Quality control procedure for marine water quality logger data

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Executive Summary

TropWATER recognises the importance of providing reliable data that aligns with best-practice quality assurance and quality control (QA/QC) procedures. By implementing robust quality control procedures to our workflows, we can ensure consistency across datasets and provide the highest confidence in our data products. Our QC procedures are science-based and align with those used by government agencies nationally and internationally when dealing with marine logger data.

This report outlines the quality control process we apply to data collected from loggers in our marine water quality monitoring programs. Data goes through both automated and manual quality control steps. There are twelve quality control tests in the automated step followed by semi-formal manual quality control by a trained operator. A flagging system is used to communicate the results of quality control tests to the end user with flag values assigned to each sensor value. The flagging system assigns values from 1 to 99, with the end user most commonly seeing flag values of 1 (good data), 2 (probably good data), 3 (probably bad data), 4 (bad data), or 9 (missing data).

The end user can then decide what level of data 'quality' they wish to use for their application, and unwanted data can easily be masked in MS Excel or other data management programs by filtering by 'QC flag'. For most applications we suggest 'good data' and 'probably good data' is acceptable, 'probably bad data' may be used with caveats, and 'bad data' should be discarded. Retaining all data 'as is' along with its QC flags through to the end user maintains data integrity.

Introduction

Quality assurance (QA) and quality control (QC) procedures are methodologies implemented to limit the introduction of error into analytical data. Quality assurance is the proactive approach of quality which focusses on guidelines, policies and procedures designed to prevent errors at the data acquisition level, for example, standard operating procedures, staff training, equipment inspection, maintenance, and testing. Quality control by contrast, is the reactive approach of quality which works by finding errors in the data, for example, false readings due to a water quality sensor being out of water, instrument failure, or an unexplainably high/low data value. Together, QA and QC procedures are vital to identify and correct data acquisition problems and deliver a more robust data product.

TropWATER has introduced a stringent quality control process for water quality logger data obtained by our suite of water quality loggers. The QC process is science-based and designed around published methodologies used across the industry. Development of our bespoke procedures leaned heavily on the Quality Assurance of Real-Time Oceanographic Data (QARTOD) program (Bushnell et al., 2019; Fredericks, 2007), The QARTOD program is considered best-practice for handling of marine data and has been adopted in Australia by the Integrated Marine Observing System (IMOS) (Morello et al., 2014), and Great Barrier Reef Marine Monitoring Program (GBRMPA, 2021), among others (EuroGOOS, 2010; Schallenberg, Jansen, & Trull, 2017; Zhou, Qin, Xu, Sadiq, & Yu, 2018). The flag system has parallels to quality code systems used for weather and hydrological data from national and state agencies which end-users may also be familiar with (BOM, 2023; DRDMW, 2023). The QC process complements our quality assurance which includes maintaining a current list of standard operating procedures (SOP's), training of staff on all SOPs and equipment use, and systematic record keeping of all field and laboratory data.

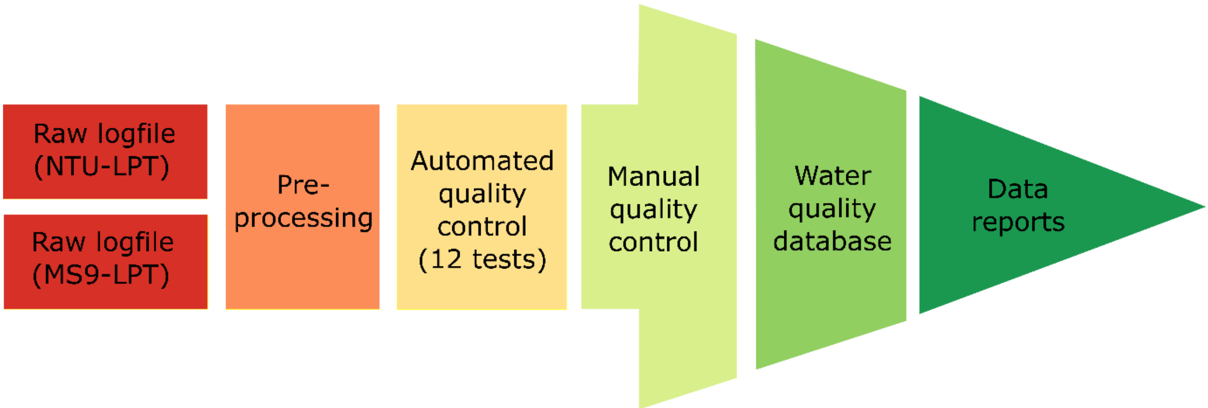

Figure 1. Simplified workflow diagram showing the steps taken from raw instrument data to final data reports sent to client

