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Quality control procedure for IMOS real-time meteorological and sea surface observations, and air-sea fluxes from research vessel and mooring platforms

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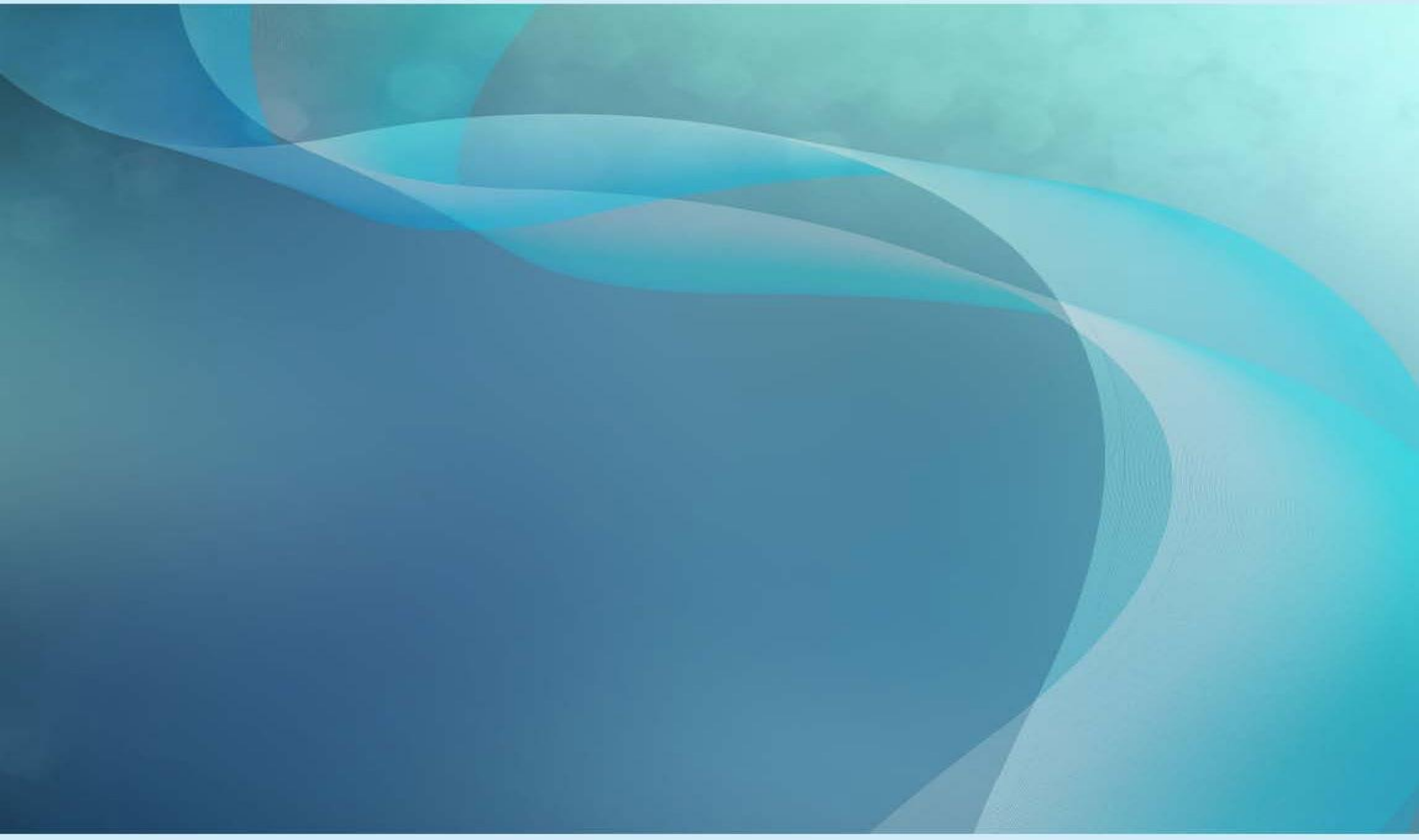

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EXECUTIVE SUMMARY

This document outlines the automated Quality Control system implemented at the Bureau of Meteorology as part of the Integrated Marine Observing System, to process the real-time marine meteorological and surface ocean observations and air-sea fluxes obtained from ships and moorings.

