of a staggered scheme, with alternate stations sampling the pressure mid-points, provides improved overall (over multiple station) resolution of vertical gradients. Such a scheme conceptually looks like this:

```

Station #-> D
. . . . . e
. . . . . p
. . . . . t
. . . . . h
. . . . . l
. . . . . v

```

But on many cruises some key parameters of interest are sampled only every second station. This is often the case for some of the carbon and CFC parameters, for example. In such cases the alternate-station staggering scheme does not provide the benefits of staggering to those parameters. A staggered sampling scheme more appropriate to resolving the every-second-station parameters might look like this:

```

Station #-> D
.. .. . e
. . . . . p
.. .. . t
. . . . . h
.. .. . l
.. .. . v

```

Niki Gruber and Paul Robbins suggested that a three-station sampling pattern might provide the best overall vertical resolution on long, basin-scale oceanographic transects, where lateral gradients are relatively small. Conceptually, such a pattern looks like this:

```

Station # ->      D
. . . . . . . e
. . . . . . . p
. . . . . . . t
. . . . . . . h
. . . . . . . l
. . . . . . . v

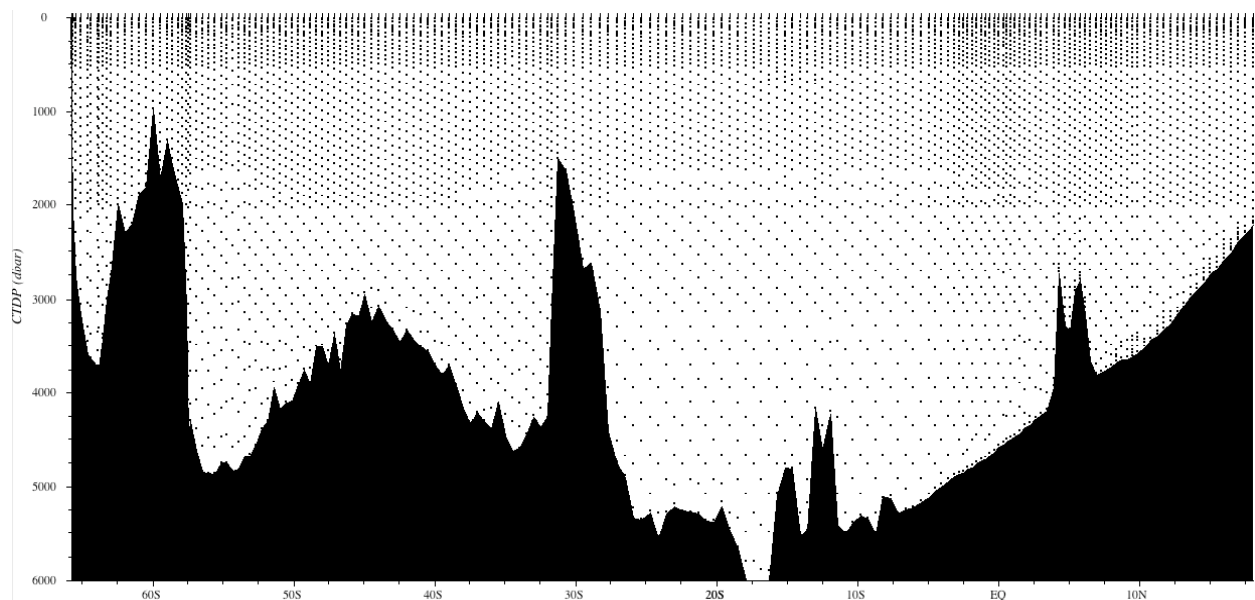
```

This scheme has since been adopted by some groups, such as the US team carrying out ocean carbon and repeat hydrography transects; these are repeats of key WOCE Hydrographic Program lines. On a given transect, the three schemes are rotated in order, with occasional adjustments for boundaries and water mass changes. The Pacific Ocean version of the team's sampling levels is shown in the table below:

<i>bottle count</i>	Scheme 1	Scheme 2	Scheme 3
1	5	5	5
2	25	35	20
3	55	70	45
4	80	95	85
5	105	120	110
6	130	145	135
7	155	170	160
8	180	195	185
9	215	220	210

10	250	270	235
11	300	320	285
12	350	370	335
13	400	420	385
14	450	470	435
15	500	540	485
16	600	640	570
17	700	740	670
18	800	840	770
19	900	940	870
20	1000	1040	970
21	1100	1140	1070
22	1200	1240	1170
23	1300	1340	1270
24	1400	1440	1370
25	1500	1540	1470
26	1600	(1640)	1570
27	(1700)	1740	(1670)
28	1800	(1840)	1770
29	(1900)	1940	(1870)
30	2000	2100	1970
31	2250	2350	2170
32	2500	2600	2420
33	2750	2850	2670
34	3000	3100	2920
35	3400/(3250)	3500/(3350)	3250/(3170)
36	3800/(3500)	3900/(3600)	3650/(3420)
	4200/(3750)	4300/(3850)	4050/(3670)
	4600/(4000)	4700/(4100)	4450/(3920)

The figure below shows the distribution of water samples on a long transect from Antarctica to Bangladesh carried out by this team in 2007, using the three-scheme approach:



### **3. KEY ASPECTS OF PRACTICE**

In the context intended for this document, these key aspects of practice lead to improved reliability and documentation of water sample data:

organizing data and records in a logical manner,

recording the information needed to put together disparate linked data and to unambiguously identify and document unusual events,

verification of the collection depth and unambiguous association of that depth with a unique sample identifier,

understanding the degree to which the water which issued from the sampling spigot matched the characteristics of the ambient water from the collection level,

verification that all data values associated with a water sample are correctly matched to the water sample identifier, and

determination if the values for each parameter are correct.

#### **3.1 Data organization**

Bottle data can usefully be organized in a hierarchy as system/cruise/station/cast/sample.

- At the system level are the master files, e.g. for CTD configurations, a history of CTD and thermometer calibrations, and oxygen flask volumes.
- At the cruise level there should be a station/cast description, a weather log, cruise-specific identifiers for winches and instruments, and a set of directories which hold the raw and processed data for the cruise as well as a “doubtful data” directory which holds a complete record of all sample-related data problems and the actions taken because of them.
- At the station level there are files for the raw and processed data. The "doubtful data" directory can alternatively reside as a set of individual files, one per station.
- Cast number is part of the record for each water sample. Hence when cast number is specified, only data from the requested cast(s) are retrieved or examined.
- Data should be identified and retrievable by sample number.

#### **3.2 Record keeping**

The key to data assessment is the availability of proper records, meaning a path of overlapping records of all relevant information. Record keeping follows the pessimist approach and should include redundancy of all critical information, all of which must be verified. There are several reasons for this. First of all, blunders are insidious, especially on oceanographic expeditions where many people handle samples, forms, and data. At sea, persons may be ill or tired, and so

may more commonly than usual miss or transpose numbers, replace sample containers in improper positions, fill sample containers from the wrong rosette bottle, and so on — almost everything imaginable goes wrong at some time or other. Electronic record keeping has helped a great deal, but there is always a human element somewhere, plus electronic records can be disrupted or lost. A typical example of failure of electronic records lies in the software used to capture CTD information during rosette bottle trips: Because there is no absolute confirmation of bottle closure, the number of apparent bottle closures recorded by the computer can be less or more than the actual number, leading to a data processing and evaluation challenge, i.e. bottle data incorrectly offset one or more levels for one or more samples.

Procedures for maintenance and availability of the records must be strictly enforced. A certain level of redundancy provides added security, plus discrepancies can point to areas of confusion which need to be sorted out by the data quality assessors.

### *3.2.1 CTD Console Operations Log.*

A log sheet should be maintained by the person who operates the central CTD operations area for each cast. The information is partly redundant to that recorded by the computers, and so provides valuable back-up and cross-check. There are four types of information to consider: (1) cast headers, (2) cast data, (3) CTD information at bottle trips, and (4) documentation of unusual events. This may well be the only record of information related to the human element in console operations. Most important of all: this is usually the *only* record of the *intended* bottle depths (which may differ grossly from the actual depths if there is failure of correct operation of the underwater package). This log sheet is thus one of the first items a data analyst turns to for information.

Support for **cast header** information (e.g., expedition, station number, date, time, position, depth to bottom) may be partly or even fully automated by some data acquisition systems. Some acquisition systems prompt the console operator to enter the information from the keyboard, or the header data may be added or modified later in data processing. In any event, it is wise to keep a manual record of key header information in the event of confusion or electronic data loss. The names or initials of the operators should also be noted.

"**Cast data**" are the records of attempted closure of the bottles. This includes a list of the identification numbers on the bottles in or with the intended order of closure, a list of the intended bottle depths, a list of the actual wire out at the time of each closure, and a log of each and every attempt to close a rosette bottle including the outcome of that attempt. [There should be one mark on the console operations log sheet for each 'button push', i.e., attempt to close a bottle by some physical action such as pushing the 'fire' button on a water sampler deck unit. A "check mark" indicates confirmed closure (via whatever information is available) and a "0" indicates any other outcome. The console operator should also write notes on the margin of the console operations log sheet regarding further details of the circumstances accompanying unconfirmed closure attempts. After each cast the number of confirmed and unconfirmed trips, and the number of closed and open bottles, should be compared to the actual post-cast disposition of the water sampler. Discrepancies indicate mechanical and/or electrical problems and a likely problem in assignment of closure level/pressure/depth to the water samples. Note especially that *the intended sample level can differ grossly from the actual depth of closure when*



*there is a tripping or sequencing problem in the rosette system.* Hence the hand-recorded cast data provide essential information for bottle data evaluation.

Considering that the output of a CTD system is a time series of data, noting the times of various events can be useful in sorting out discrepancies in the electronically recorded data vis-à-vis various cast events. Times to record might include those of cast start, maximum wire out, cast end, winch stops, and attempted bottle closures. It is also important to note the time of any untoward events, such as a temporary data loss, sudden/suspect data offsets, and so forth. Time or elapsed time records are often useful to locate bottle trips in the recorded CTD data stream if the cast's CTD data must later be recovered from a backup.

Any **CTD information at bottle trips** (lanyard release) written on a log sheet is almost certainly redundant with that recorded by the computer during the cast. But the CTD operator should consider what information, written on a log during the cast, would help to definitively sort out a bottle sequence, sample level, or related problem uncovered later during data processing. At a minimum, writing onto the log sheet the CTD pressure value at the time of attempted bottle closure can be useful in later reconstructing correct closure depths when there is a closure sequence problem, such as a serious mismatch between the actual closure depth and the assumed closure depth.