Water quality logger data is handled through a series of scripts in the R environment (R Core Team, 2023). A simplified workflow diagram showing the steps taken from raw instrument data to final data reports sent to the end-user is shown in Figure 1. Initially, the raw logfiles are pre-processed in preparation for quality control testing. The pre-processing step documents the deployment details (metadata) and converts the raw logfiles into the format required for the following steps. The rule-based automated QC process takes place in a script-based R environment. The automated scripts allow the QC process to be repeatable and removes human bias. There are twelve automated quality control tests which the data sequentially goes through (Table 1). The result of each test is recorded as a QC flag. Each flag is accompanied by a comment which describes which test the data failed and how it failed. In the case of multiple QC tests failing, the 'worst' flag for each value is reported with the final data reports but the information of the other tests is also retained. Following completion of the automated QC tests, one of our scientists or trained technicians familiar with the water quality logger program will perform semi-formal manual quality control steps. Finally, once the data has been fully checked it is ingested into our custom-made water quality database ready for further analysis and reporting.

Table 1. The twelve automated quality control tests

QC test 1: Syntax test	QC test 5: Regional range test	QC test 9: Stationary test
QC test 2: Impossible date test	QC test 6: Impossible depth test	QC test 10: Standard deviation test
QC test 3: In/out water test	QC test 7: Spike tests	QC test 11: Burst count test
QC test 4: Global range test	QC test 8: Rate of change test	QC test 12: Orientation test

Instrumentation

TropWATER utilise optical water quality loggers manufactured by Insitu Marine Optics (IMO), Perth, Australia (https://insitumarineoptics.com) and include:

- NTU-LPT turbidity logger
- MS9-LPT multispectral light logger

These loggers are standalone units which measure water depth, water temperature, tilt, and either turbidity (in NTU), or photosynthetically active radiation (PAR) and irradiance at nine specific wavelengths. The loggers are mounted on stainless steel frames to be placed on the seafloor where they log data continually (or as programmed) for up to two-month deployments at a time (Figure 2). Upon retrieval, data is downloaded from the loggers and entered into the QC workflow where automated and manual flags are applied.

Figure 2. Turbidity and light loggers attached to instrument frame ready for deployment on the seafloor.

Quality control flagging system

Primary flags

Primary flags are the flagging level which accompany the end-user data. A primary flag is set to the worst flag for each measurement of each parameter from the automated and manual quality control tests (i.e. worst secondary flag). The primary flags applied to the IMO loggers in the QC process are based on the Integrated Marine Observing System (IMOS) flag schematic (Morello et al., 2014) (Table 2).

Table 2: Primary QC flags as applied to the IMO logger data.

QC flag	Description	Definition
0	No QC performed	Raw data
1	Good data	All QC tests passed
2	Probably good data	Probably good data
3	Probably bad data	Probably bad data as it has failed a minor QC test. There is potential for the data to be manually corrected.
4	Bad data	Bad data. The data has failed a major QC test
5	Value changed	A value has been manually changed by the data reviewer
6	Not used	
7	Not used	
8	Estimated value	Estimated value (interpolation, extrapolation, or other estimation)
9	Missing value	Missing value
99	Masked data	Masked data where multiple loggers were deployed

Secondary flags

Secondary flags are retained with the logger data in the water quality database. These flag values contain detailed information about the conditions and outcome of each QC test. The secondary QC flag values are encoded in a way which is not end-user friendly. The secondary flags may be decoded when the need arises, but generally enough information for the end-user is contained in the primary flag and accompanying comment.

