DEPARTMENT OF ECOLOGY
State of Washington

Standard Operating Procedure EAP130, Version 1.0

Short-term Continuous Data Collection with a Multiparameter Sonde, Part 2: Data Processing

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Purpose of this Document

The Washington State Department of Ecology develops Standard Operating Procedures (SOPs) to document agency practices related to sampling, field and laboratory analysis, and other aspects of the agency's technical operations.

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Contact Information

For more information contact:

Publications Coordinator
Environmental Assessment Program
Washington State Department of Ecology
P.O. Box 47600
Olympia, WA 98504-7600

Phone: (360) 407-6764

Washington State Department of Ecology – ecology.wa.gov

- Headquarters, Olympia 360-407-6000
- Northwest Regional Office, Bellevue 425-649-7000
- Southwest Regional Office, Olympia 360-407-6300
- Central Regional Office, Union Gap 509-575-2490
- Eastern Regional Office, Spokane 509-329-3400

Original Author – Nuri Mathieu, Modeling and TMDL Unit, Western Operations Section
Tighe Stuart, Eastern Operations Section
Date – 6/30/2018

Original Reviewer – Jim Carroll, Eastern Operations Section
Date – 7/37/2018

QA Approval – Arati Kaza, Ecology Quality Assurance Officer

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SOP Revision History

Revision Date	Revision History	Summary of changes	Sections	Reviser(s)
6/12/2018	1.0	Original draft completed	All	Nuri Mathieu
6/30/2018	1.0	Review and major contributions	All	Tighe Stuart;
7/30/2018	1.0	Reviewer	All	Nuri Mathieu
5/14/2019	1.0	Approval	All	Arati Kaza

1.0 Purpose and Scope

1.1 This document is the Environmental Assessment Program (EAP) Standard Operating Procedure (SOP) for the preparation of technical SOPs.

1.2 This document is the Environmental Assessment Program (EAP) Standard Operating Procedure (SOP) for processing, reviewing, and finalizing short-term (less than 6 months) continuous data sets collected using a deployed multi-parameter sonde. This SOP is intended for a variety of types of water quality studies, including Total Maximum Daily Load (TMDL), effectiveness monitoring, toxic loading, and other focused water quality studies.

1.3 For data collection procedures associated with this SOP see Part 1, SOP EAP129.

1.4 Several of the methods and information presented in this SOP were taken or adapted from the USGS techniques and methods 1D-3: *Guidelines and Standard Procedures for Continuous Water Quality Monitors: Station Operation, Record Computation, and Data Reporting* (Wagner et al., 2006).

2.0 Applicability

2.1 This document should be used for processing data from sondes deployed in freshwater rivers, streams, and other waterbodies for project-level water quality assessments of limited duration (less than 6 months). Deployments of great than 6 months involve a larger dataset and a more dynamic range of deployment conditions. These long-term deployments should be conducted in consultation with EAP’s freshwater monitoring unit.

3.0 Definitions

3.1 Data adjustment — raw data values changed based on a factor or equation that accounts for observed bias or drift.

3.2 Fouling — the accumulation of unwanted material on solid surfaces to the detriment of function. The fouling materials can consist of either living organisms (biofouling) or a non-living substance (inorganic and/or organic).

3.3 Instrument Drift — a change in the accuracy of an instrument’s measurements over time.

3.4 RMSE — Root Mean Squared Error, the square root of the average of the differences between two measurements.

3.5 Sonde — an instrument probe that transmits or logs information about its surroundings underground, under water, in the atmosphere, etc.

4.0 Personnel Qualifications/Responsibilities

4.1 Staff must be trained in processing, reviewing, and adjusting water quality sensor data.

4.2 Job classifications that typically perform data processing work: Natural Resource Scientist 1/2/3, Environmental Engineer 1/2/3, Environmental Specialist 1/2/3/4/5, Hydrogeologist 1/2/3/4. Entry-level staff should not perform data review or adjustment without oversight from experienced senior staff.

5.0 Equipment, Reagents, and Supplies

5.1 Computer with data processing software such as Microsoft Excel/Access, R, Hydstra, Aquarius, etc.

6.0 Summary of Procedure

6.1 Reviewing and qualifying the field-check instrument data

6.1.1 The first step in processing the continuous data from the deployed sonde is to make sure that the field-collected “check” data used to assess it is of acceptable quality.

6.1.2 For all parameters except dissolved oxygen (DO), the post-check results (see SOP EAP129, Part 1; section 6.9) are used to calculate the difference between the field-check instrument values and reference material values.

6.1.3 The calculated differences are compared to the criteria in table 1 and used to assign a data-quality rating for data collected with each field-check instrument. When multiple reference checks are conducted, the larger of the two differences should be used to assign the rating. For example, if the instrument was 0.15 pH units high, compared to the pH 7 buffer, and 0.22 units high, compared to the pH 10 buffer, then the instrument pH should be assigned a quality rating of “Qualify” based on the 0.22 value.