Note: CTD parameter data values manually recorded onto the Console Operations Log from the CTD readouts during bottle closure should be used for emergency backup purposes only<sup>1</sup>.

Regarding the CTD data electronically recorded at the time of bottle closure (bottle trips), various schemes are in use in the community. One goal is to have the best feasible agreement between the water represented by the CTD values and the water in the rosette sample bottle. The rosette bottle is not co-located with the CTD sensors, and it contains a much larger volume of water -and different water at that -than the volume sensed by the CTD. Most important for best CTD-versus-bottle agreement is that the rosette sample bottle be well flushed. Generally, this means waiting for the time of two ship rolls -and at least 20 seconds (the time it takes for the rosette wake to clear the bottles -to close the bottle. (Some investigators report statistically-improved agreements waiting one minute as opposed to 20 seconds.) A 2-second average of the processed up cast CTD data near the time of bottle closure may be sufficient. Some groups, however, average data over the period of one ship roll (ca. 7-10 seconds). For best agreement with the water samples, these would include ca. 50% CTD data from before closure of the bottle and ca. 50% from after closure, since this may help to better represent bottle property shifts during final flushing. If an SBE-35 reference thermometer is in use, the SBE-35 records its temperature value for N seconds (set by the CTD technician) after the bottle trip signal. Thus the best CTD-versus-SBE-35 agreement would be obtained by recording the CTD data beginning immediately after the bottle closure. Considering all factors, when an SBE-35 is in use, it is probably best to record the CTD data for the bottle trip immediately after bottle closure. Also, the CTD operator must wait for the SBE-35 reading to complete (and the CTD data at bottle closure to be recorded) before resuming raising the rosette.

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<sup>1</sup> Any laboratory relying on manual entry of CTD data at bottle trips should realize that errors are rife in such efforts, for example in estimating the 'average' of a fluctuating electronic display, misreadings of displays, errors in displays (due to malfunctions), transpositions of digits, and the like. All laboratories should thus adopt automated recovery of CTD information at bottle trips (for example a 2-second average or other suitable statistical assembly).

An experienced CTD operator — knowing what may turn out to be key information later during data assessment — also keeps track on the log sheet of all **unusual events**, problems or hints of problems. It is worth remembering that having a console operations log sheet at hand also provides the back side of the sheet to write details of problems and unusual events.

A console operations log sheet can become untidy, for example when changes in intended sample levels are made mid-cast or when there are problems. No matter: it is meant to be a working document, not necessarily one to be archived beyond stored records of the science team at sea. Nonetheless, for safekeeping and to ease distribution of the completed log sheets within the seagoing team, it is strongly recommended that when each console operations log sheet is complete, it should be scanned and the file saved for inclusion in the electronic records of the expedition.

A sample blank CTD console log sheet is included as [Exhibit A](#), and an example of a filled-in sheet is included as [Exhibit B](#). (Note that in Exhibit B some of the information on the form has not been filled in. This is normal in routine operations. But places for extra information, for unusual circumstances, are provided by the CTD group which uses this form.)

### *3.2.2 Sample Log Sheet.*

This document is the master record for water sampling, and is another critical source for extra information for the data assessor.

Before sampling, the sample log is prepared by the scientists in charge of the cast, who supply various header information, the approximate intended depth for each rosette bottle, and a list of which parameters will (or will not) be drawn from which rosette bottle. Note that the Niskin bottle numbers and the intended depths should match exactly those on the Console Operations Log sheet.

Most of the sample log is completed on deck during water sampling. Where there are many sampling programs, it is sometimes useful to appoint a ‘sample cop’ armed with the sample log sheet. When many properties are being sampled at once from a large rosette by a group of 3-6 samplers, the function of the sample cop in directing samplers to available bottles, keeping sampling in order, and in writing comments and sample identification numbers is invaluable.

When the cast is being recovered, the sample cop first records any observations from the deck crew, such as “#15 leaking from bottom cap during recovery; stopped when tapped”, “lanyard fouled in top cap of #11, no sample”, “pylon rotor on position #1 — not position #24 — at end of cast”, or “raining during sampling; rosette bottles removed to wet lab”. Then, as each sampler draws samples, the sample cop records sample container numbers in the blank spaces for each bottle, and writes down the samplers’ comments, if any. The latter are most often from the first sampler to open the bottle, who might say, for example, “#7 has an air leak” [water issues from the spigot when it is tested before the air vent is opened], “air vent not closed on #3”, or “#9 leaks from bottom cap after air vent opened”.<sup>1</sup> Records of this type are invaluable to the analyst

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<sup>1</sup> The first person to draw a water sample from a bottle has a special obligation to note the condition of the bottle, test its integrity, and report any discrepancies at once to the sample cop. The suggested procedure: (1) Verify that the number on the bottle is the one expected. (2) Inspect for water leaks from the spigot or the bottom cap. If there is a small leak from the spigot try to stop it. If there is a small leak from the bottom cap, tap the bottom cap to see if

later attempting to ascertain the cause for unusual data values. By the way, it is much preferred to record each water sample identification number on the sample log sheet at the time of drawing rather than to fill out the list for the entire cast before or after drawing. The usual procedure is for the sampler to notify the sample cop (e.g., “drawing oxygen 1124 from Niskin 27”), which is in turn noted on the log sheet by the sample cop who responds by verifying the numbers (e.g., calling back, after writing the numbers, “OK, oxygen #1124 from Niskin #27”).

Any additional information relevant to sampling should be recorded, such as serial numbers, if any, of the boxes, cases or trays used to hold sample bottles, and the names or initials of the persons drawing each type of water sample.

An example blank sample log sheet (two-part) is included as [Exhibit C](#), and an example of a filled-in sheet (also two-part) is included as [Exhibit D](#).

### *3.2.3 Instrument and deck log sheets.*

Log sheets or books should accompany the CTDs, rosette, and each instrument used to analyze water sample data. Usually standard tables are prepared to hold repetitive information with provision for more detailed comments, for example relative to specific samples or events. The logs record all relevant details of the operation and standardization of the instruments in question, providing a continual stream of ancillary information, including a record of instrument set up and adjustments, cruise-specific procedures, problems, calibration, standardization, and any other noteworthy material over the whole of the expedition. These are a useful source of information when a sample or CTD cast is noted to be unusual or in some other way suspect of error.

The technicians should also maintain a deck log, which keeps a running account of every cast activity, including all modifications or alterations to the rosette and attached instruments and harnesses. All unusual or noteworthy occurrences are logged, such as minor damage or repairs, striking the ship or the bottom, and so forth. This is where changes to lids, bottles, and O-rings are noted. This log provides to the analyst a running assessment of the performance of the underwater package. If an underway surface water measurement system is in operation, there are also log sheets for recording check samples and system performance data.

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the leak stops (in which case the leak is due to a seating problem). (3) Open the spigot; then close it. If more than a few drops of water issued, there is an air leak from the top cap or the air vent. The force of any ‘spurt’ is a rough guide to the severity of the leak and should be noted. Check the seating of the top cap and the sealing of the air vent. Note any discrepancies and try to fix them, for example by closing the inadvertently left-open air vent. Now re-try opening the spigot to see if the problem was correctly identified. (4) Open the air vent. Check for leaks from the bottom cap. If there is a leak, attempt to re-seat bottom cap — via a tap — if necessary. (5) Note any problems in (2)-(4) to the sample cop. (6) Proceed with sampling.

### 3.3 Sample identifiers and verification of the collection depth

Because many types of scientific analyses of oceanographic water sample data require reference to the level (pressure or depth) from which a particular sample was collected, water sample data may be unusable from bottles for which the sampling level cannot be unambiguously determined. The issue at hand rests not so much in the precision or accuracy to which the sampling level is known as it is does with regard to whether or not it can be determined that the sample container closed - fully closed - at the intended level.

Closely associated with the sampling level is the sample identifier, i.e. some code unique to that water sample which forever tags it. For the WHP, the identifier was the combination of the expedition code ("EXPOCODE"), station, cast, and sample (or bottle) numbers.<sup>1</sup>

Ambiguity creeps into any sample identifier system from two sources: (1) Despite all labels, checks with others in the sampling room, etc., the person drawing water samples occasionally draws a sample from the wrong Niskin bottle, or uses a sample container labeled or otherwise intended for a different Niskin bottle. (Simple sequential numbering schemes for rosette and sample bottles can help, though in practice out-of-sequence numbers must be permitted.) With a careful system of checks and cross checks this occurs only rarely and is often relatively easy to identify in data quality evaluation. (2) For CTD/rosette casts the sample identifier must be matched to CTD information. Problems occur when the identifier assigned to the CTD data at bottle closure by the computer or the computer operator is not in reality associated with the specific Niskin bottle the computer or operator assumed. This is, of course, where the difficulty lies, i.e. in seeing that the two data paths are in 100% agreement. The problem is not trivial because there is not absolute confirmation of actual bottle closure at the time of intended bottle closure. Many instances are known, including with equipment which provides a confirmation signal, of the data acquisition computer or the CTD console operator mis-matching the bottle identifier to the CTD data. Almost every imaginable type of "wrong level" malfunction occurs, and some expeditions experience continual problems. When bottle identifier vis-à-vis CTD data problems are not cleared up at once, on board, the situation rapidly approaches chaos.

With this in mind it is obvious that the number one issue in water sampling is to collect a water sample from the intended level and the number one issue in data assessment is to verify the collection level and unambiguously associate that level with a unique sample identifier.

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<sup>1</sup> Some institutions use different coding schemes with the same intent to provide uniqueness. For example, the Bedford Institute of Oceanography assigns to each bottle on the rosette (or wire) a unique, one-time identification number used for the bottle and all water samples drawn from it. Sheets of adhesive labels with these numbers (one number per sheet, and ca. 12 labels per sheet) are prepared, with one label applied to each Niskin bottle on the rosette before it goes into the water and, before sampling, to each of the unfilled sample containers. The persons who sample the rosette need only verify that the label on the sample container in their hand matches that on the Niskin bottle from which they are drawing the sample to unambiguously establish that they are drawing from the correct Niskin bottle. This is especially useful for situations when not all Niskin bottles are sampled for all parameters. Yet it should be noted that despite having the identification number on both the Niskin bottle and the sample container, samples still are drawn from the incorrect Niskin from time to time - no system is foolproof.