1. INTRODUCTION

This document outlines the automated Quality Control (QC) system implemented at the Bureau of Meteorology as part of the Integrated Marine Observing System (IMOS: https://imos.org.au), to process the real-time marine meteorological and surface ocean observations and air-sea fluxes obtained from ships and moorings as part of facilities 2c (Sea Surface Temperature Sensors for Australian Vessels), 2d (Research Vessel Real-Time Air-Sea Fluxes) and 3ab (Southern Ocean Time Series Observatory). The QC procedure is based on the system developed by the Center for Ocean-Atmospheric Prediction Studies (COAPS), Florida State University, for the Shipboard Automated Meteorological and Oceanographic System Initiative (SAMOS: http://samos.coaps.fsu.edu) and as documented in Smith et al., (2010) (see http://www.oceanobs09.net/proceedings/cwp/Smith-OceanObs09.cwp.83.pdf). Research vessel observations from IMOS sub-facility 2d are submitted as a contribution to SAMOS. The IMOS QC attempts to maintain compatibility in procedure, QC flag sets, file formats and versioning where possible.

2. PRE-PROCESSING

All incoming data is archived in its original form. Data is converted to the SAMOS NetCDF format (Rolph and Smith, 2005) and changed to standard units if required. The default QC flag is 'Z' and this is assigned to all data values. Checks are performed to confirm the expected number of variables, their order, dimensions and attributes. The existence and order of the time, latitude and longitude variables is verified. All three must exist for an observation to be valid. If there is a known instrument malfunction then the variables produced by that instrument are assigned the QC flag of 'M' for the duration of the malfunction and no more QC flags will be assigned to that variable.

3. QC PROCESSING

The QC procedure is automated and runs routinely as the real-time data arrives – for one-minute data this is typically several times an hour. Sub-daily QCd data is available for immediate submission to the near-real-time Global Telecommunication System (GTS) for the World Meteorological Organisation. Once all data for a particular date has arrived a daily QC is performed and data is made available for submission to the IMOS Australian Ocean Data Network.

The QC procedure is applied to the observations at each time entry and involves a number of sequential tests which are performed until a test fails, at which point the relevant QC flag is assigned (Smith et al., 1996). If all the tests are passed then the default 'Z' QC flag is retained. Note that whatever the outcome of the QC tests the data remains unchanged.

The QC flags are based on the original SAMOS flag set available at: https://samos.coaps.fsu.edu/html/docs/samos_quality_flag.pdf, and https://www.coaps.fsu.edu/woce/docs/qchbook/qchbook.htm.

The SAMOS QC flag set and associated tests are in Table 1, with bold flags indicating those used in the IMOS QC system.

Table 1 QC flags

Flag	Description
A	Units not provided, so determined by climatology or some other method
B	Physical bounds
C	Time sequential
D	Air temperature
E	True wind
F	Platform speed
G	Climatology
H	Time discontinuity
I	Interesting feature found in data.
J*[1]	Data are of poor quality by visual inspection
K*	Data suspect, has obvious errors, but no specific reason for determined
L	Position over land
M*	Known instrument malfunction
N	Vessel in port
O*	Original units differ from those listed in the original_units variable attribute
P*	Position of platform or its movement are uncertain.
Q	Exhaust emission contamination of air temperature/humidity, or SST from SBE48 vessels & VHW6005 are near stationary, or VLMJ keel not extended
R	Interpolated value applied prior to arrival at the DAC.
S*	Spike in the data
T	Time duplicate
U	Suspect (statistical)
V	Spike (statistical)
X	Step/discontinuity (statistical)
Y	Suspect values between X-flagged data (statistical)
Z	Data passed evaluation

[1] indicates QC flags which may be assigned manually to particular variables and for specified periods of time based on external knowledge provided by the platform operator or manual visual inspection of the data.

The tests are, in order of application & relevant QC flag:

1. Physical bounds (‘B’)
2. Time (‘C’, ‘H’, ‘T’)
3. Position (‘L’)
4. Platform speed (‘F’)
5. Water temperature (‘Q’)
6. Exhaust contamination (‘Q’)
7. Air temperature (‘D’)
8. True wind (‘E’)
9. Statistical (‘U’, ‘V’, ‘X’, ‘Y’)
10. Climatological bounds (‘G’)

3.1 Physical bounds

The bounds test establishes if the data (including time, latitude, longitude and other observed quantities) are within expected physical bounds (Table 2). Failed data is assigned a ‘B’ QC flag.