Table 1. Measurement quality objectives for field-check instruments using post-check data

Measured field parameter	Post-check Reference	Accept	Qualify as Estimate	Reject
Water temperature	NIST-certified Thermometer	≤ ± 0.2°C	> ± 0.2 – 0.8°C	> ± 0.8°C
Specific conductance[a]	NIST-certified Buffer/s	≤ ± 10%	> ± 10 – 20%	> ± 20%
pH	NIST-certified Buffers (2-3pt)	≤ ± 0.2 units	> ± 0.2 – 0.8 units	> ± 0.8 units
Turbidity	NIST-certified Buffer/s	≤ ± 1.0 units or ≤ ± 10% [b]	> ± 1.0 – 2.0 units or > ± 10 – 20% [b]	> ± 2.0 units or > ± 20% [b]

[a] *Except for zero-check*
[b] *Whichever is greater*

6.1.4 For DO, it is recommended that field checks be assessed and, if necessary, adjusted (see section 6.5) based on regression with Winkler samples. Winkler-adjusted DO field checks can be rated based on the degree of agreement between the adjusted values and the Winkler samples (Table 2). In the absence of "accepted" Winkler data, the field-check instrument should be rated based on the percent saturation post-check (Table 2).

6.1.5 For large short-term surveys with many deployed sondes and one field-check sonde, a good approach is to collect a large number (e.g. 10+) of Winklers alongside the check sonde, across a range of values. This provides a strong basis for bias correction of the check sonde. A minimum of 5 Winklers are required to adjust field-check data.

6.1.6 Using the Winkler-adjusted field checks to assess the deployed instruments combines the accuracy and standardization of Winkler samples with the precision of optical DO sensors (Figure 1).

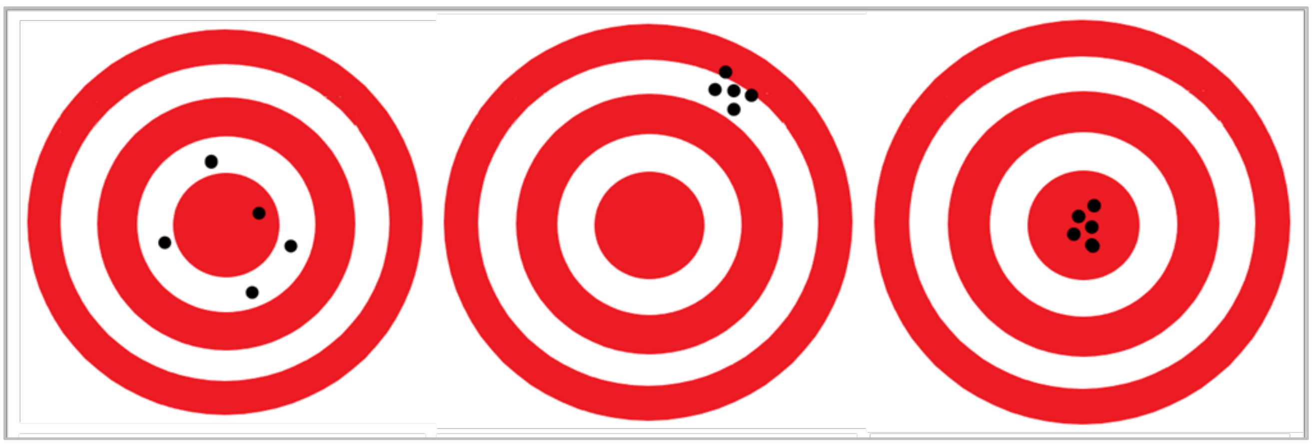

Figure 1. Illustration of accuracy vs. precision, as applied to Winkler and optical DO methods
Additional text describing Figure 1:

Left: The chemical basis of Winkler samples ensures they are generally accurate, but they are not precise, often having up to 0.3 mg/L error.

Middle: Optical DO probe results are very precise, down to a few hundredths of a mg/L. However, they can be inaccurate (biased) up to 1 mg/L off because of inherent problems with saturation calibrations.

Right: Applying a bias correction to optical DO probe results using several Winkler results provides a way to be both precise and accurate.

Table 2. Dissolved Oxygen measurement quality objectives for field-check instruments equipped with optical DO probes, post adjustment.

Measured field parameter	Quality Rating Method Preference	Post-check Reference	Accept	Qualify as Estimate	Reject
Dissolved Oxygen	Primary	Winkler samples	≤ ± 0.5 mg/L	> ± 0.5 – 1.0 mg/L	> ± 1.0 mg/L
Dissolved Oxygen	Secondary	Saturation Check	≤ ± 5%	> ± 5 – 15%	> ± 15%

6.1.7 Winkler data quality is assessed by collecting replicate samples in the field and by performing sodium thiosulfate normality checks with potassium bio-iodate during titration.

6.1.8 If the normality check is off by greater than ±0.2 mg/L, then an attempt will be made to correct the problem (i.e. replace the thiosulfate, check equipment, etc.). A second normality check will then be performed. If the problem is corrected (check now <±0.2 mg/L), then the Winkler samples titrated prior to that normality check may be adjusted by the offset (difference between first and second check). If the second normality check is greater than ±0.2 (problem not corrected), then the Winkler samples will be qualified as estimates. If the second check is greater than ±0.8, the Winkler samples will be rejected.

6.1.9 The programmatic QAPP (McCarthy and Mathieu, 2017) states that the median absolute difference for DO Winkler replicate pairs should be less than 0.2 mg/L.

6.2 <u>Preliminary data rejection and removal</u>

6.2.1 The first step in reviewing a time series raw data file for a deployed sonde is to remove all measurements where the sonde was not deployed in the water column or had not yet equilibrated. If the log file was not enabled/disabled in the field (or power was supplied early), then there may be numerous measurements on either end of the record.