### 3.4 Understanding the quality of the water in the sample bottle

The second most important issue in water sampling and data quality assessment is to understand the degree to which the water which issues from the sampling spigot matches the ambient characteristics of the water from the collection level. This issue includes many different facets. For example, the rosette and cable disturb the water; the rosette bottle may be incompletely flushed; the water in the rosette bottle can be affected by warming as the rosette is brought through warmer layers or in air, by cooling or even freezing if the rosette is brought on board during winter, and by leaking of air or water past the seals in the end caps, spigot, or air vent. The water in the rosette can also be contaminated from substances from other equipment on the rosette, from the CTD armored cable, or from the bottle interior, seals, or spring.

Sometimes contamination is immediately suspected, for example when a bottle comes on board with a lanyard caught in the top lid. Sometimes the effects are subtle and require much detective work.

During the time water samples are drawn, contamination or other sample degradation can come from the sampling equipment or sample containers, from spray, particulates, or aerosols in the sampling area, and by exchanges with gases in the head space above the water in the Niskin bottle or in the region of the sample container. Some of these affect only an individual water sample, but others, such as gas exchange in the head space, potentially affect the entire sequence of water samples for gasses from a Niskin bottle, with the magnitude of the degradation increasing with time. For this reason samples are generally drawn in the order of decreasing sensitivity to such exchanges. [The sampling order currently recommended is CFC,  $^3\text{He}$ ,  $\text{O}_2$ , and  $\text{CO}_2$  parameters. Then AMS  $^{14}\text{C}$ , nutrients, salinity, alkalinity, and any other samples may follow in unspecified order.<sup>1</sup>]

Sample degradation information is critical to the measurement technicians for each parameter, who are eager to identify faulty data before they are sent onward. Yet the individual analysts do not always have at hand the combined picture of how associated water characteristics co-vary. For this reason it is often the data quality assessor who determines — by examining the totality of the characteristics — whether or not the quality of water in the sampling container is unusually suspect. [The first check in this regard is comparison of the water sample salinity and CTD salinity differences for the cast. One also can compare CTD and bottle oxygen values on some cruises.]

Weather information is sometimes noted on cast log sheets. Air temperature provides a clue to on-deck warming (and possible degassing) or freezing (especially harmful to salinity samples). Wind speed or sea state clue the analyst to possible sample contamination by wave slap during recovery, or provide a rationale for an aborted cast. Precipitation is potentially damaging to

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<sup>1</sup> With demonstrated at-sea net precision for dissolved oxygen now near  $\pm 0.05\%$  for a few groups doing this type of work, oxygen sampling perhaps should precede helium sampling. But a better way to think about this is that CFC, helium, and oxygen sampling should follow upon each other in close succession, especially when duplicate CFC or helium samples are to be drawn. [The authors has noted clear degradation in bottle oxygen — presumably from addition of headspace gas — when larger-than-usual amounts of water were drawn before oxygen sampling or when there was untoward delay in availability of a Niskin bottle for oxygen sampling once the air vent was opened.]

samples collected without benefit of weather protection. Hence it can prove worthwhile to provide the data analyst with weather data via routine weather logs or expanded station headers.

### 3.5 Matching laboratory data values to the water samples

When the analysts for each water property complete their work in the laboratory, they report their values to a person or group designated to merge their data with other bottle data parameters (and the CTD data associated with the closure of the Niskin bottle). **It is crucial that the scheme used to identify and merge co-located data not be dependent upon the value of any measured parameter.** By far the most common mistake in this regard is use of depth (or pressure) as an index parameter for bottle data. The laboratory analyst should not report the outcome of a measurement as "the value at station X at YYY meters". What if the CTD/rosette team later determined that the bottle actually closed at some other depth than originally assumed? Instead, the laboratory should report with respect to a unique and unchangeable index number.

**It is very strongly recommended that all reported water sample data be indexed by cruise, station, cast, and sample (or bottle) number.** The ideal data delivery from the analyst will then be something akin to an ASCII table, each column clearly labeled, with the first four columns being cruise, station, cast, and sample (or bottle) number, followed by columns for the measured parameters and (usually) the data quality codes for each parameter from that analyst. Once this scheme is established with all groups who are reporting water sample analysis results, this greatly simplifies and makes much more reliable the task of the person(s) who will merge the disparate data from various analysts together to provide the total data for each rosette bottle.

## 4. ASSESSING THE QUALITY OF THE MEASURED PARAMETERS

Assessment is a key aspect of the production of reference quality hydrographic data, especially when accompanied by documentation of the activity and results. Various approaches and schemes are used by different specialists. In general the care and experience of the analyst and the analyst's access to complete records are of greater importance than the particular approach or scheme used.

Data evaluation should begin at sea. This is usually the only time all involved personnel and all records are together. There the analyst can work with each measurement team to help determine if the values for each parameter are correct. And early intervention at sea makes it possible to correct repetitive problems before they can further degrade the data.

The analyst must determine if the appropriate standards were met by the bulk of the data, and that quality standards are applied consistently. Emphasis should be placed on adherence to proven, documented methodology over agreement with historical data. The analyst also determines which individual data values are suspect. This is partly a matter of identifying outliers and assessing their severity and cause, or verifying by absence of cause or coincidence with other data that the anomalies are likely genuine. Suspicion of a data problem based on a data value alone, without probable cause for an erroneous value, should normally not of itself be cause to demote the quality of a value. Finally, the analyst should work with the measurement teams to see that apparent problems are corrected if possible.

The analyst's report is a crucial element of the data documentation. It and a report of subsequent actions must be archived. It is best to include these in a cruise data report which also contains information about the cruise, a summary of data acquisition and processing methodology, data quality information, and a complete list of contacts for further information regarding the cruise, methodology, and the data.

The data evaluator endeavors to uncover causes for problems and, if possible, make corrections. With patience, luck, and complete records, it is interesting what can be accomplished with an open mind and a relentlessly thorough approach. There are many different approaches to data evaluation, depending on the oceanographic regime, the parameters available and/or in question, and the preferences of the analyst. Although each cruise is unique, there are several primary questions, in general following a hierarchy:

- (1) Is each parameter correctly identified with all its companion values?
- (2) Did the quality of the water in the water sample meet expectations?
- (3) Are there problems with any of the individual analyses?

Because so many sources of data errors are solvable if one has access to the original methods and data, the primary data evaluation should be done by the data originators at sea. An evaluator not affiliated with the cruise can often provide only educated guesses and offer suggestions on methods to improve measurements in the future.

Providing strong and routine (i.e. daily) data evaluation at sea is especially important for the obvious reason that the sooner problems (e.g., leaky or contaminated bottles) are uncovered, the sooner they can be fixed. While some problems with the casts are obvious to the sampling crew, other problems, such as unseen rust on a bottle spring (which contaminates  $\text{PO}_4$  analyses in particular), are uncovered by only one analyst, who may or may not have time or tools to examine the data.

One advantage of rigorous, complete record keeping is that if no probable cause for error can be uncovered, and if the characteristics of a suspicious water sample do not violate some solid physical/chemical principle, one can more readily and with relatively clear conscience leave the suspicious value flagged as "good", i.e. simply assume it is correct.

Also, it is usually easier to identify problem data when there are few of them. And so the situation becomes more challenging for the analyst when problems occur at multiple levels within the hierarchy. On the other hand, many types of problems reoccur until solved, and so show up in a distinctive pattern. The main problem then is to distinguish the pattern of the error from the patterns generated by true oceanographic signals.

Documenting and understanding the quality of the water sample inside the Niskin bottle is carried out jointly with assessing the water sample data for individual chemical characteristics, i.e. the performance of drawing and analyzing the sample, and standardizing the result. Hence because water sample results are used for sampling level verification, checks of sample integrity, and assessment of the analytic performance, there is interdependency that can lead to confusion.

Excessive noise and errors indicate a failure of methodology, so it is always important to examine failures and problems with an eye toward methodology. Replicate sampling programs can provide a useful guide to the field precision of the analyses, and hence to the expected noise level in the data set. Also, the method of drawing and storing the water samples should be taken into account by the data analyst. For example, sample storage is known to produce degradation of results, such as the tendency for salinities to be randomly high (due to evaporation from improperly sealed samples), for silicate to polymerize in frozen samples, and so forth.

Depending upon the amount of information available, some of the techniques discussed in the following may be useful. More important than any specific scheme, however, is the care of the analyst and access to complete records.

#### **4.1 Preparing for the data examination**

The first task of the data analyst is to assemble the records from the expedition, including the data files in the expected configuration and formats. Ensure that the data files are resident on a computer which supports the graphics packages used for evaluation. Preparing the data files is not always straightforward. For example, some data evaluation techniques require that data be considered on a cast-by-cast basis, and where multiple casts exist at a station, these must be sorted out. But the formats of the data as received may not provide for cast discrimination in the manner required by the graphics software on the evaluator's computer. (It's amazing how much time is spent just getting all the pieces together.)

At this point it is useful for the analyst to review the records, with an eye to omissions and errors, but most importantly to obtaining a sense of the overall performance of the sampling programs during the expedition. Were there unusual problems? Do the records indicate adherence to accepted methodologies? The experience of the analyst is crucial at this stage in evaluation, partly because it is during this review that the overall correctness (or accuracy or standardization) of the data is first assessed.

#### **4.2 Examining header and index data**

The various header and index data should be reviewed. Missing values should be completed, data entry errors corrected, and any omissions noted in the assessor's records. Often there are small adjustments necessary to preliminary values for these parameters, such as taking into account the transducer depth for depth-to-bottom values.

Thinking of the bottle data file as an ASCII table or spreadsheet-like document, it is important that the analyst verify that the headers for each column of the bottle data file are exactly correct and complete. Does every column have a title (header)? Is every header correctly aligned with its data? Does every column of measurement values have the units listed? Are the units shown exactly correct? (More about units later in this document.)

The bottle data file should be arranged so that the list of stations and casts is temporally ordered, from the first cast at the first station to the last cast at the last station. The WOCE protocol of reporting data on a cast basis should be followed. In other words, if there are multiple casts at one station, all the data from the first reported bottle cast should appear as a sequence, followed by the bottle data from the next reported cast, and so on. The data from multiple casts at a single



station should not be interleaved, for example mixed together and sorted by pressure. Also, it is strongly preferred that the data for each cast be sorted by increasing pressure.