Interpretation and use of QC flags

Retaining all data 'as is' along with its QC flags through to the end user maintains data integrity. The end user decides what level of data 'quality' they wish to use for their application. For example, for most applications we suggest 'good data' and 'probably good data' are acceptable, 'probably bad data' may be used with caveats, and 'bad data' should be discarded. Unwanted data can easily be masked in MS excel or other data management programs by filtering by 'QC flag'.

Automated quality control steps

The first steps in the quality control process are completed by a collection of automated scripts written in the R programming language. The script assesses the data against twelve quality control rules in a series of tests. QC flags are added to any data which fails any of these rules. The 12 rules are as follows:

QC test 1: Syntax tests

The syntax test checks that each value is recorded in the correct data format for that parameter. For example, the timestamp is in ISO8601 datetime format, temperature is numeric class as a double-precision vector (i.e., numeric with decimal), Site_code is a character vector. Any values which are of incorrect syntax will throw an error and be flagged. The expected syntax is shown in Table 3. This test is a pass/fail test where the result is either ‘good data’ or ‘bad data’.

Table 3. Expected syntax (data format) for values of each parameter

Parameter	Syntax	Example
Timestamp_10min	Datetime (ISO 8601)	2022-06-05 08:54:23.200
Temp	Numeric double-precision	23.574
Depth	Numeric double-precision	6.53
NTU	Numeric double-precision	3.2
PAR	Numeric double-precision	300
Tilt	Numeric double-precision	91.50
Region	Character vector (string)	Mackay
Site_code	Character vector (string)	MKY_AMB1
Site_name	Character vector (string)	Freshwater Point

Test	QC Flag	Description
Syntax is correct	1	Good data
Unassigned	2	Probably good data
Unassigned	3	Probably bad data
Syntax is incorrect	4	Bad data

QC test 2: Impossible date

The impossible date test checks whether the timestamp has a sensible date. The earliest possible date is set at 2020-07-01 which corresponds with when TropWater commenced deploying the IMO loggers. The latest possible date is set as the current day, i.e. the day the logfile is being processed. Any timestamps with dates outside this range will throw an error and be flagged. Generally, when the data fails this test, the raw logfiles are scrutinised and the date/time is corrected where possible. The corrected logfiles are then rerun through the pre-processing and automated QC steps.

Test	QC Flag	Description
Date within possible date range	1	Good data
Unassigned	2	Probably good data
Date outside of possible date range	3	Probably bad data
Unassigned	4	Bad data

QC test 3: In/out-water test

The in/out water test flags the first 30 minutes of obtained logger data due to the high chance that either the logger is still at sea level and has yet to be placed on the sea floor, or the logger sensors have not yet stabilised. The outcome of test is further scrutinised during the manual QC tests.

Test	QC Flag	Description
Timestamp beyond first 30 minutes of deployment	1	Good data
Unassigned	2	Probably good data
Timestamp is within the first 30 minutes of deployment	3	Probably bad data
Unassigned	4	Bad data

QC test 4: Global range test

The global range test checks whether the sensor value is i) within the manufacturer's specifications, and ii) within the range of what is typically expected from field measurements (user specified range). The test is completed in two steps. I) test the values against manufacturers specifications (Table 4), then ii) test the values against the user thresholds (Table 5) and adjust the QC flags as necessary.

The upper limit of the NTU loggers optical sensors are nominally 400 or 1000 NTU depending on their build. In reality, due to optical imperfections, each turbidity sensors range is generally tuned slightly higher than the nominal value and is known as the 'NTU cut-off' value. Each logger has a unique NTU cut-off value which is recorded in the loggers internal configuration file. The user 'very high range' threshold is based on this cut-off value.

Any values which are outside of the global range will throw an error and be flagged. For example, the PAR logger can often show small negative values when PAR is zero due to the difficulty in obtaining a perfect calibration. Negative PAR values are flagged as 2, probably good data, as they can be considered as zero.