6.2.2 Deployment, retrieval, and site-visit times should be used to remove data points where the sonde was out of water. If field activity time is missing, specific conductance values at or near zero can be used to identify times when the sonde was out of the water. As a general rule, any measurements logged near-in-time to placing the sonde in the water should be removed if they are out of line with other measurements in the record. All removed data should be documented in the project files.

6.2.3 pH may take multiple log intervals to equilibrate. Additional values may be removed from the beginning of the pH time series record based on visual review.

6.2.4 Figure 2 provides an example of data points removed from the raw data file that were collected prior to deployment and after retrieval.

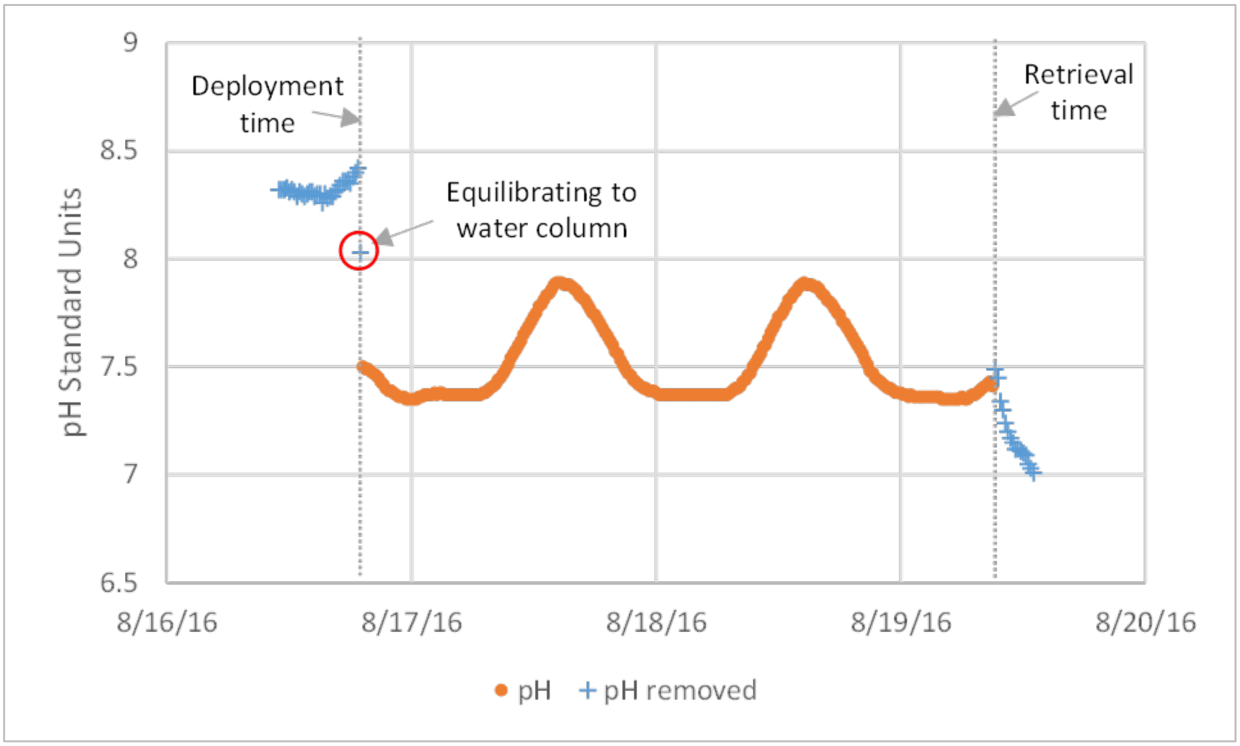

Figure 2. Example of preliminary data removal prior to deployment and after retrieval.

6.2.5 In some cases, temporary interference or fouling may create artificial noise in the data record. Data filters and/or manual review may be used to remove or qualify spurious data points. This level of data processing requires careful review and thorough documentation of any rejected data in the project files.

6.2.6 Figure 3 provides an example of specific-conductance data processing to remove unexplained noise in the data. First, a rate of change filter is applied, and, then, additional noise is removed manually by visual review. The daily signal is retained, and the average of the data changes by 1.1% between raw and processed data.

6.2.7 Removal or rejection of noisy data points should be thought of as a conservative process, whereby data with less certainty associated to it is not reported.

6.2.8 Do not perform data averaging or smoothing to remove noise on continuous sonde data.

6.2.9 Only noise that appears randomly distributed should be removed. Continuous “spikes” in the data should NOT be removed, as they likely represent real discrete changes in water quality due to a temporary discharge or condition. If it is unclear whether the noise is random, qualify, rather than reject the data.