Errors in cast dates and times may be found in preliminary data files. For example, if, as recommended, the position, date, and time of the cast reported are those attending to the time the cast was at its deepest level, it is understandable that the cast date could get confused when a cast takes place over the time of a date change<sup>1</sup>. The analyst should thus stepwise inspect the list of cast dates and cast times to see that they are sequential and without unexplained gaps.

Errors in reported station position arise from a variety of causes. Thus the analyst should make a computer plot of the station positions - using the values in the data files - on a map at an appropriate scale, with bathymetry if feasible. Station numbers should appear on the map in logical sequence without duplication, and in general the layout of the cruise track and station positions should match expectations. The depth-to-bottom listed for each station should conform to known aspects of local bathymetry.

Some analysts use station start and end times, plus positions, to calculate implied on-station drifts speeds and inter-station transit speeds, with unusual values pointing to probable errors in reported station times and/or positions.

It can be useful for bottle section data to prepare a section plot showing simply one symbol for each sampled level. (Such a plot would be similar to the plot in Section 2.1.) This plot can draw the analyst's attention to unexpected gaps in plotted horizontal or vertical coverage, or unusual incidence of multiple casts at a single station (sometimes an indication of problems).

### 4.3 Quality codes (quality flags)

The data files should contain quality codes (also called quality flags or quality bytes) for each measurement and for the water bottle itself. Standard community data formats, such as the WHP-exchange formats recommended for WOCE and CLIVAR CTD/rosette data, provide for quality codes. The simplest implementation - this is what is used in the WHP-Exchange formats - is to provide a data column for a quality code immediately to the right of each parameter. There are different schemes for assignment of quality codes. Here we will show both the WOCE and IGOSS - Integrated Global Ocean Services System - quality code schemes. It is very important that each quality code column be labeled with a name that unambiguously associates it with the correct parameter and with the quality code scheme used. The suggested scheme is to form a one-word column label which combines the name of the parameter, the word "FLAG", and a mnemonic for the quality code scheme, as in NO3\_FLAG\_W, from:

Quality Code	value of "a"	Comments
PARAMETER_NAME_FLAG_a	W = WOCE quality flag. I = IGOSS quality flag.	The parameter name of a data flag should be identical to the actual parameter name, followed by "FLAG" and then by a character indicating the type of quality flag, with underscores between each word.

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<sup>1</sup> The time the cast is at its deepest level is usually the time when the first (and deepest) bottle on that cast is closed, and so can be thought of as the time of the beginning of the bottle cast.

Some users may wish to translate the WOCE quality codes into the more widely recognized IGOSS quality codes. See table below.

The WOCE quality codes for the water bottle itself are:

- |   |  |
|---|--|
| 1 | Bottle information unavailable.  |
| 2 | No problems noted.   |
| 3 | Leaking.   |
| 4 | Did not trip correctly.  |
| 5 | Not reported.  |
| 6 | Significant discrepancy in measured values between Gerard and Niskin bottles.  |
| 7 | Unknown problem.   |
| 8 | Pair did not trip correctly. Note that the Niskin bottle can trip at an unplanned depth while the Gerard trips correctly and vice versa. |
| 9 | Samples not drawn from this bottle.  |

Flags 6, 7, and 8 apply primarily to large volume samplers.

The WOCE bottle parameter data quality codes are:

- |   |  |
|---|--|
| 1 | Sample for this measurement was drawn from water bottle but analysis not received. Note that if water is drawn for any measurement from a water bottle, the quality flag for that parameter must be set equal to 1 initially to ensure that all water samples are accounted for. |
| 2 | Acceptable measurement.  |
| 3 | Questionable measurement.  |
| 4 | Bad measurement.   |
| 5 | Not reported.  |
| 6 | Mean of replicate measurements (Number of replicates should be specified in the .DOC file and replicate data tabulated).   |
| 7 | Manual chromatographic peak measurement.   |
| 8 | Irregular digital chromatographic peak integration.  |
| 9 | Sample not drawn for this measurement from this bottle.  |

The WOCE CTD data quality codes are:

- |   |                                     |
|---|-------------------------------------|
| 1 | Not calibrated.                     |
| 2 | Acceptable measurement.             |
| 3 | Questionable measurement.           |
| 4 | Bad measurement.                    |
| 5 | Not reported.                       |
| 6 | Interpolated over >2 dbar interval. |
| 7 | Despiked.                           |
| 8 | Not assigned for CTD data.          |
| 9 | Not sampled.                        |

The WMO IGOSS observation quality codes are:

0	No quality control yet assigned to this element
1	The element appears to be correct
2	The element is probably good
3	The element is probably bad
4	The element appears erroneous
5	The element has been changed
6 to 8	Reserved for future use
9	The element is missing

A perfect translation is probably not feasible, but the following WOCE-to-IGOSS (not IGOSS-to-WOCE) translation rules as reasonable:

	WOCE	IGOSS
<b>bottle</b>		
	1	0
	2	1
	3	3 (see <a href="#">note #1</a> )
	4	4
	5	0
	6	4
	7	4
	8	4
	9	9
<b>water sample</b>		
	1	0
	2	1
	3	2 (see <a href="#">note #2</a> )
	4	4
	5	0
	6	2
	7	2
	8	2
	9	9
<b>ctd</b>		
	1	0
	2	1
	3	2 (see <a href="#">note #2</a> )
	4	4
	5	0
	6	2
	7	2
	9	9

Note #1:	In the interest of being conservative, it is preferred to translate the WOCE bottle quality code 3 into IGOSS quality code 3. A leaking water sample bottle typically results in a discrepancy or error in gas samples, such as oxygen and CFCs, but less often results in data discrepancies for salinity and nutrients. It is suggested that data users who wish to import only "good" data not import any water sample data from bottles with a WOCE code 3 or IGOSS code 3. A data user who is willing to entertain slightly greater risk might choose to import non-gas sample data (e.g., salinity and nutrients) from a WOCE code 3 or IGOSS code 3 water sample bottle, and allow import of gas sample data (e.g. oxygens and CFCs) for bottles with IGOSS Code 2. (The CCHDO is not, however, currently assigning IGOSS code 2 to water sample bottles; but future data originators or data centers may wish to use code 2.)
Note #2:	The CCHDO has noted that in general, data originators tend to be conservative and so in DQE reports many WHP code 3 ("questionable") water sample parameter data are deemed WHP code 2 ("good") by the examiners. The IGOSS code 2 ("probably good") seems to be a reasonable interpretation. The CCHDO is not currently assigning IGOSS code 3 ("probably bad") to WHP water sample data values.

#### 4.4 Examining data values

There are three key questions: (1) Have the appropriate standards been met by the bulk of the data? (2) Which data are suspect? This has to do both with determining which data deviate from the appropriate standards and also with determining that all data have been assigned to the correct trip level/depth. (3) Can the problem(s) be corrected? This recognizes that many problem data can be recovered either wholly or to a useful degree.

Assessment of the first involves — ideally — following the paper and file trail for each parameter to see that the methodology was followed and in particular that standards were applied correctly.

Assessment of the second and third issues — given a positive response to the first — is mostly a matter of identifying outliers and assessing their severity and cause. It must be emphasized that suspicion of a data problem based on an outlying data value alone, without probable cause for an erroneous value, should normally not of itself be cause to ‘flag’ a value as questionable. And, of course, it is often not clear exactly what causes an outlier.

This is worth expanding upon: The term “outlier” denotes bad or incorrect data in the minds of many, especially statisticians not familiar with real ocean variability. After examining many routine profiles, one tends to be lulled into thinking that it is ‘known’ what the ocean ‘should look like’, and then one too quickly flags unusual data points as questionable, or even omits them from the reported data. Outliers *are* cause for careful examination of data recording, standardizations, and computational correctness, but having done that, if no specific causes are found and the suspect value remains within the general realm of plausibility, it is usually best to let the value go as is. Often, when one can see together all of the data, including calculated parameters such as density, from a single station, the inter-relationships come clear between the various measured parameters of an unexpected or novel oceanographic feature.

Some anomalies are real features of the ocean. Larry Armi's story about discovering that samples from several "Meddies" (small blobs of relatively undiluted Mediterranean water in the North Atlantic) had been deleted from the old WHOI data files — due to their seemingly out of place very high salinities — comes to mind. Also, when stations are not spaced closely enough to resolve eddies, the eddies can be difficult to recognize. The meeting of water masses can result in considerable interleaving (though density compensated), seen not only on the CTD trace, but in chemical signatures also. Some examples of regions where that sort of interaction has been observed are the confluence of the Falkland and Brazil currents, the Kuroshio-Oyoshio extension, regions with Gulf Stream-Slope water interactions, the Mediterranean outflow, regions of sinking shelf waters off of the Adelie coast, the Agulhas retroflection, and probably many other regions as well. Seamounts have been implicated as well in shedding eddies and intermingling waters, the Maud Rise for example. Thus there is ample reason for exercising caution in rejecting 'odd-looking' data.

Any unusual features should be carefully checked in the original data and calculations. Many turn out to be simple errors and are easily correctable. Misread poor handwriting is most often the cause, and simple key entry errors, even after proofing, often slip by. Anomalies in one property are likely to be reflected in other properties. An inversion in oxygen is usually seen in inflections or inversions in phosphate, although if both persist in the same Niskin bottle, it could be due to exposed metal inside the bottle (this happened on the SIO Marathon expedition due to exposed metal bolts on the handle brackets). Also, a persistent isolated deep NO<sub>2</sub> maxima may be traceable to a particular dirty Niskin bottle, the 'feature' disappearing after scrubbing out the bottle. Extraneous NO<sub>2</sub>s have also been traced to particular sample collection tubes that had not been cleaned out often enough<sup>1</sup>.

#### *plot software*

Often, data evaluators have at hand software for plotting, data quality code assignment, and other tasks. There are also various public domain software packages useful in data evaluation. The program "Ocean Data View" (<<http://odv.awi.de/>>) is used by some. The author and developer John "Oz" Osborne created the application Java OceanAtlas (<<http://www.oceanatlas.com/>>) partly with data evaluation tasks in mind. Both Ocean Data View and Java OceanAtlas work on a wide range of computer operating systems (Windows, Mac OS X, Linux, and UNIX). The newest versions of Java OceanAtlas (JOA 5 and above) contain editors for assigning and changing bottle and parameter quality flags, and can export WHP-Exchange data files. The CLIVAR and Carbon Hydrographic Data Office (CCHDO) has - and can distribute - a version of JOA which can merge the parameters from a bottle data cast received from the various analysts.

