

Southern Ocean Time Series (SOTS) Quality Assessment and Control Report Salinity Records 2009-2020

Version 1.0

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October 2021



Citation

Jansen P, Shadwick EH and Trull TW (2021). Southern Ocean Time Series (SOTS) Quality Assessment and Control Report Salinity Records Version 1.0. CSIRO, Australia.

DOI: [10.26198/rv8y-2q14](https://doi.org/10.26198/rv8y-2q14)

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Acknowledgments

SOTS is supported by the NCRIS IMOS program, CSIRO Oceans and Atmosphere, Bureau of Meteorology, Antarctic Climate and Ecosystems CRC, Australian Marine National Facility, Australian Antarctic Program Partnership, and Australian Antarctic Division.

Data was sourced from Australia's Integrated Marine Observing System (IMOS) – IMOS is enabled by the National Collaborative Research Infrastructure Strategy (NCRIS). It is operated by a consortium of institutions as an unincorporated joint venture, with the University of Tasmania as Lead Agent.

Executive summary

The Southern Ocean Time Series (SOTS) Observatory located near 141°E and 47°S provides high temporal resolution observations in Subantarctic waters. It is focused on the Subantarctic Zone because waters formed at the surface in this region by deep wintertime convection slide under warmer subtropical and tropical waters, carrying CO₂ and heat into the deep ocean, where it is out of contact with the atmosphere. This process also supplies oxygen for deep ocean ecosystems, and exports nutrients that fuel ~70% of global ocean primary production. Local biological production also impacts carbon cycling and the SOTS moorings measure several variables important to these processes.

This report describes the quality control (QC) procedures applied to salinity data collected from the SOTS moorings between 2009 and 2020. These measurements help to quantify heat and freshwater transfers, help to distinguish Eulerian from Lagrangian influences on seasonal records, and contribute to understanding controls on surface mixed layer depth (and thus light availability to primary production). The quality-controlled datasets are publicly available via the Australian Ocean Data Network (AODN) Portal: [Open Access to Ocean Data \(aodn.org.au\)](https://aodn.org.au). This report should be consulted when using the data.

The QC procedures apply automated tests following QARTOD recommendations for in-situ temperature and salinity data quality control (Bushnell and Worthington, 2020), with the test parameters tailored to reflect regional oceanography. QARTOD is an initiative of the US Integrated Ocean Observing System for Quality Assurance of Real Time Oceanographic Data: <https://ioos.noaa.gov/project/qartod/>. The procedures yield QC flags for each observation, as well as uncertainty estimates for the overall results, but do not produce an adjusted or gridded data set (that task will be addressed in a subsequent report).

1 Introduction

The Southern Ocean Time Series (SOTS) Observatory provides high temporal resolution observations in Subantarctic waters. Observations are broad and include measurements of physical, chemical and biogeochemical parameters from multiple deep-water moorings in the Subantarctic Zone southwest of Tasmania (Figure 1). The emphasis is on seasonal and inter-annual variations of lower atmosphere and upper ocean properties and their influence on exchange with the deep ocean. The continuous time-series information allows the study of ocean physics and chemistry, climate change, carbon cycling and biogeochemical controls on marine productivity. These moorings provide cost-effective observations and overcome the infrequent availability of ships in the region. The Southern Ocean Time Series is an Australian contribution to the international OceanSITES global network of time series observatories (www.OceanSITES.org) and is one of the few comprehensive Southern Ocean sites globally. More information on the SOTS Sub-Facility is available on-line at <http://www.imos.org.au/>.

The Southern Ocean (south of 30°S) is responsible for ~40% of the total global ocean uptake of human-induced CO₂ emissions, and 75% of the additional heat that these emissions have trapped on Earth. The Southern Ocean Time Series site is focused on the Subantarctic Zone because waters formed at the surface in this region, the Subantarctic mode and Antarctic Intermediate waters, slide under warmer subtropical and tropical waters and carry this CO₂ and heat into the deep ocean, out of contact with the atmosphere. This process also supplies oxygen for deep ocean ecosystems, and exports nutrients that fuel ~70% of global ocean primary production. The Subantarctic Zone and these processes are expected to change with global warming, but the potential impacts of these changes are not yet known.

The Southern Ocean Time Series site southwest of Tasmania is comprised of a number of elements including a deep ocean sediment trap mooring (SAZ), a surface biogeochemistry mooring (Pulse) and an air-sea flux mooring (SOFs). Located in the Subantarctic Zone near 141°E, 47°S, the site is particularly vulnerable to the extreme weather events that typify the area including very large waves, strong currents and severe storms, presenting significant technical and engineering challenges.