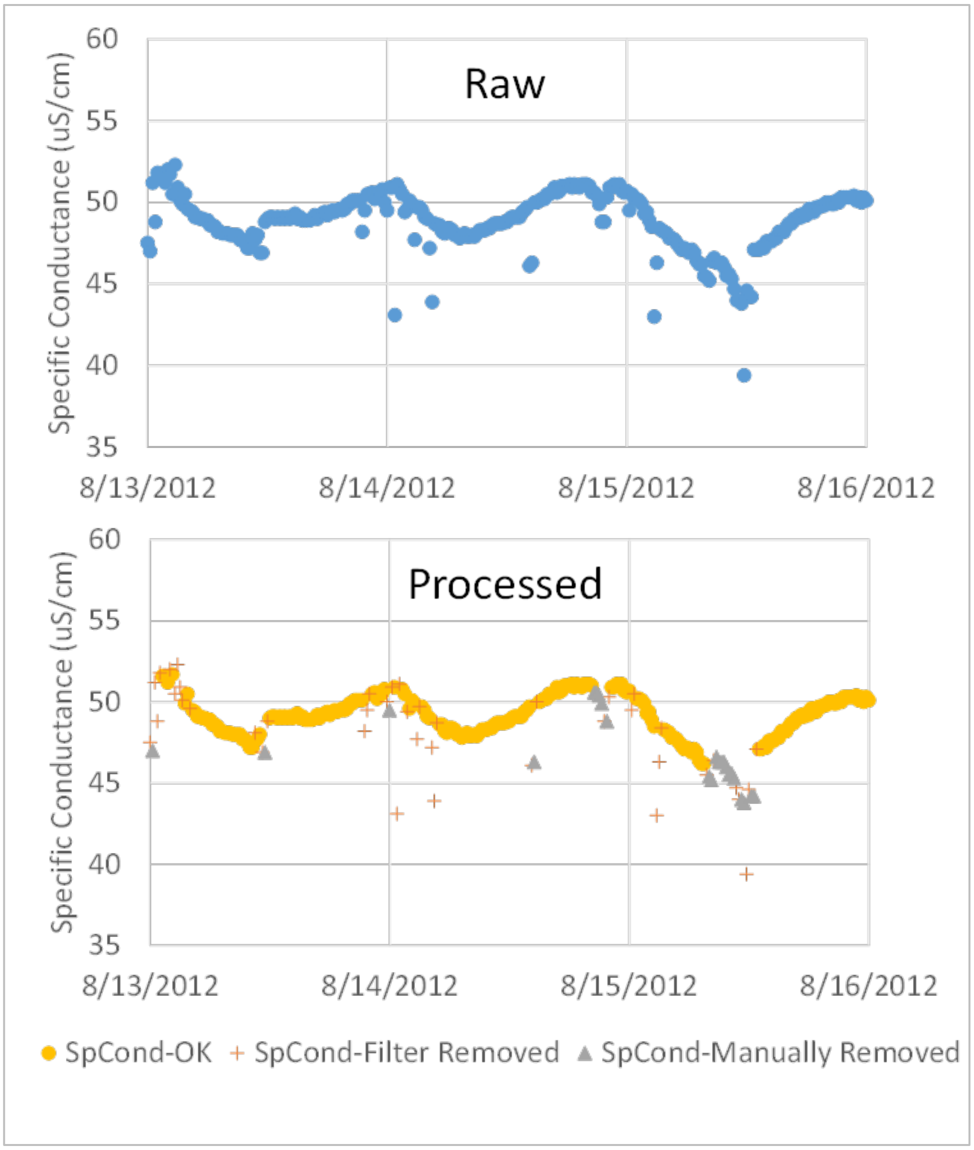

Figure 3. Example of removal of unexplained noise in the data record

6.2.10 When a sonde experiences extreme fouling, sediment burial, or major interference, part of the data file may be salvaged, if a specific fouling or interference event can be identified. Figure 4 provides an example where Sonde A was found buried in sediment following a large storm event. Flow data from a gage in the watershed and water quality data from the nearby unburied Sonde B were used to identify the time of burial. Only results after the identified burial event were removed from the final record.