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<sup>1</sup> Genuine "odd" NO<sub>2</sub> features are possible where the ambient water dissolved oxygen concentrations are extremely low, such as in the northern Indian Ocean and off Peru. When that occurs, the NO<sub>2</sub> is from the reduction of NO<sub>3</sub>, and so in those circumstances there will be a local reduction in NO<sub>3</sub> concentration as well.

From the ODV web site (in the grey box):

Use ODV to produce:

- \* [property/property plots of selected stations](#) (45kB),
- \* [scatter plots for sets of stations](#) (120kB),
- \* [color sections along arbitrary cruise tracks](#) (70kB),
- \* [color distributions on general isosurfaces](#) (100kB),
- \* [temporal evolution plots of tracer fields](#) (47kB),
- \* [differences of tracer fields between repeats](#) (49kB),
- \* [geostrophic velocity sections](#) (68kB).
- \* [animations](#) (3MB).

ODV can display original data points or gridded fields based on the original data. ODV has two fast weighted-averaging gridding algorithms built in and also allows integration of the advanced [DIVA gridding software](#) as an optional package (ODV version 3.4 and higher). Gridded fields can be color-shaded and/or contoured. ODV supports five different map projections and can be used to produce high quality [cruise maps](#) (20kB). ODV graphics output can be sent directly to printers or may be exported to PostScript, gif, png, or jpg files. The resolution of exported graphics files is specified by the user and not limited by the pixel resolution of the screen.

The ODV data format allows dense storage and very fast data access. Large data collections with hundred thousands of stations can easily be maintained and explored on inexpensive desktop and notebook computers. Data from the [World Ocean Circulation Experiment \(WOCE\)](#), the [World Ocean Database](#), the [World Ocean Atlas](#), and the [Medar/Medatlas projects](#) can be directly imported into ODV. Ready-to-use versions of the WOCE data, the gridded World Ocean Atlas 2005 and 2001 as well as many other important geo-science datasets are available for [download](#).

ODV also supports the [netCDF](#) format and lets you explore and visualize [CF, COARDS, GDT and CDC compliant](#) netCDF datasets. Climate data in netCDF format are available [here](#).

Optional high-resolution coastline, bathymetry and topography sets are available for [special regions](#). Additional sets for your region of interest can be produced on [request](#). Note that there is a charge for this extra service.

ODV is used by more than 9000 scientists at leading research institutes world wide. The [UNESCO Ocean Teacher](#) project employs ODV as one of its main analysis and display tools. In addition, ODV is used as visualization tool for the [Pangaea](#) information system. Pangaea data sets can be easily converted into ODV collections using the [Pan2Applic](#) application. Data in TGM-3M format can be converted using the TGM2ODV Windows application ([english](#) / [russian version](#)).

From a Java OceanAtlas-related web site (in the grey-shaded box):

Java OceanAtlas (or simply JOA) is a software application for viewing and manipulating oceanographic profile data. JOA was designed primarily for oceanographic sections but is also useful for looking at data also in the latitude-longitude domain. Here's a brief list of what JOA can do:

**Open a wide variety of standard oceanographic profile data files** including EPIC netCDF (bottle, CTD, and XBT), WOCE bottle and CTD "EXCHANGE" files, WOCE netCDF bottle and CTD files, spreadsheet or tab-separated value, NODC SD2, and Mac OceanAtlas binary files. JOA can also open EPIC pointer files and zip files containing any of the accepted individual file formats. CTD files can optionally be decimated to a user-defined interval, standard depths, or to custom depths. JOA can perform sophisticated filtering of WOCE data values by quality codes.

**Powerful data collection filtering and selection via [NdEdit](http://www.epic.noaa.gov/epic/ewb).** NdEdit allows a user to open an EPIC pointer file (created by 'epicselect' on UNIX systems or the web version of epicselect at <<http://www.epic.noaa.gov/epic/ewb>>), filter in latitude, longitude, depth, and/or time and open the selected data files directly into JOA for analysis. See the following page for more information about NdEdit: <http://www.pmel.noaa.gov/epic/software/JavaNdedit.htm>.

**Property-property plots, profile (waterfall) plots, station value plots, contour plots, residual contour plots, and maps in a variety of projections with coastlines and bathymetry.** Property plots and profile plots are automatically colored by a third parameter and T-S plots can have optional isopycnal overlay. Contour plots and residual contour plots can be created using distance offset between stations or offset by latitude or longitude. Maps can optionally color station symbols by value of a parameter interpolated onto an isosurface. For example, you could make a map of salinity interpolated onto pressure surfaces or plot the surface temperature. All plots are resizable and areas of interest can be extracted to new plot windows.

**Linked browsing between all views.** Clicking on a point in any plot will identify the same point in all other views. A central data window shows the values of parameters at the selected point.

**Wide variety of built-in calculated parameters** including (potential temperature, density (built-in and custom reference pressures), heat storage, specific volume anomaly, spiciness, sound velocity, O2 saturation, AOU, NO, PO, Brunt-Vaisala frequency, squared Brunt-Vaisala frequency, potential vorticity (all buoyancy frequency calculations have settable e-folding length), alpha, beta, acoustic travel time, net heat content, potential energy anomaly, and geo-potential anomaly. A custom calculator can be used to create new parameters by arithmetic operations and derivatives on existing parameters.

**Station Calculations.** JOA can calculate the mixed-layer depth using a variety of techniques (slope, surface layer, and difference) with user-settable tolerance. JOA can calculate the integral (or weighted average) of any parameter between surfaces defined by any other parameter. For example, the integral (or weighted average) of salinity can be computed between two user-settable density surfaces.

**Plots can be filtered by station or observation criteria.** Station filters include geographic region, missing parameters, and individual station selection (include or exclude selected stations). Observation filters consists of up to 4 criteria that can be grouped using and/or logic. A criterion can test whether a particular parameter is inside (or outside) a given range or whether it's quality code (if present) matches a certain value. Plots can show or highlight the observations that match the filter criteria.

**Extensive customization for your data or area of interest.** JOA has tools for creating color bars (used for coloring plots as well as contouring), interpolation surfaces (used for contour plots), and color palettes. JOA also can save custom map settings, observation filter settings, and custom CTD decimation schemes. Existing sections can be sorted by latitude, longitude, date, and station number.

**Plot output can be printed, saved to GIF files or "printed" to Postscript files** (Windows and UNIX). MAC OS-X can print graphics to PDF files.

Instructions for the use of Ocean Data View or Java OceanAtlas are outside the scope of this document. One obvious point should be noted, however, and that is that inconsistencies in data files - compared to the format definitions - can easily disrupt importing data into ODV, JOA, or any other plotting or editing application. Thus one of the first tasks of the data evaluator is to see that the data files are prepared to be compliant with the data import requirements of the plotting and editing applications. This is sometimes difficult. One suggestion is that one take a careful look at a data file which successfully imports into the application vis-à-vis the data file at hand. Often this will promote the insight needed to make the necessary file adjustments for successful data import.

#### *single- and multi-parameter plots of profile data*

A scatter-plot of the data for a given parameter, plotted against pressure, can help to locate egregious outliers as well as clusters of similar values, and can be used to determine the axis ranges appropriate to shallow, intermediate, and deep layers. If the plotting program permits values on the scatter plot to be highlighted one cast at a time, for example by joining the values for that cast by lines (JOA has this feature on property-property plots), the individual profiles can be quickly examined vis-à-vis their peers; outliers may pop into view.

A plot useful for uncovering a chronically leaking bottle is to plot the bottle oxygen and/or CFC data versus bottle number (instead of versus depth or pressure). Non-oceanographic high numbers over a group of stations may indicate a leaking bottle. Plotting PO<sub>4</sub> versus bottle number can sometimes help locate a bottle with rust on its spring. (The author has also tried plotting dissolved oxygen data - and/or the CTD-minus-bottle oxygen difference - versus the oxygen flask number to help ferret out a suspected miscalibrated oxygen flask.)

Although it is useful and proper to closely examine the data for each parameter individually, valuable insight into data quality issues can be obtained by examining data for multiple parameters collectively, one station at a time or in small groups of stations. For example, profile data for a suite of parameters can be plotted versus depth or pressure, using axis scales for each parameter that allow each parameter to be viewed with sufficient sensitivity to detect subtle features. For example, as part of his evaluations of the "routine hydrography" bottle data (CTDO



at bottle trips, S, O<sub>2</sub>, and nutrients), the author makes 7-parameter plots against pressure - choosing from  $\theta$ , bottle S, CTD S (the CTD S corresponding to the bottle S), O<sub>2</sub>, CTD O<sub>2</sub>, SiO<sub>3</sub>, NO<sub>3</sub>, NO<sub>2</sub> and PO<sub>4</sub>, or a density parameter - one cast at a time (but with "live" switching to profile plots for adjacent casts) with axis ranges optimized for either shallow or deep parameter ranges in order to increase the resolution of deep, low-gradient zones. The author also routinely examines PO<sub>4</sub> versus NO<sub>3</sub> plots and  $\theta$ -S plots, as well as any others which can help illuminate the data and data problems. Oceanographic signals feature co-variability in certain parameters that is usually unlike the signal of error in an analysis. It should be noted, however, that an "oceanographic-like" property signature can accompany a serious in-water malfunction of a water bottle - for example a bottle for which one end cap closed at the intended level but the other end cap did not close for minutes (and many meters) later. The bottle may only partly flush in the interim, giving rise to all the measured properties appearing to represent some odd, erroneous blend of water from different levels. Sometimes such errors take place for the same bottle on successive casts, and if the bottles are tripped near the same level at those casts, one might assume the odd values are genuine. This can be a data assessment challenge, but usually some aspect of the situation convinces the data assessor that there is a problem with the bottle.

#### *plotting vertical sections*

Another rewarding way to view the data is via sections of the characteristics. Besides providing a spatial perspective on the data, vertical sections highlight problems with depth assignments for the bottles, at least when the error in assignment exceeds the depth variations reasonable from the local gradients. By scanning through the parameters, and by fine tuning the contour intervals, one can quickly and profitably explore a data set.