Table 4. Manufacturers specifications used by the global range test

Sensor	Low	High
Temperature (°C)	-55	125
Turbidity (NTU)	0	400/1000
Irradiance (µW cm^{-2} nm^{-1})	0	400
PAR (µmol m^{-2} s^{-1})	0	10,000
Pressure (depth) (m)	0	90

*NTU sensors come in low range (up to 400 NTU) and high range units (up to 1000 NTU)

Table 5. User thresholds used by the global range test

Sensor	Very low	Low	High	Very high
Temperature (°C)	0	15	35	NA
Turbidity (NTU)	-10	-1	0	NTU cut-off
Irradiance (µW cm^{-2} nm^{-1})	-10	0	400	NA
PAR (µmol m^{-2} s^{-1})	-10	0	8000	NA
Pressure (depth) (m)	NA	1	30	NA

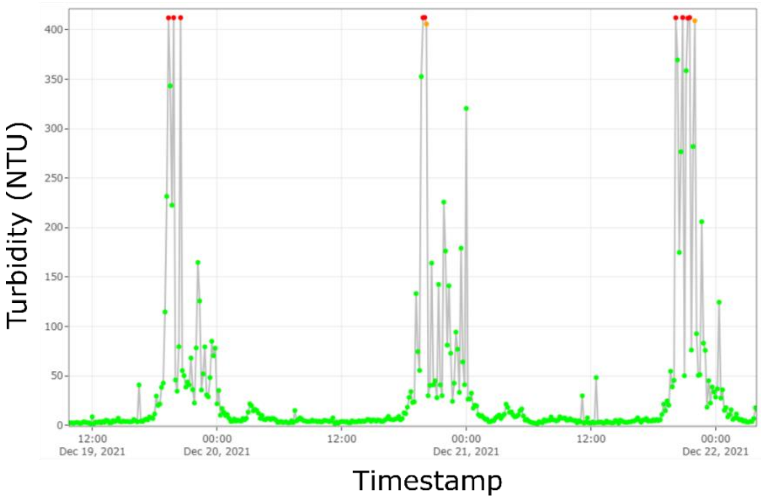

Figure 3. Example of global range test on NTU-LPT turbidity sensor data. In this case, the sensor was returning values greater than the manufacturers specifications. When this occurs, the values are 'clipped' to the maximum value of the digital-analog converter in the instrument and it is not possible to ascertain whether the value is real, or the real value is much higher. Green points indicate good data, orange points indicate values which were slightly above the instrument specifications and deemed 'probably bad data', red points indicate values which were outside of the instrument specifications and designated 'bad data'.

Test	QC Flag	Description
Sensor value is between the low and high manufacturers specifications	1	Good data
Sensor value is greater than the very low user threshold and less than the low user threshold, or sensor value is greater than the high user threshold and less than the very high user threshold	2	Probably good data
Sensor value is less than the low manufacturers specification or greater than the high manufacturers specification, or Sensor value is	3	Probably bad data
Sensor value is below the very low user threshold or above the very high user threshold	4	Bad data

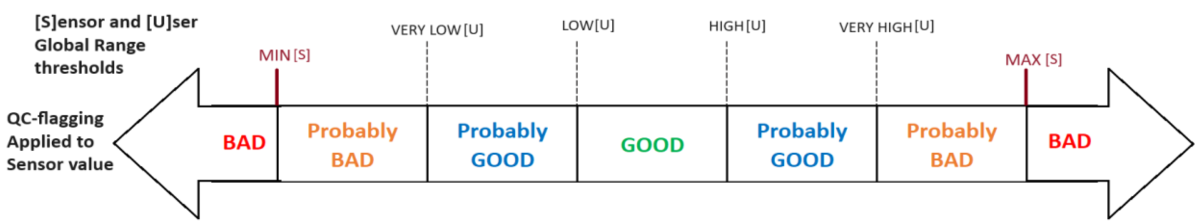

Figure 4. Global range test showing manufacturers specifications and user thresholds used.

QC test 5: Regional range test

The regional range test checks whether the water temperature and depth values are within expected range at the regions/sites where loggers are deployed in the coastal ocean. Temperature and depth thresholds (ranges) where determined from historical logger data collected from each region. Any values which are outside of the regional range will throw an error and be flagged as 'probably bad data'.

Table 6: Regional range thresholds for temperature and water depth for regions where loggers are deployed.