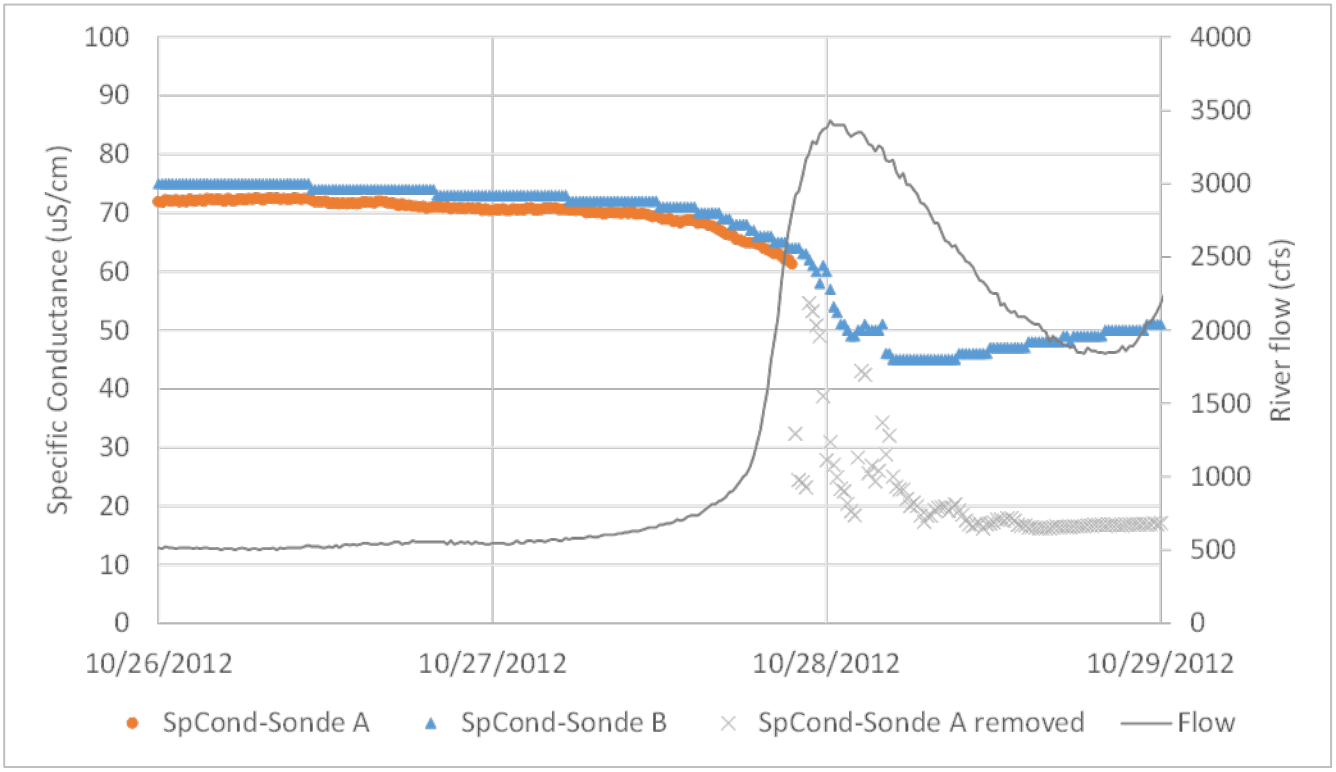

Figure 4. Example of data removed due to sediment deposition during a runoff event.

6.2.11 A log of all removed data (including dates, times, and justification for removal) should be kept with the project files.

6.2.12 In EIM, observations should be entered for data removed/rejected mid-deployment. It is not necessary to enter observations into EIM for data removed from either the beginning or end of the record. See EIM time series data entry guidance for additional detail.

6.3 Fouling adjustments

6.3.1 Fouling adjustments are necessary when fouling checks (see EAP SOP 129, Part 1 section 6.7), collected before and after cleaning, reveal a bias due to sensor fouling. Fouling adjustments should be reviewed and completed before any other type of data adjustment.

6.3.2 Fouling adjustments, while rare, are applied as a drift correction that is a linear interpolation based on the start time, zero, the stop time and the final offset due to fouling.

$$\text{The final fouling offset} = (DS_{post} - DS_{pre}) + (FC_{pre} - FC_{post})$$

Where DS= Deployed Sonde Value; FC = Field-check Value; Pre/Post= Before/after cleaning.

6.3.3 Changes in the "clean" field-check instrument values, before and after the deployed sonde cleaning, are used to separate the "true" changes in water chemistry that elapsed while the deployed sonde was being cleaned from the changes in the deployed sonde readings due to removal of fouling.

6.3.4 Figure 5 illustrates a minor drift-fouling adjustment of DO data based on a final fouling offset of 0.15. The fouling offset was calculated as (8.73 - 8.60) + (8.79 – 8.77).