Table 2 Range bounds

Variable	Lower bound	Upper bound	Units
Time	00:00 (1/1/1980) (UTC)	Current date and time	Minutes since 1980-01-01 00:00 (UTC)
Latitude	-90	90	Degrees
Longitude	0	359.999	Degrees
Platform heading	0	360	Degrees
Platform speed	0	25	ms^{-1}
Relative wind direction	0	360	Degrees
Relative wind speed	0	100	ms^{-1}
Wind direction	0	360	Degrees
Wind speed	0	100	ms^{-1}
Air pressure	850	1050	mb (hPa)
Air temperature	-30	50	Celsius
Wet bulb temperature	-30	50	Celsius
Dew-point temperature	-30	50	Celsius
Water temperature	-2	40	Celsius
Relative humidity	0	100	%
Visibility	0	10000	m
Precipitation	0	55	mm
Rain rate	0	4.2	mm $minute^{-1}$
Short wave radiation	0	1400	Wm^{-2}
Long wave radiation	100	450	Wm^{-2}
Photosynthetically active radiation	0	6000	μEm^{-2}
Compass direction	0	360	Degrees
Conductivity	0	6	Sm^{-1}
Salinity	0	40	psu
GPS height	-30	100	m
Keel extension	0	10	m

3.2 Time

The time variable is tested to ensure the times are sequentially increasing and by the expected amount. The expected time difference between adjacent data points is known as the data interval – normally 1 minute for research vessels, 60 minutes for SOFS mooring (real-time) and 1 through to 60 minutes for other vessels including AVOF – see http://imos.org.au/fileadmin/user_upload/shared/SOOP/SST_Sensors_for_Australian_Vessels/IMOS_ship_SST_table_02Oct2019.pdf. If a time is less than the previous one the value is considered non-sequential and a 'C' QC flag is applied. Duplicate values are QC flagged with 'T'. If the time difference between two adjacent data points exceeds the expected data interval a time discontinuity is indicated with a 'H' QC flag.

3.3 Position

The position test is performed to verify that the platform (vessel or mooring) is not located over land. A high resolution (~1km) land/sea map with distance from land from the U.S. Naval Oceanographic Office (downloadable from https://www.ghrsst.org/ghrsst-data-services/tools) is used as a land mask covering 80.3°N to 80.3°S, 0-360°E and includes coastal regions and lakes. If a position is over land latitude and longitude are assigned an 'L' QC flag.

3.4 Platform speed

The platform speed test determines if the speed of the platform exceeds a threshold. Platform speed is determined using selected sequential latitude and longitude positions of the vessel. The vessel speed is determined from the great circle path on a perfect sphere. For all data with a data interval of at least three minutes, velocities are calculated using sequential latitude and longitude values. For 1-minute data, to reduce noise in position data and inaccuracy in velocity, speed is computed from positions 3 minutes apart (in original SAMOS procedure 1-minute data are averaged up to 3-minutes). The threshold value is shown in Table 1. If the speed exceeds the threshold, or if the speed is negative (possibly when speed cannot be computed because time, latitude or longitude are not present or are suspect), both the latitude and longitude are flagged with an 'F'. To be compared with the threshold, speed must be computed over a time gap of at most 3 hours.

3.5 Water temperature

This test assigns a QC flag 'Q' to the water temperature if the SST instrument type is SBE 48 and the ship speed is low (below 2.5 ms^{-1}), or for VHW6005 (RV Linnaeus), which has an SBE 38 sensor, when its speed is less than 0.5 ms^{-1}, or for VLMJ (RV Investigator) if the port drop keel is not extended. Up until 6th September 2017 water temperature measurements from VMQ9273 (RV Solander) and VNCF (RV Cape Ferguson) were also assigned a QC flag 'Q' when vessel speeds were less than 0.5 ms^{-1}.

3.6 Exhaust contamination

This test determines if the air temperature and humidity observations may have been affected by emissions from the ship engine exhausts. A wind direction from the aft sector of the ship will trigger a fail and application of QC Flag 'Q' to both port and starboard air temperature and relative humidity. The aft sector is defined for each individual vessel depending on relative locations of the exhaust and the air temperature and humidity instruments. This test requires relative wind. This test is applied to the RV Investigator from October 2021.

3.7 Air temperature

If dry-bulb (air temperature), dew-point and wet-bulb temperatures are present then a test is performed to confirm that dry-bulb >= wet-bulb >= dew-point temperature. The QC flag 'D' is applied if the test fails.

3.8 True wind

The calculation of true wind speed and direction is tested if the relative wind and ship velocity is available. A failure threshold of 2.5 ms^{-1} and 20 degrees is used. The QC flag 'E' is applied if the test fails.