Region	Temperature threshold	Depth threshold
Bowen	18 < value < 32 °C	6 < value < 25 m
Whitsunday	19 < value < 32 °C	5 < value < 15 m
Mackay	16 < value < 32 °C	4 < value < 16 m
Weipa	22 < value < 33 °C	2 < value < 7 m

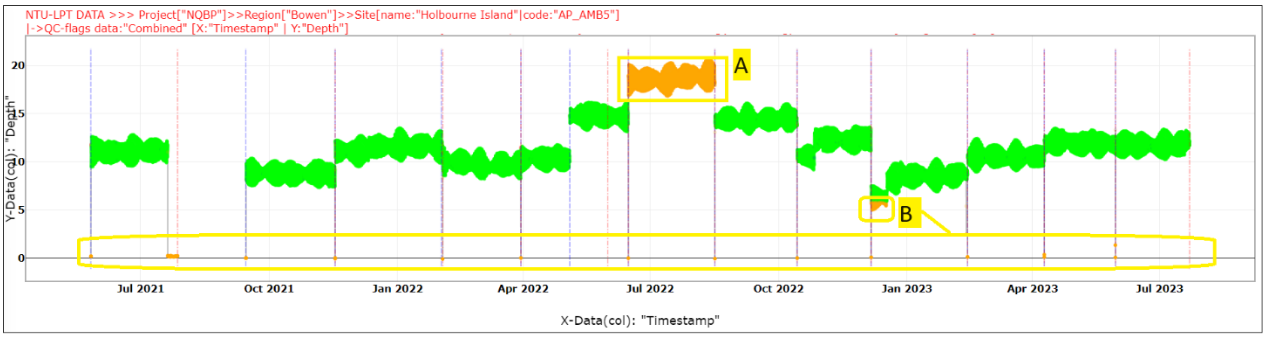

Figure 5. Results of regional range test on depth data from Holbourne Island. The orange points indicate data where depths exceed upper (A) and lower (B) depth thresholds for the Bowen region.

Test	QC Flag	Description
Sensor value within expected regional range	1	Good data
Unassigned	2	Probably good data
Sensor value outside of expected regional range	3	Probably bad data
Unassigned	4	Bad data

QC test 6: Impossible depth test

The impossible depth test closely follows the previous global and regional range tests. This test checks whether depth measurements are i) within a particular range of possible depths that we would measure for any deployment, or ii) significantly different (> z-score) from all other measurements across the deployment data. Minimum depth is set to 1 m to identify periods when the logger is out of water. For example, at the start and end of a deployment (Figure 6).

Table 7. Possible depth range for regions where the loggers are deployed.

Parameter	Value
Minimum depth	1 m
Maximum depth	30 m
Reasonable depth z-score	3 σ

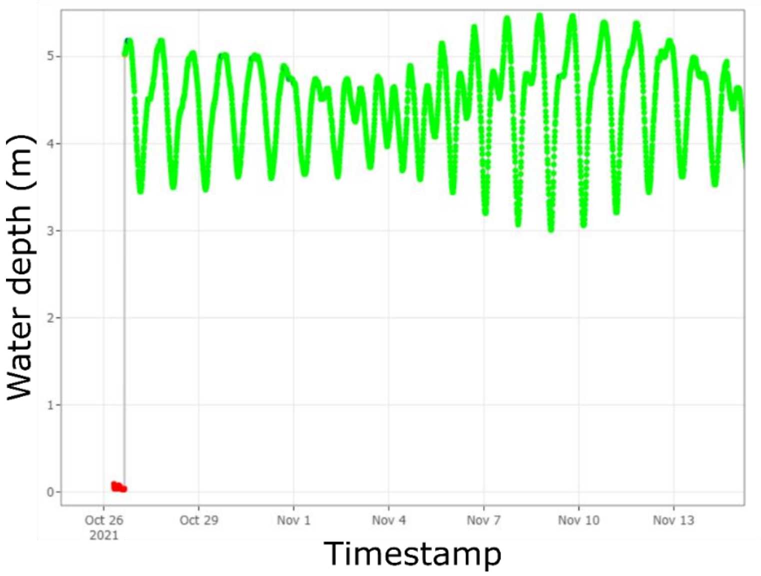

Figure 6. Example of the impossible depth test. The test flagged water depths less than 1 m as 'bad data'. this commonly occurs when there is a delay between when the logger is activated and when it is placed on the seafloor.