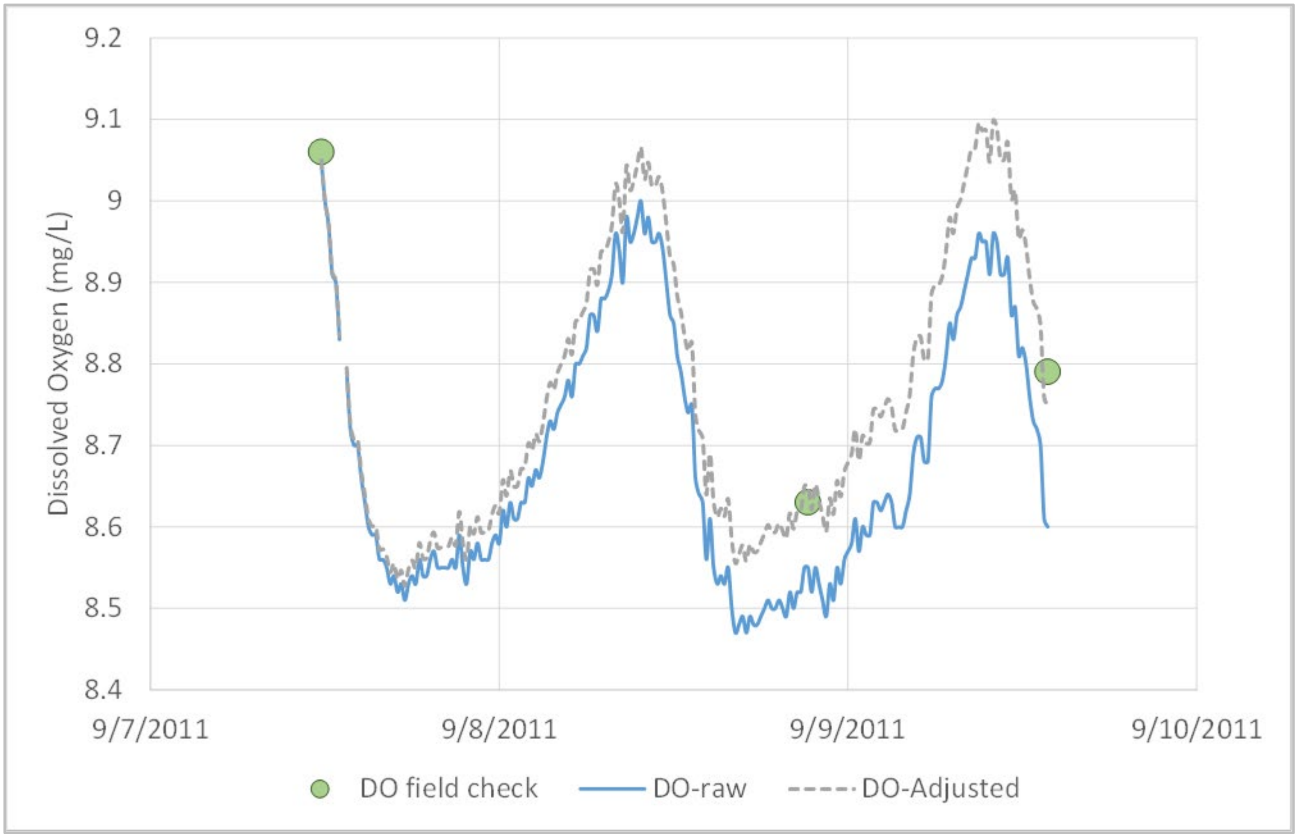

Figure 5. Example of a minor drift-fouling adjustment of DO data based on a final fouling offset

6.4 Determining final adjustment period

6.4.1 The period of adjustment may be different for each parameter. For fouling, the adjustment period will always be limited to in between cleanings. For final adjustments (section 6.5), the period ends when the sonde is recalibrated. This typically coincides with retrieval on short deployments, but not always.

6.4.2 For optical DO sensors, it is recommended to not recalibrate the deployed sensor, if it continues to meet the QAPP specific MQO, until the end of a project. The deployed sensors measurements can then be compared to a larger number of Winkler samples and field-check measurements. Bias or regression adjustments are then made on a larger period of data, based on a larger sample size of quality checks.

6.5 Weight of evidence adjustment based on quality checks

6.5.1 Once the steps of data removal/rejection and fouling review/adjustments have been completed, the final data quality review and adjustment (if applicable) process is started.

6.5.2 All the available information should be used in evaluating whether or not a data adjustment is warranted. A weight-of-evidence approach is used that considers the following information:

- Post-deployment checks against NIST reference.
- Post-deployment checks against other reference (for example air-saturated water).
- Field checks using instrument with “Accept” quality rating (see Table 1 and 2).
- Field checks from Winkler samples with “Accept” quality rating (DO only).
- Deployed measurement values at a nearby location on the same waterbody. *Note: Use caution when considering nearby data; if there are significant inflows, significant biological productivity, or long residence times between the two sites, then this approach is not warranted.*
- Consideration of physical, biological, or chemical processes (for example DO appears supersaturated at all times).
- Field observations (for example, debris accumulated on deployment tube).
- Field-check instruments or DO Winkler samples with a “Qualify” rating are generally not used in the weighing of evidence for adjustments.
- Field-check instruments or DO Winkler samples with a “Reject” rating should never be used in the weighing of evidence for adjustments.

6.5.3 Typically, choose the adjustment that results in the smallest residuals and bias between the adjusted values and QC checks (post and field checks). Best professional judgement and visual review are necessary to confirm the adjustment.

6.5.4 **If the evidence is weak or inconclusive, do not adjust the data**.

6.5.5 There are three primary types of data adjustments:

6.5.5.1 Bias offset: Data are typically adjusted by the average difference between the QC checks and deployed sonde. The majority of QC checks must show bias to use this method. An adjustment for representativeness may also be made, based on the average difference from cross-section surveys or area weighted mean measurements (see SOP EAP129, Part 1).

6.5.5.2 Regression (slope + offset): Data are adjusted using regression, typically linear, between QC checks and deployed sonde. This accounts for both a slope and offset adjustment. The regression must have at least 5 data points and an R^2 value of >0.95 to use for adjustment. Use extreme caution when extrapolating regressions beyond the range of the QC checks.

6.5.5.3 Calibration Sensor Drift: Data are adjusted using linear regression with time from calibration or deployment to post check or retrieval. The majority of QC checks, particularly post checks, must confirm the pattern of drift (the drift-adjusted sonde values should more closely match most of the QC checks). This adjustment is applied in a manner similar to a fouling-drift correction (Figure 4); however in this case, rather than fouling, the drift is due to a sensor degrading, losing power, or not holding a calibration over time.

6.5.6 Table 3 and Figure 6 provide an example of a bias adjustment of 7.1% applied to a specific-conductance deployment based on the average bias from both field and buffer post checks. Table 4 shows the adjusted values and the associated reduction in bias (from 7.1% to -0.4%) and the RMSE (From 7.4% to 2.1%), compared to the QC checks.

Table 3. Example of bias in a deployed sonde, compared to buffer and accepted field checks.