3.9 Statistical

This test and the associated parameters (Table 3) are based on the SAMOS automated Spike And Stair Step Indicator (SASSI) procedure (Smith et al., 2010). Outliers, spikes and steps or discontinuities in data are detected by identifying where (absolute) differences between selected successive data values exceed a threshold. The threshold is set as the maximum of (i) the product of the standard deviation of the 99th percentile of successive data differences and a standard deviation scale factor equal to 3, and (ii) a background threshold (Table 3). The background threshold has been set for each variable based on examining the natural variability and data precision (a combination of instrument and data processing performed on the platform). Outliers are assigned the 'U' QC flag. Spikes are assigned the 'V' QC flag. 'X' QC flags indicate steps or discontinuities and 'Y' QC flags indicate suspect values between 'X' QC flags. The statistical test is applied only to datasets with a data interval less than 3 minutes and with more than 200 data values, usually at the daily QC.

Table 3 Statistical test

Variable	Background Threshold
Air pressure	0.6 hPa
Air temperature	0.5 Celsius
Relative humidity	1.5 %
Water temperature	0.5 Celsius
Salinity	0.3 psu
Conductivity	0.3 Sm^{-1}

3.10 Climatological bounds

Water temperature is compared against blended satellite SST analysis data: The Regional Australian Multi-Sensor Sea Surface Temperature Analysis (RAMSSA) and Global Australian Multi-Sensor Sea Surface Temperature Analysis (GAMSSA) products (Beggs et al., 2011; Zhong and Beggs, 2008). If an absolute difference between analysis and platform value exceeds 3°C, the QC flag is set to 'G'. Observations of wind speed, air pressure, air temperature, water temperature and relative humidity are compared against the daSilva climatology (da Silva et al., 1994). The QC flag 'G' is applied if the observation lies more than 4 standard deviations from the mean. The water temperature comparison against the daSilva climatology ceased after November 2019. Note that prior to October 2021 this test was performed before the statistical test.

4. QC INFORMATION

The output SAMOS-format netCDF data files contain the original input data accompanied by a QC data array with dimensions matching the time and number of variables. The QC data array contains QC flags corresponding to the QC quality of each data value in the file. For distribution via IMOS AODN the netCDF files are in IMOS netCDF format and contain, for each measured variable, a dedicated QC data array which depends only on time.

5. AIR-SEA FLUX PROCESSING

Air-sea fluxes are calculated using the bulk method (Fairall et al., 2003).
Fluxes are only calculated when all the input data is available, has appropriate QC flags ('Z' or 'G') and includes observation height from the water for some variables. Therefore, the air-sea flux datasets do not include QC flags.

- The bulk method requires the following data: time, latitude, longitude, platform heading, platform speed, relative wind direction, true wind, air temperature, water temperature, humidity, air pressure, precipitation, incoming longwave radiation, incoming shortwave radiation.
- Height above water is required for the following observations: true wind, air temperature, water temperature, humidity and air pressure.
- Water intakes (for SST and salinity) located on retractable keels (i.e. the RV Investigator), must be in the extended position for the calculation to proceed.
- Negative incoming radiation observations are assigned zero.
- Dual sensor long-wave radiation observations must agree to 20 Wm^{-2}.
- Small variations and small negative trends in precipitation (due to evaporation) are removed by smoothing using a 2-hour running mean.
- Missing air pressure values are assigned a value of 1013.25 hPa for the SOFS platform. For ship platforms the calculation will not proceed.
- Many platforms have two or more sensors collecting the same observation type. An observation from one sensor only must be selected for the bulk flux calculation.
    - For wind, air temperature and humidity, the upwind sensor (based on relative wind direction) is selected to minimise the effects of the instrument mounts and mast.
    - In addition, for ship platforms the observations are excluded if the wind direction is from the aft of the ship, to minimise exhaust emission contamination and deck heating of air temperature and humidity observations. The relative wind directions defining 'aft' are set for each platform to account for different smoke stack and instrument siting configurations. This condition is indicated by the 'Q' QC flag applied to air temperature and humidity.
    - The highest value of short-wave radiation is used (low values are assumed to be due to shading from ship superstructure).
    - The lowest value of long-wave radiation is used (high values are assumed to be due to heating from roosting birds or hot superstructure in the field of view).
- The selected input observation data and output air-sea flux data are provided together in the output file for reproducibility.

6. ACKNOWLEDGEMENTS

Ruslan Verein created the first draft of this document (unpublished).

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