Test	QC Flag	Description
Depth is possible and within reasonable depth z-score	1	Good data
Unassigned	2	Probably good data
Depth is within possible range but exceeds reasonable depth z-score	3	Probably bad data
Depth is not within possible range	4	Bad data

QC test 7: Spike test

The spike test checks for any anomalous data 'spikes' in the temperature, pressure, turbidity, and light sensor data. Any values which are identified as spikes will throw an error and be flagged. The flag thrown depends on the threshold exceeded. The test looks for data spikes in three ways i) the value is compared to immediate neighbour and flagged if value is very different, ii) using a threshold equation.

$$Test\ value\ (fail) = \left|V_n - \frac{(V_{n+1} + V_{n-1})}{2}\right| - \left|\frac{(V_{n+1} + V_{n-1})}{2}\right| > threshold$$

The thresholds used for the spike test are shown on

Table 8. When a spike measurement is below the low threshold ‘good data’; when spike measurement is between the low and high threshold the ‘probably good data’, and when spike measurement is above the high threshold it is flagged as ‘probably bad data’ (Figure 7).

Table 8. Spike test thresholds for each sensor.

Sensor	Low threshold	High threshold
Temperature	0.5	2
Pressure (depth)	0.5	1
Turbidity	50	100
Irradiance (individual channels)	25	50
PAR	100	300

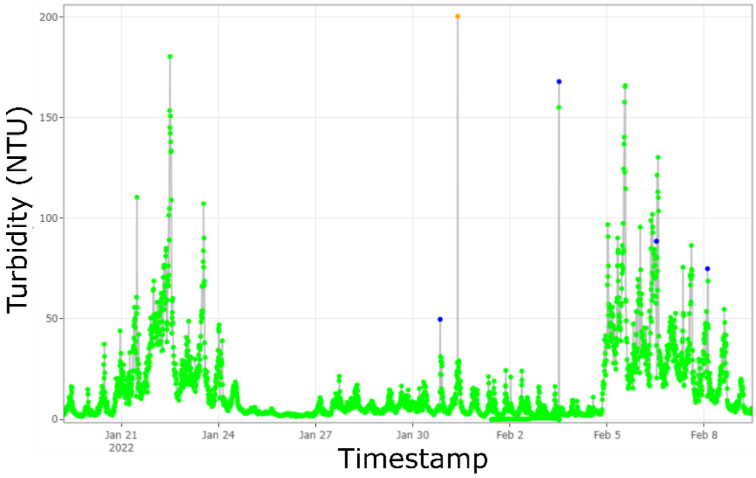

Figure 7: Example of spike detection on NTU-LPT turbidity sensor data. Green points indicate good data, blue points indicate spikes which were deemed 'probably good data', orange point indicates a spike which was designated 'probably bad data'.

Test	QC Flag	Description
Spike value does not exceed low threshold	1	Good data
Spike value exceeds low threshold but does not exceed high threshold	2	Probably good data
Spike value exceeds high threshold	3	Probably bad data
Unassigned	4	Bad data

QC test 8: Rate of change test

The rate of change test checks if a particular measurement significantly changes across neighbouring measurements (exceeding a certain threshold).

$$Test\ value\ (fail) = (|(V_n - V_{n-1})| - |(V_n - V_{n+1})|) > 2 * Threshold$$

Table 9 shows low and high thresholds applied for each parameter. When a series of measurements rate of change is below the low threshold the data is flagged as ‘good data’; when measurement rate of change is between the low and high threshold the data is flagged ‘probably good data’; and when measurement rate of change is above the high threshold the data is flagged ‘probably bad data’.

Table 9: Rate of change test thresholds

Sensor	Low threshold	High threshold
Temperature	0.5	2
Pressure (depth)	0.5	1
Turbidity	100	200
Irradiance (individual channels)	25	50
PAR	150	300

Test	QC Flag	Description
Rate of change is less than the low threshold	1	Good data
Rate of change is greater than the low threshold but less than the high threshold	2	Probably good data
Rate of change is greater than high threshold	3	Probably bad data
Unassigned	4	Bad data

QC test 9: Stationary test

The stationary test looks for 'stuck' values. It is expected that under natural conditions the values recorded for all sensors on the loggers should show some natural variation and not return the same value for an extended period. Stuck values may occur when a sensor malfunctions and repeatedly returns the same value. Any values which are stuck will throw an error and be flagged.