#### *effect of numerical methods*

The numerical methods used in data processing can themselves produce various data problems. Different numerical techniques applied to similar data, or inconsistent application of numerical techniques, can lead to often overlooked effects on reported parameter values. A good example is in the processing of CTD data, and this is quite apart from any issue of subjectivity arising from processing by different analysts. Some common sources of problems:

- Pressure reversals due to ship roll during CTD cast operation are treated differently by different CTD groups and institutions. Inclusion in vertical bin averaging of CTD scans from upward CTD excursions (caused by ship roll) during CTD down casts can increase the amount of unstable density structure reported from a vertical profile, particularly for data collected when the ship is riding a rough swell. This is undesirable.
- Despiking routines which are not based on the known physics of the sensors can lead to fictitious T-S features in a CTD profile. Examples of unsound techniques are averaging or interpolating through spikes. In general it is preferable to leave a gap in a record, or if quality bytes are associated with each reported CTD level, to use a "bad" or "doubtful" quality indicator, rather than to substitute artificially "clean" values for measured values.
- Station-number-dependent CTD conductivity calibration corrections should properly reflect the observed changeable behavior of the conductivity sensor, and at the time scale appropriate to that sensor. If a station group is not fine or accurate enough, calculated CTD

salinity for entire stations can be biased. Such biasing will not be revealed through a single, entire-cruise standard deviation value of the salinity residuals (e.g. CTD minus bottle salinity). Instead the progressive change of standard deviation and mean between individual stations must be closely examined.

- The order in which the following numerical steps are applied can lead to subtle differences in profile structure:

treatment of pressure reversals  
application of sensor lag filters  
vertical binning of data  
application of calibration coefficients.

- Different methods for surface pressure offset calculation can lead to correction values differing by up to 1 dbar.

#### *sample indexing and offsets*

The data values in the final bottle data file for a cruise are typically merged from several different sources, some fundamentally different from others. For example, during the cast itself the computer may assign to each sample identifier a set of CTD values garnered at the time each bottle is closed (or, more correctly, at the time the bottle is *assumed* to have been closed). These "CTD data values at bottle trips" may be slightly adjusted by subsequent CTD data processing, or be grossly corrected when errors in sample identifiers vis-à-vis sampling levels are corrected. (Note that some of the chemical analysts who copy down preliminary information from the CTD may not learn of the data problems uncovered post-cast, and even months or years later still be working from wrong CTD information.)

Because the pressure value at sampling time may be mis-assigned or later corrected it is critical that data for individual parameters *not* be indexed by pressure or depth. Instead, unique sample identifiers *must* be used. This is especially critical for the shore-analyzed tracers, which should always have non-depth-based identifiers as their primary labeling. Any marking of sampling depth on sample containers should be ancillary to the primary cruise/station/cast/sample label and labeled "intended depth" or "provisional depth". Shore laboratories should never trust a depth value taken from a label on a sample container labeled at sea before or during sampling.

Each original data sheet for the station at hand is looked at for any comments as to problems and how they were resolved. Occasionally the temperature curve will look fine — it is derived from the CTD — but the water samples will appear to be one or more levels off. Careful comparison with the CTD bottle closure/trip file and the *intended* sampling depths recorded on the console operations log sheet will verify that the water samples have been assigned the wrong depths (and temperatures), usually caused by a ramp-shaft error on the pylon or redundant trips recorded and mis-assigned.

Once the correct trip depths have been verified by comparison of the lab data with the CTD, detailed examination of the station data is begun.

Thus during data assessment the data originators should carefully comb through the merged files to see that all bottle data are correctly identified and merged. The sample identifiers are the key, of course, much reinforcing the notion that *any problems with sample identifiers must be sorted out at sea as soon as possible after a cast.*

## *QC*

The data for each profile for each parameter should be examined closely. This is most profitably done first at sea, by the analysts for each parameter if they have appropriate expertise. Sometimes when student or temporary analysts are assisting in the analyses (often the case for salinity analyses, for example), it is necessary that a senior analyst take on this task.

### *a. bottle QC*

Small leaks in bottles can be an especially difficult problem to detect. For air leaks gas samples are the key, with oxygen values often the primary choice. But when high-quality CFC data are available, the CFC values can in some cases provide a better air leak indicator than oxygen values, because atmospheric CFC concentrations are high compared to values over most of the water column. The turnaround time for preliminary CFC results is usually only a few hours. All gas samples must be discarded from a bottle with an air leak visible in the CFC or oxygen data. However, it is not always necessary to discard (or flag) the data for dissolved matter (salinity, nutrients) from such bottles.

In-water leaks have a different effect on the data, essentially contaminating the entire sample, resulting in discard of data for the entire level (unless the CTD values which were set aside at the bottle trip are still desired in the discrete data file). The signatures of some in-water leaks are subtle, and so the analyst must examine the data with an eye for a suite of measured values showing signs of addition of water from those parts of the water column passed through after bottle closure. If the leak was generated at the sea surface -the mechanical stresses on the bottle lids are higher there (for example, consider wave slap) -it can be simpler to identify such leaks because surface waters usually have high gas concentrations and distinct patterns for other tracers.

### *b. salinity QC*

The bottle minus CTD salinity should be examined near the beginning of data evaluation, because for bottles with correct ("good") salinities this check helps to verify that the sample really came from its intended sampling location. In ocean regions with a vertical salinity gradient this check is sensitive. But the bottle salinity values themselves must be correct. For example, a common cause of larger than usual bottle minus CTD values arises when the salinometer drifts during successive fills during analyses. Usually the best agreement will be in the first few fills of the salinometer, in which case that is the "best" bottle salinity and should be the value reported.

Station to station analytical salinity consistency may be examined by plotting the mean bottle salinometer salinity minus the raw CTD salinity for each station versus time. This scatter plot is most useful for detecting CTD sensor drift or sudden offsets, but it can also be used to identify poor salinometer runs (most often due to faulty standard seawater ampoules — a problem more common in some batches than in others). If a plot of the raw CTD  $\theta$ -S in some deep uniform part of the profile is similar to that from adjacent stations, but the bottle-CTD salinity differences are not, then the salinometer results are suspect.

There is a tendency to throw out salinities that do not agree closely with the CTD, yet those salinities may truly represent the water that is in the Niskin bottle. This can be a problem, especially in high gradient regions. The CTD is commonly mounted below the water sample bottles, and thus real differences may arise when the trips occur in strong vertical gradients in salinity. Also, all sampler bottles have a finite mixing length (Weiss, 1971) and require a pause at the desired sampling depth, with duration longer than one or two ship rolls, to collect a sample best representative of that depth. If the console operator trips the bottle immediately upon arriving at the desired depth<sup>1</sup>, the bottle will still contain some water from below and will not be quite representative of the desired depth. Not only the salinity but also all of the other analyses from that bottle will be slightly contaminated with deeper water. (This type of error is most readily visible in high gradient regions.) If the salinity analysis itself is not suspect, the salinity truly reflects what is in the bottle at the time of closure, so it should not be deleted, because it serves to indicate that values for the other parameters are likely somewhat depth-smeared also. [There is also the effect of wire and rosette wake to be considered.]

One must remember that salinity is a calculated, not measured, parameter. Errors in CTD pressure and temperature may strongly affect calculated CTD salinities. [For this reason, CTD processing technicians are advised to correct CTD conductivity, not salinity, by converting bottle salinities to conductivities after CTD pressure and temperature have been corrected.] Similarly, density is a calculated parameter, and so indexing data examination to density-related parameters introduces potential interdependencies that can mask the true cause of an apparent problem.

The tabulation of the differences between the individual bottle salts and the CTD salinities are scanned for consistency to verify that the rosette sampler did indeed sample the water from its assigned depth.

### *c. oxygen QC*

A "bottle minus CTD" bottle oxygen check may be better than a salinity check for verifying the actual sample depth in regions where the salinity structure is weak, but where there is significant vertical gradient in dissolved oxygen. Consistency helps to verify that the rosette sampler did indeed sample the water from its assigned depth.

Regarding apparent dissolved oxygen outliers, the data analyst should examine the analytical data to see if there are any obvious errors in titration end point detection, or if the correct flask volume was used in the calculation.

On the oxygen standard graph, the oxygen analyst should look to see if two or more iodate standards were used on the leg and gave reasonable agreement ( $\pm 0.1\%$ ) on the normality of the thiosulfate. If not, either a weighing or preparation error has occurred (a bad batch from one manufacturer was identified on a past cruise), and the correct one must be resolved. Plots of reagent blanks are also examined, but it is not unusual for reagent blanks to change with a

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<sup>1</sup> An extra 20-second wait at each winch stop (for bottle closure) on a 120-station cruise with a 36-place rosette will add one day to the cruise duration. But it can be shown that the wake of the rosette takes approximately that long – up to 20 seconds – to clear the vicinity of the rosette when the winch is stopped.

change in pickling reagents (particularly sodium iodide). Any individual high or low standardizations are looked at to make sure that the data calculations were not adversely affected.

If there are oxygen samples from multiple bottles in the surface mixed layer - or another layer known to be homogenous with respect to dissolved oxygen - the degree to which the oxygen concentrations from different bottles agree will provide an indication of the achieved total precision. On some cruises that agreement has been near the  $\pm 0.01 \text{ ml l}^{-1}$  level.

#### *d. nutrient QC*

During nutrient QC, one common error for which the nutrient analysts should be on alert regards the peak height value. A spike in the colorimeter peak may be incorrectly tabulated as the sample peak value. Such mistakes can be corrected by the nutrient analyst if the complete peak data are retained and plotted.

Deviations from linear  $\text{PO}_4/\text{NO}_3$  slopes may point toward erroneous nutrient values, but also may be true where reduction in  $\text{NO}_2$  has happened, or in data from anoxic basins where the  $\text{NO}_3$  is reduced, and where  $\text{PO}_4$  is released from the sediments (results in an odd hooked shape  $\text{PO}_4/\text{NO}_3$  plot).

Plots of nutrient standards usually reveal the inherent instability of automated nutrient analyses; some methods are quite sensitive to ambient operating temperature conditions. The technique is also operator sensitive, some producing much more consistent results than others. While the plots are usually noisy, they may help sort out apparent shifts in one parameter relative to another. For example, if the nitrate curve shifts relative to bracketing stations but phosphate does not, the standard graph may help sort out the problem. It may turn out that the raw sample absorbances are similar to those from adjacent stations but the calculated concentrations are not, pointing to a likely standardization error. Plots of Beer's Law are also checked for linearity and to see if the non-linearities common to the nitrate and silicate analyses were handled satisfactorily. On a cruise in 1985, the data analyst discovered an interesting "diel" signal in upper water column silicate values: silicates from samples collected at night consistently differed slightly from those collected during the day watch. He subsequently traced this to the fact that the filled nutrient sample containers from the night watch were stored in the refrigerator, and the nutrient analyst - who was working the day watch - was inadvertently failing to re-warm the stored samples to the same temperature as that of the daytime samples which were being run immediately following collection, without chilled storage.