Date & Time	SpCond Deployed	QC type	SpCond QC	Field-check rating	% Difference
9/24/2012 12:40	66.9	Field Check	70.2	Accept	4.7%
9/25/2012 11:00	66.0	Field Check	72.9	Accept	9.5%
9/25/2012 16:40	65.2	Field Check	71.7	Accept	9.1%
9/27/2012 11:40	69.0	Field Check	73.7	Accept	6.4%
9/28/2012 10:00	94.0	Buffer Check (Post)	100		6.0%
Average QC Difference (Bias) =					7.1%
RMSE QC Difference =					7.4%

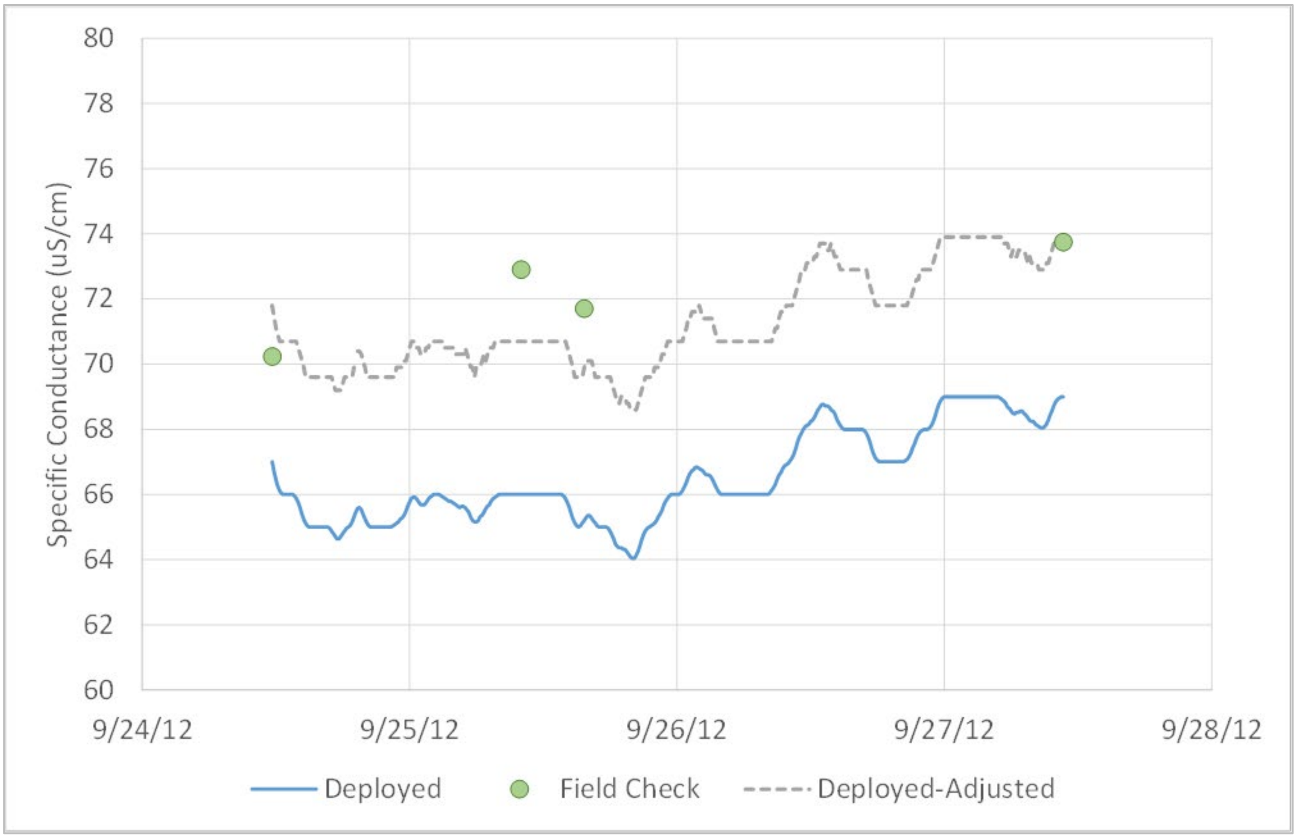

Figure 6. Example of bias adjustment.

Table 4. Adjusted deployment data and residuals/fit with quality checks.

Date & Time	SpCond Adjusted	QC type	SpCond QC	Field-check rating	% Difference
9/24/2012 12:40	71.8	Field Check	70.2	Accept	2.2%
9/25/2012 11:00	70.7	Field Check	72.9	Accept	-3.0%
9/25/2012 16:40	69.9	Field Check	71.7	Accept	-2.5%
9/27/2012 11:40	73.9	Field Check	73.7	Accept	0.2%
9/28/2012 10:00	101.0	Buffer Check (Post)	100		1.0%
				Average QC Difference (Bias) =	-0.4%
				RMSE QC Difference =	2.1%

6.5.7 If any data are adjusted, detailed documentation of the QC data and justification for adjustment must be retained with the project files.

6.6 Final data quality ratings and data qualifiers

6.6.1 The final deployed sonde data, adjusted or not, is assigned a quality rating by comparing the final RMSE QC difference to the criteria in Table 5. For example, the adjusted data from Table 4 would receive an "Accept" quality rating, based on an RMSE of less than 10%, post-adjustment (2.1% RMSE).

6.6.2 The RMSE is the square root of the average of the squared residuals between the final deployed data and the QC check (both field and post check). For specific conductance, the RMSE is calculated with the square of the percent difference, instead of the residual.

Table 5. Final data quality ratings based on the RMSE between quality checks and adjusted/final deployed readings.

Measured field parameter	Accept	Qualify as estimate	Reject
Water temperature	≤ ± 0.2°C	> ± 0.2 – 0.8°C	> ± 0.8°C
Specific conductance	≤ ± 10%	> ± 10 – 20%	> ± 20%
Dissolved Oxygen	≤ ± 0.5 mg/L	> ± 0.5 – 1.0 mg/L	> ± 1.0 mg/L
pH	≤ ± 0.2 units	> ± 0.2 – 0.5 units	> ± 0.8 units
Turbidity	≤ ± 1.0 units or ≤ ± 10%	> ± 1.0 – 2.0 units or > ± 10 – 20%	> ± 2.0 units or > ± 20%

For "or" criteria, use whichever is greater.