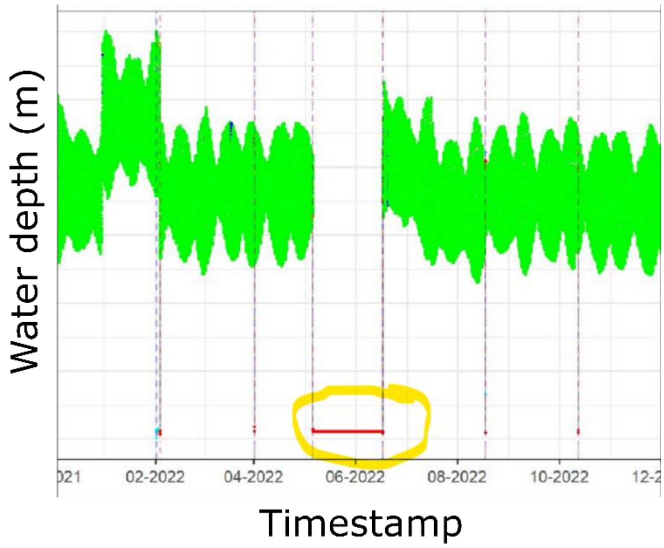

Figure 8. Example of water depth data failing the stationary test. In this case the pressure sensor malfunctioned, and the measurements were stuck at 0.00 m for the entire deployment. Values which were flagged as 'bad data' are shown in red.

Test	QC Flag	Description
Value is non-stationary	1	Good Data
Values are stationary for less than 60 minutes	2	Probably good data
Values are stationary for more than 60 minutes and less than 24 hours	3	Probably bad data
Values are stationary for more than 24 hours	4	Bad data

QC test 10: Standard deviation test

Placeholder. This test is not currently used.

QC test 11: Burst count test

The burst count test checks that the correct number of measurements were recorded for each 'burst' that occurs for each 10-minute interval, e.g., the loggers are programmed to record a burst of 50 samples at 5 Hz every 10 minutes. If there were only 5 values recorded for the 10-minute period, the data would be flagged.

Test	QC Flag	Description
Correct number of measurements recorded	1	Good Data
At least ¾ of the measurements have been recorded	2	Probably good data
Between ½ and ¾ of the measurements have been recorded or more measurements have been recorded than expected	3	Probably bad data
Less than ½ of the measurements have been recorded	4	Bad data

QC test 12: Orientation test

The tilt sensor on the instrument is used to assess whether the logger is orientated correctly on the seafloor. It is possible that the instrument frame may be disturbed, and its orientation changed by adverse weather such as strong wind, tidal current, or large seas, vessel activity (i.e., fishing trawlers), or members of the public. The optimal orientation for the MS9-LPT light logger is vertical (0°). The maximum allowable off-vertical angle for the MS9 irradiance sensor is 60° as cosine correction beyond 60° is not within specifications of the instrument. Light data is flagged 2 (Probably good data) for instances where 10° < tilt < 60° and flagged 4 (Bad data) for instances where 60 < tilt < 180°. The optimal orientation for the NTU-LPT turbidity logger is 90°. Turbidity data is flagged 2 (Probably good data) for instances where 0° < tilt < 60° and 120 < tilt 150°. Turbidity data is flagged 4 (Bad data) for instances where 150° < tilt < 180° (Figure 9).