#### *doubtful data record*

The data analyst, working together with the data provider(s), must prepare a record of the examination, including a summary report, identification of problems, and suggestions and/or actions on corrections. The report should be archived with the data records.

For example, below are the data examination records from two stations occupied during the WOCE Hydrographic Program "A24" expedition, copied from the on-line data report <<http://cchdo.ucsd.edu/data/onetime/atlantic/a24/a24do.pdf>>.

#### **Station 025**

Cast 1 Sample Log: "Forgot to remove O2 sensor cover." No CTDO reported.

122 SiO<sub>3</sub> appears low. Nutrient Analyst: "Large gradient in nutrients." Data are acceptable.

118 Salinity is slightly high. No analytical problem found. PI: "High gradient." Salinity is acceptable.

117-120 NO<sub>3</sub> and PO<sub>4</sub> are high. Nutrient Analyst: "Large gradient in nutrients." Data are acceptable.

101 Salinity is high. Autosol diagnostics indicate 4 tries to get a good reading, indicating a problem with the samples. The first readings gave better results and are used in this salinity calculation. Salinity is acceptable.

101-131 Oxygen sensor cover left on. CTDO lost.

The station 025 record tells the future data user why there are no CTD oxygens at this station (the sensor cover was inadvertently left on). Some nutrients or salinities on cast 1, bottles 17-20 and 22, appeared high or low on first examination but the analyst noted first (not in the record) that no problems were uncovered with the analytical procedures or nutrient calculation. The analyst's subsequent observation that these somewhat high or low nutrient values came from high-gradient portions of the water column offered what seemed to that analyst to be sufficient rationale that those values could be left with a "good" quality code. The salinity for bottle 01 - the deepest bottle - was high (compared to the CTD). Apparently (the note is not completely clear on this) the salinity value finally reported was from early in the analytic run.

#### **Station 053**

122 High on N:P plot. Nutrient analyst: "Gradient, data is acceptable."

108 Sample Log: "Vent is open." Oxygen as well as other data are acceptable. SiO<sub>3</sub> is low. Nutrient analyst: "Probably bad, code questionable."

105 Delta-Sat 1618db is -0.0035. No analytical problems noted. Salinity agrees with adjoining stations. Gradient area, salinity is acceptable.

103 O<sub>2</sub> high. PI: "Doesn't fit in CTDO. Freon did not measure to assist in this. Doesn't match CTDO, but similar to Stas. 054 & 055. Oxygen is acceptable."

102 Oxygen: "PC lock-up, lost sample."

The station 053 record tells the future data user that a suspicious nutrient value from cast 1, bottle 22, was from a high gradient portion of the water column and so should probably keep a "good" quality code. [See author's note, above, regarding "high-gradient" notes in the station 025 record.] Bottle 08 was found by the sampling crew to have its vent open, but the oxygen data were acceptable so it was decided to keep the bottle and most parameter data coded "good". But a low silicate value at that bottle was out of place and so was coded "questionable". The CTD versus bottle salinity difference for bottle 05 was

a bit large (-0.0035) but was concluded to be acceptable. An oxygen anomaly at bottle 03 did not fit with the CTD oxygen (these are pre-SBE-43 CTD oxygen data), but did match a similar feature at the next two stations so was left as "acceptable". And, finally, the note explains why there is no bottle oxygen value for bottle 02 (problem with the oxygen rig's computer).

One can see that such notes, included in the on-line documentation, help future data users to understand the data, and alert them to issues they may wish to re-examine. Sometimes the notes are cryptic - but the added value is clear.

All groups generating reference-quality data are urged to implement a report system for data comments and to include at least a summary - if not the complete document (preferred) - for the archived documentation which will accompany the data files.

### *comparisons with historical data*

In general, the same types of plots useful for the internal consistency check are useful for the inter-cruise comparisons. Usually comparisons are made in some regime where low spatial and temporal variability are expected, i.e. a deep region well away from boundaries. Inter-cruise differences may help direct the analyst to specific data records and focus attention on likely problem areas. We tend to expect the more recent cruise to report the higher quality data, but this is occasionally not so.

Comparisons with archived data are important, but can be risky. Historical data are useful to find out what has been seen before in the region but they are not to be taken as 'truth' (e.g., cf. Mantyla, 1994). Secular changes do occur and frontal zones do migrate. Historically, oceanographers have noted that the deeper portions of many basins (but well above the bottom) can be remarkably uniform with no discernible differences between cruises (Saunders, 1986). From that viewpoint historical data can provide comfort and useful insight when they too show apparently anomalous features (provided that no one has deleted them first).<sup>1</sup> But temporal variations in deep ocean properties have been increasingly reported. Among the most widely and earliest recognized were deep changes in the northern North Atlantic Ocean, relatively close by water mass formation regions. But during the early 2000s, investigators carrying out repeat occupations of WOCE Hydrographic Program basin-scale transects began to report inter-cruise property differences at nearly all levels of the water column, in nearly all the oceans. The deep water changes were subtle, but consistent on a basin scale. If these changes are genuine, then (1) the deep water "reference" is only as useful as the size of the changes, and (2) the only way such changes can be observed reliably is via closely monitored, reference quality observations, following all aspects of recommended practice.

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<sup>1</sup> On a GEOSECS cruise to the southwest Atlantic, the CTD oxygen sensor showed five oxygen extrema, unlike anything one scientist had seen before. He cried out, "You would never see that on a Nansen cast!" Another scientist on the ship pulled down Sverdrup's 1942 "The Oceans" and found that Sverdrup had discussed all 5 features: they had been observed on a *Meteor* cruise in the late 1920's. Also, a Nansen profile done on the same GEOSECS station, but sampling blind (without reference to the CTD data), picked up evidence of all five extrema, though not at the extremes.

## Acknowledgments

Arnold Mantyla (SIO), the grand master of this craft, contributed text and a wealth of insight; he also reviewed the drafts. Mark Rosenberg (CSIRO) supplied much-appreciated advice and text regarding numerical processing methods applied to CTD data. This report rests on traditions of the Scripps Institution of Oceanography, and as such represents the contributions of many individuals who have helped shape knowledge and practices here. In particular Hans Klein directed the Data Collection and Processing Group at SIO, turning it into a first class operation, and Arnold Bainbridge directed the Scripps GEOSECS Operations Group, which took DCPG methodology into expanded realms. The author owes much to the past and present technicians at the Scripps Oceanographic Data Facility (the product of the merger of DCPG and GOG), whose dedication and expertise provide much to his research. Jerry Kappa edited and formatted the text and made many helpful suggestions. The author gratefully acknowledges the US National Science Foundation's support, which has enabled him to go to sea to learn and practice the methods discussed here, and their patience, which permits him to write non-research reports such as this one.

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# CONSOLE OPERATIONS LOG

Ship:		Expedition/Leg:			Operator:		Station/Cast:			CTD#	Raw Pressure on Deck: Start   End		Target Depth:		
Position	Bottle	TIME (UTC)			RAW READOUTS			Wire Out	Desired Depth	Comments:					
No.	No.	Stopped	Tripped	Confirm	Pressure	Temperature	Conductivity								
1															
2															
3											Cast Start: Date (UTC)				
4															
5											Time (UTC.HH:MM)				
6															
7											Latitude				
8															
9											Longitude				
10															
11											Depth, uncorr. M				
12															
13											Cast at Bottom: Time (UTC.HH:MM)				
14															
15											Latitude				
16															
17											Longitude				
18															
19											Depth, uncorr. M				
20															
21											Maximum CTD Corr. Pressure,DB				
22															
23											Distance above Bottom				
24															
25											Maximum Wire Out				
26															
27											Cast End: Time (UTC.HH:MM)				
28															
29											Latitude				
30															
31											Longitude				
32															
33											Depth, uncorr. M				
34															
35											Other Equipment:				
36															
Confirm Column: Enter check mark if confirmation received, O if no confirmation.												There must be a mark for every attempt to trip a bottle			

## SCHEME 2

## CONSOLE OPERATIONS LOG

Ship:		Expedition/Leg:			Operator:		Station/Cast:		CTD#		Raw Pressure on Deck:		Target Depth:	
Revelle		Iqn			SM/EK		138/1		381		Start 0.2 End 0.2		4600 4720 4730 4735	
Position	Bottle	TIME (UTC)			RAW READOUTS			Wire	Desired	Comments:		Station/Cast		
No.	No.	Stopped	Tripped	Confirm	Pressure	Temperature	Conductivity	Out	Depth					
1		00:57:05	00:57:45	✓	4785.5			4735	BOTTOM			13811		
2		01:01:27	01:01:58	✓	4598.1			4550	4550			Cast Start: Date (UTC)		
3		01:06:45	01:07:16	✓	4343.6			4300	4300			April 10, 2007		
4		01:14:45	01:15:16	✓	3937.4			3900	3900			Time (UTC.HH:MM)		
5		01:22:45	01:23:46	✓	3529.5			3500	3500			23.30		
6		01:31:06	01:31:39	✓	3123.9			3100	3100			Latitude		
7		01:36:30	01:37:01	✓	2870.4			2850	2850			2° 12.10S		
8		01:41:57	01:42:35	✓	2619.4			2600	2600			Longitude		
9		01:47:25	01:47:57	✓	2365.1			2350	2350			94° 7.92E		
10		01:52:37	01:53:08	✓	2112.9			2100	2100			Depth, uncorr. M		
11		01:56:30	01:57:00	✓	1950.6			1939	1940			4724		
12		02:00:54	02:01:24	✓	1749.8			1740	1740			Cast at Bottom: Time (UTC.HH:MM)		
13		02:05:18	02:05:48	✓	1548.3			1540	1540			00:57		
14		02:08:14	02:08:54	✓	1448.3			1440	1440			Latitude		
15		02:11:05	02:11:45	✓	1347.0			1340	1340			2° 12.1008S		
16		02:13:57	02:14:37	✓	1247.4			1240	1240			Longitude		
17		02:16:44	02:17:24	✓	1145.6			1140	1140			94° 7.9200E		
18		02:19:34	02:20:16	✓	1045.6			1040	1040			Depth, uncorr. M		
19		02:22:28	02:23:08	✓	945.5			940	940			4724		
20		02:25:18	02:25:58	✓	845.4			840	840			Maximum CTD Corr. Pressure.DB		
21		02:28:09	02:28:49	✓	743.8			740	740			4785.5		
22		02:30:57	02:31:38	✓	646.0			640	640			Distance above Bottom		
23		02:34:12	02:34:52	✓	525.7			520	520			9.6 ✓		
24		02:36:27	02:37:07	✓	476.1			470	470			Maximum Wire Out		
25		02:38:35	02:39:15	✓	424.8			420	420			4735 ✓		
26		02:40:45	02:41:26	✓	375.4			370	370			Cast End: Time (UTC.HH:MM)		
27		02:42:53	02:43:33	✓	325.2			320	320			03:15		
28		02:44:56	02:45:33	✓	275.4			270	270			Latitude		
29		02:46:55	02:48:54	✓	224.5			220	220			2° 12.07S		
30		02:50:18	02:50:49	✓	174.7			170	170			Longitude		
31		02:52:06	02:52:48	✓	144.5			140	140			94° 8.03E		
32		02:53:44	02:54:25	✓	125.0			120	120			Depth, uncorr. M		
33		02:55:45	02:56:28	✓	94.8			90	90			4726		
34		02:57:29	02:58:10	✓	74.8			70	70			Other Equipment:		
35		02:59:21	03:00:53	✓	41.0			35	35			Problems Noted:		
36		03:12:30	03:13:11	✓	2.4			-6	SURF	oil sheet noted on surface moved ship around before bringing rosette to surface				

Confirm Column: Enter check mark if confirmation received, O if no confirmation.