6.6.3 Bias adjustments can typically be applied with more confidence, compared to fouling/calibration drift or slope adjustments where the linear relationship cannot be confirmed between quality checks. For this reason, adjusted data where a drift or slope adjustment exceeds the thresholds in Table 6 should be qualified as estimates, regardless of whether or not the final RMSE meets accept criteria.

Table 6. Threshold for when to qualify data based on drift or slope adjustment applied

Measured Field parameter	Drift or slope adjustment threshold for qualifying data
Water temperature	> 0.4°C
Specific conductance	> ± 20%
Dissolved Oxygen	> ± 1.0 mg/L
pH	> ± 0.4 units
Turbidity	> ± 2.0 units or > ± 20% [c]

6.6.4 Adjusted data from a deployed sonde should be designated as adjusted in the EIM database (See section 6.7 data reporting).

6.7 Data Reporting

6.7.1 Table 7 contains names, method codes, units, and digit conventions for continuous deployment data reporting.

Table 7. Reporting units and conventions for continuous data parameters.

EIM Parameter Name or Alias	Reporting Unit/s	EIM Method Code	Reporting Conventions
Temperature, water	°C	TEMPTHERM	To nearest 0.01 °C.
Specific conductance	µS/cm	CONDMETER	<1 to the nearest 0.01 1-100 to the nearest 0.1 > 100 to the nearest whole number
pH	pH	PHMETER	to the nearest 0.01
Dissolved Oxygen	mg/L	DO-OPTICAL DO-CLARK[1]	to the nearest 0.01
Turbidity	FNU/NTU	TURBM	0–10, to nearest 0.1 10–100, to nearest 1 >100, to nearest 10

[1] *Most sensors used by EAP are optical LDO technology (EIM method code = DO-OPTICAL), a few Clark-cell technology sensors are actively maintained (DO-CLARK). Only optical sensors should be used for field-check instruments.*

6.7.2 Dissolved oxygen percent saturation from deployed sondes is generally not reported in EIM. For this data type, temperature, specific conductance, and elevation data are available in EIM. These data can be used to calculate the percent saturation outside of the database.

6.7.3 The EIM help center provides specific guidance on how to enter adjusted time-series data into EIM. Table 8 summarizes this guidance in the context of this SOP. Time-series data is entered into EIM using a specific template and the associated help document.

6.7.4 It is recommended to enter information specific to the data adjustment into EIM Result comment field (see Table 8 comment example).

Table 8. EIM data entry guidelines for adjusted and non-adjusted time-series data from short term deployments.

Final Data Quality Rating	**Result Data Qualifier[1]**	**Result Data Qualifier Description**	**Comment (Example)[2]**
Non- Adjusted Data			
Accept	-	-	-
Qualify	EST	Measurement value reported is estimated. See comment for additional detail.	RMSE >0.5 mg/L based on data quality checks; reported result is an estimate and should be used with caution.
Adjusted Data			
Accept	IA	Instrument result adjusted; reported result meets study objectives	Result Value adjusted for linear instrument drift identified post deployment.
Qualify	EST	Measurement value reported is estimated. See comment for additional detail.	Result Value adjusted; considerable instrument drift during deployment, reported result is an estimate and should be used with caution.

[1] (Column S in Time-Series Result Template)

[2] (Column U in Time-Series Result Template)

7.0 Records Management

7.1 All original data files should be retained in their raw electronic form (.csv, .txt, etc.) in one data folder or database.

7.2 A "final" file or database should be retained for each deployment that includes at a minimum: final data after processing and/or adjustment, any field check or buffer check data associated with the deployed sonde, and any factors or equations used to adjust the data.

7.3 Any information used to review or adjust data should be retained with the project files.

7.4 All files and databases should be stored on a network drive that is routinely automatically backed up.

8.0 Quality Control and Quality Assurance

8.1 The quality control and assurance guidelines are embedded throughout Section 6 in the order that they are encountered during data processing.

8.2 Specific QA/QC criteria are included in tables 1, 2, 5, and 6.

8.3 The Part 1 SOP includes field procedures related to data quality.

8.4 Additional applicable quality assurance guidelines can be found in the programmatic QAPP for water quality impairment studies (McCarthy and Mathieu, 2017)

9.0 Safety

9.1 For further field health and safety measures refer to the EAP Safety Manual (EAP, 2019).

10.0 References

10.1 Environmental Assessment Program (EAP), 2019. Environmental Assessment Program Safety Manual. Washington State Department of Ecology. Revised 03/19.

10.2 McCarthy, S. and N. Mathieu, 2017. Programmatic Quality Assurance Project Plan: Water Quality Impairment Studies. Washington State Department of Ecology, Olympia, WA. https://fortress.wa.gov/ecy/publications/SummaryPages/1703107.html.

10.3 Wagner, R.J., Boulger, R.W., Jr., Oblinger, C.J., and Smith, B.A., 2006, Guidelines and standard procedures for continuous water-quality monitors—Station operation, record computation, and data reporting: U.S. Geological Survey Techniques and Methods 1–D3, 51 p. + 8 attachments; http://pubs.water.usgs.gov/tm1d3.