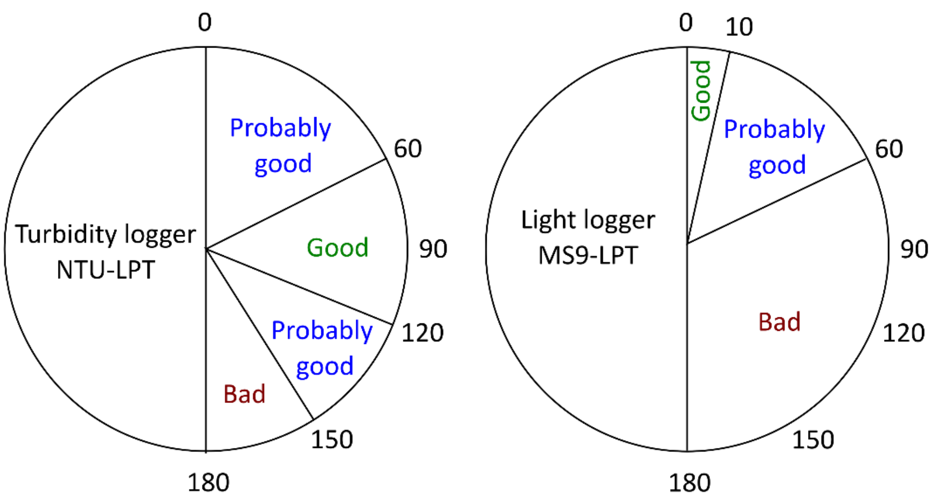

Figure 9. Tilt thresholds for MS9-LPT and NTU-LPT loggers. The optimal orientation of the turbidity logger is horizontal (90°) while the light logger is vertical (0°)

Test	QC Flag	Description
Sensor is orientated within normal angle	1	Good Data
Sensor is orientated outside of normal angle but within maximum allowable angle	2	Probably good data
Unassigned	3	Probably bad data
Sensor is orientated outside of maximum allowable angle	4	Bad data

Manual quality control steps

The data is reviewed by a trained operator once the automated quality control steps have been completed. This allows for problems which are difficult to see from a machine perspective to be flagged by an operator. The operator may choose to either modify the QC flag value, add new or additional comments, or make corrections (such as a timestamp correction) and reprocess the data.

Manual check 1: Review of data that fails an automated QC test.

The first step is to review the data and inspect regions in the dataset where QC flags have been thrown. The operator may add further QC flags and manual comments to the dataset. For example, a spike in NTU data flagged by the automated spike test may have an explainable reason, such as elevated wave activity (as seen in the depth RMS data), or nearby known dredging activity. In these cases, data flagged 'probably bad data' may be reassessed as 'probably good data' and comments added. Another example may be depth sensor data originally flagged as 'probably bad data' by the regional range test being valid on further inspection. In this case the logger was deployed to a slightly deeper depth than usual, which was apparent when reviewing the field notes and deployment GPS waypoint.

Manual check 2: Timestamp check

The operator who is reviewing the logger data checks that the start and end date and time of the logfile correspond with the start and end date and time of the deployment recorded on the field datasheets. This check is done on top of the impossible date test as the automated test can only tell if the date is realistic, not if it aligns with an actual deployment event. The operator may choose to either modify the QC flag value, add new or additional comments, or make corrections (such as a timestamp correction) and reprocess the data.

Manual check 3: Sensor stability check

This check looks at the period at the start of each deployment when the logger has been placed on the seafloor, but the sensors have potentially not stabilised to their surrounds. The operator looks at depth and water temperature looking for pattern in the temperature data which indicates the sensors are still stabilising. This generally only affects the initial 3 or 4 measurements of any deployment and is intentionally overly cautious. All parameters while the temperature sensor is returning unstabilised data are assigned flag 4 (Bad data).

Manual check 4: Sensor baseline drift check

This check does a visual eyeballing of plotted data for sensor baseline drift, along with 'funny' looking values. Some drift around the zero baseline is expected from the optical sensors but excessive drift is a sign of the sensor falling out of calibration. If a sensor is shown to be drifting significantly from its baseline it will be removed from operation, serviced, and recalibrated. The operator may modify the QC flag value and add comments to the dataset.

Manual check 5: Overlapping data check

Occasionally two loggers will be deployed at the same site with overlapping deployment windows. The most common reason for this is where a logger has been temporarily 'lost' and a new logger has been deployed in its place as scheduled. The lost logger has later been found and successfully retrieved and the data downloaded. The operator manually selects which values keep and which values to mask/discard. Generally, the newly deployed logger values are kept, and the values from the logger which is being retrieved are discarded. The masked data is given a flag value of 99 (Masked data). This flag is generally not encountered by the end-user.

Manual check 6: Missing data

Periods of missing data are identified and a flag value of 9 (Missing data) is assigned. The QC comments of the missing data are manually updated to include details about the cause of missing data.

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