There must be a mark for every attempt to trip a bottle

# I8S RV REVELLE SAMPLE LOG

Page 1 of \_\_\_\_\_

STATION/CAST:		Date:		UTC Start:		UTC End:		O <sub>2</sub> Box:	NUTRIENT RACK:		SALT BOX:	
Niskin No.	Intended Depth	Freon Syringe	Helium Tube	Oxygen Flask	O <sub>2</sub> Draw Temp	TCO <sub>2</sub> Bottle	TALK Bottle	<sup>14</sup> C	DOC/DON	Tritium Bottle	Nuts Tube	Salt Bottle
1												
2												
3												
4												
5												
6												
7												
8												
9												
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31												
32												
33												
34												
35												
36												
Sampler Initials				600ml		-----		1500ml		70ml	200ml 1500ml	
REMARKS:												
Sample Cop:												

# I8S RV REVELLE SAMPLE LOG

STATION/CAST:		Date:		UTC Start:		UTC End:						
Niskin No.	Intended Depth	CDOM	CHL	BACT	CARB	POC						
1												
2												
3												
4												
5												
6												
7												
8												
9												
10												
11												
12												
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24												
25												
26												
27												
28												
29												
30												
31												
32												
33												
34												
35												
36												
Sampler Initials												
REMARKS:		100ml	550ml	60ml	70ml							
Sample Cop:												



STATION/CAST:		Date:		UTC Start:		UTC End:		O <sub>2</sub> Box:	NUTRIENT RACK:		SALT BOX:	
042/01		28 FEB 2007		08:07		10:00			BLV		C	
Niskin No.	Intended Depth	Freon Syringe	Helium Tube	Oxygen Flask	O <sub>2</sub> Draw Temp	TCO <sub>2</sub> Bottle	TALK Bottle	<sup>14</sup> C	DOC/DON	Tritium Bottle	Nuts Tube	Salt Bottle
1	4036	261 ✓		1351	3.3	A1, A37	1 ✓	6462 ✓	1 ✓		1 ✓	1 ✓
2	3870	635 ✓		1699	2.7	A2 ✓	2, 140p	6463 ✓	2 ✓		2 ✓	2 ✓
3	3670	753/274		1193	2.2	A3 ✓	3 ✓	6464 ✓	3 ✓		3 ✓	3 ✓
4	3420	754 ✓		1704	2.1	A4 ✓	4 ✓	6465 ✓	4 ✓		4 ✓	4 ✓
5	3170	265 ✓		1698	2.3	A5 ✓	5 ✓	6466 ✓	5 ✓		5 ✓	5 ✓
6	2920	756 ✓		1706	2.6	A6 ✓	6 ✓	6467 ✓	6 ✓		6 ✓	6 ✓
7	2670	—		1697	2.7	A7 ✓	7 ✓	6468 ✓	7 ✓		7 ✓	7 ✓
8	2420	623 ✓		968	2.8	A8 ✓	8 ✓	6469 ✓	8 ✓		8 ✓	8 ✓
9	2170	—		1709	3.0	A9 ✓	9 ✓	6470 ✓	9 ✓		9 ✓	9 ✓
10	1970	—		1700	3.0	A10, A38	10 ✓	6471 ✓	10 ✓		10 ✓	10 ✓
11	1770	255 ✓		1423	3.2	A11 ✓	11 ✓	6472 ✓	11 ✓		11 ✓	11 ✓
12	1670	—		1722	3.2	A12 ✓	12 ✓	6473 ✓	12 ✓		12 ✓	12 ✓
13	1570	313 ✓		1743	3.4	A13 ✓	13 ✓	6474 ✓	13 ✓		13 ✓	13 ✓
14	1470	—		1744	3.2	A14 ✓	14 ✓	6475 ✓	14 ✓		14 ✓	14 ✓
15	1370	634 ✓		1745	3.3	A15 ✓	15 ✓	6476 ✓	15 ✓		15 ✓	15 ✓
16	1270	—		1696	3.3	A16 ✓	16 ✓	6477 ✓	16 ✓		16 ✓	16 ✓
17	1170	772 ✓		1737	3.5	A17 ✓	17, 18 dop	2302 ✓	17 ✓		17 ✓	17 ✓
18	1070	—		1738	3.4	A18, A39	18 ✓	2303 ✓	18 ✓		18 ✓	18 ✓
19	970	9913 ✓		1739	3.4	A19 ✓	19 ✓	2304 ✓	19 ✓		19 ✓	19 ✓
20	870	—		1740	3.6	A20 ✓	20 ✓	2305 ✓	20 ✓		20 ✓	20 ✓
21	770	760 ✓		1741	3.6	A21 ✓	21 ✓	2306 ✓	21 ✓		21 ✓	21 ✓
22	670	—		1742	3.5	A22 ✓	22 ✓	2307 ✓	22 ✓		22 ✓	22 ✓
23	570	632 ✓		1723	—	A23 ✓	23 ✓	2308 ✓	23 ✓		23 ✓	23 ✓
24	485	—		1724	4.2	A24 ✓	24 ✓	2309 ✓	24 ✓		24 ✓	24 ✓
25	435	767 ✓		1725	4.3	A25 ✓	25 ✓	2310 ✓	25 ✓		25 ✓	25 ✓
26	385	—		1726	4.5	A26 ✓	26 ✓	2311 ✓	26 ✓		26 ✓	26 ✓
27	335	625/344 ✓		1727	5.1	A27 ✓	27 ✓	2312 ✓	27 ✓		27 ✓	27 ✓
28	285	—		1728	4.9	A28 ✓	28 ✓	2313 ✓	28 ✓		28 ✓	28 ✓
29	235	336 ✓		1729	4.4	A29 ✓	29 ✓	2314 ✓	29 ✓		29 ✓	29 ✓
30	185	—		1730	4.3	A30 ✓	30 ✓	2315 ✓	30 ✓		30 ✓	30 ✓
31	160	757 ✓		1731	4.9	A31 ✓	31 ✓		31 ✓		31 ✓	31 ✓
32	135	—		1732	5.1	A32 ✓	32 ✓	2316 ✓	32 ✓		32 ✓	32 ✓
33	85	619/761 ✓		1733	6.3	A33 ✓	33 ✓		33 ✓		33 ✓	33 ✓
34	40	—		1734	6.5	A34, A40	34 ✓		34 ✓		34 ✓	34 ✓
35	15	—		1735	7.1	A35 ✓	35, 36 dop	2317 ✓	35 ✓		35 ✓	35 ✓
36	SURF	613 ✓		1736	7.0	A36 ✓	36 ✓		36 ✓		36 ✓	36 ✓
Sampler Initials		EW		SE	SE	DG	SEA	CF/DV	CF		JS	JS

REMARKS:

600ml

-----

1500ml 70ml

200ml 1500ml

Sample Cop: JJB

1) EW notes grease on hand during sample of bottle #15.

2) No temp O<sub>2</sub> #23

3) #36 - with top vent closed and bottom valve open, it dribbles.



# I8S RV REVELLE SAMPLE LOG

STATION/CAST:		Date:		UTC Start:		UTC End:						
042/01		28 FEB 2007		09:10		10:12						
Niskin No.	Intended Depth	CDOM	CHL	BACT	CARB	POC						
1	4036	1 ✓		1 ✓		1 ✓						
2	3870	2 ✓		2 ✓								
3	3670	3 ✓										
4	3420	4 ✓										
5	3170	5 ✓										
6	2920	6 ✓		6 ✓								
7	2670	7 ✓				2 ✓						
8	2420	8 ✓		8 ✓								
9	2170	9 ✓										
10	1970	10 ✓		10 ✓								
11	1770	11 ✓										
12	1670	12 ✓										
13	1570	13 ✓		13 ✓								
14	1470	14 ✓										
15	1370	15 ✓										
16	1270	16 ✓										
17	1170	17 ✓										
18	1070	✓ 18, 37		18 ✓								
19	970	19 ✓										
20	870	20 ✓										
21	770	21 ✓										
22	670	22 ✓		22 ✓								
23	570	✓ 23, 38		23 ✓								
24	485	24 ✓		24 ✓	24 ✓							
25	435	25 ✓										
26	385	26 ✓		26 ✓	26 ✓							
27	335	27 ✓		27 ✓								
28	285	28 ✓		28 ✓	28 ✓							
29	235	29 ✓	1 ✓	29 ✓	29 ✓							
30	185	30 ✓	2 ✓	30 ✓	30 ✓							
31	160	31 ✓	3 ✓	31 ✓								
32	135	32 ✓	4 ✓	32 ✓		3 ✓						
33	85	33 ✓	5 ✓	33 ✓	33 ✓	4 ✓						
34	40	34 ✓	6 ✓	34 ✓	34 ✓							
35	15	35 ✓	7 ✓	35 ✓								
36	SYRF	36 ✓	8 ✓	36 ✓	36 ✓							

Sampler Initials

NN

REMARKS:

100ml

550ml

60ml

70ml

2500ml

Sample Cop:

CDOM taken over by Dave at bottle 13.