The SOTS site (red star in Figure 1. Location of the SOTS observatory.) is in a low current region, north of the Subantarctic Front (SAF) that marks the northern edge of the Antarctic Circumpolar Current. It is in deep waters (>4500m) west of the Tasman Rise (the shallow region south of Tasmania; with waters less than 2000m deep, shown in blue). The SOTS site exhibits oceanographic properties representative of the Australian sector of the Subantarctic Zone (from ~90 to 145°E; Trull et al., 2001). Waters flowing southward in the East Australian Current reach this region by transiting through channels in the Tasman Rise (Herraiz-Borreguero and Rintoul, 2011).

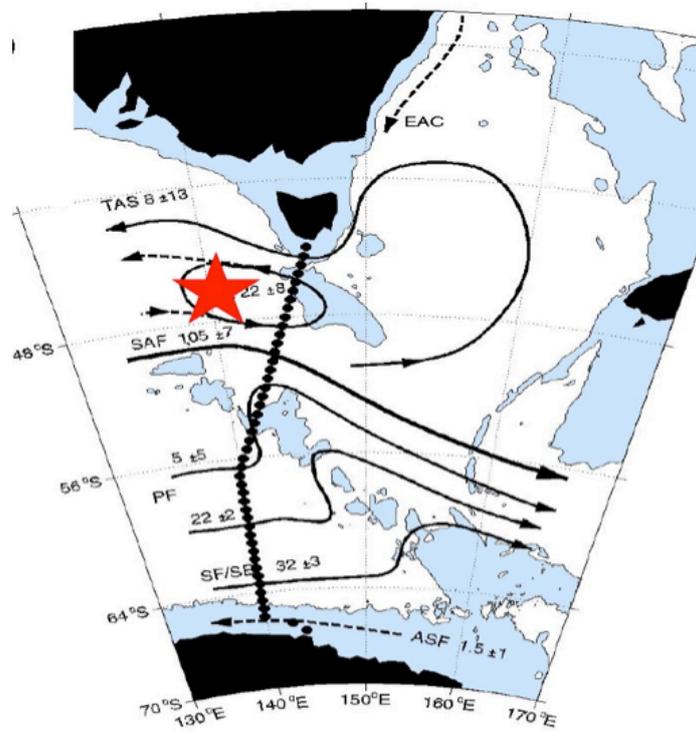


Figure 1. Location of the SOTS observatory.

EAC – East Australia Current, TAS – Tasman Sea Leakage, SAF-Subantarctic Front, PF-Polar Front, SF/SB – Slope Front/Southern Boundary, ASF, Antarctic Shelf Flow. Adapted from Herraiz-Borreguero et al., 2011

2 Moorings Description

The Southern Ocean Time Series moorings are the Pulse biogeochemistry mooring, the Subantarctic Zone (SAZ) sediment trap mooring, and the Southern Ocean Flux Station (SOFS).

The Pulse biogeochemistry mooring is used to measure upper ocean carbon cycle and phytoplankton productivity processes. Measured parameters include temperature, salinity, dissolved oxygen, total dissolved gases, nitrate, chlorophyll fluorescence and optical particulate backscatter. This mooring also collects water samples for measurements of dissolved carbon and nutrients, and phytoplankton microscopic identification.

The SAZ sediment trap mooring collects sinking particles to quantify carbon fluxes, and provides current meter measurements and a deep ocean CTD to measure heat contents below the depth of Argo profiling float measurements.

The SOFS meteorological tower mooring has dual sets of incoming solar radiometers, temperature and humidity sensors, precipitation gauges and sonic anemometers, and a pCO₂ sensor provided by NOAA. Surface photosynthetically active radiation (PAR) is also measured to help assess light available for phytoplankton production.

All three moorings are anchored to the ocean floor ~4.5 kilometres below the surface. The SOFS and Pulse moorings are s-tether designs that are longer than this, and correspondingly their surface floats move in large 'watch circles'. In contrast, the SAZ mooring is a stiff subsurface mooring with all components more than 700m below the surface. The moorings record hourly sensor observations until they are swapped with a duplicate mooring the following year.

In the 2016-17 year, the SOFS and Pulse capabilities were combined into a single prototype mooring known as FluxPulse-1. After this initial trial, the combined mooring nomenclature continued using the SOFS prefix.

Surface data collected from Pulse and SOFS are relayed back by satellite. The sub-surface data are stored and downloaded when the moorings are retrieved (approximately a year later). All data are available via the Australian Ocean Data Network (AODN) Portal.

3 Summary of Instruments

All salinity records from the SOTS moorings in the 2009-2020 period were based on conductivity measurements using Sea-Bird Electronics instruments (5 different models). All the sensors were paired with thermistor temperature measurements, some instruments were pumped and some were not. Most instruments had pressure sensors, and some also included oxygen sensors. Sampling frequency was at least hourly, and for some sensors as often as every minute (see Table 1 for details). In general, the sensors were deployed as follows:

1. On the Pulse and SOFS moorings, as sets of individually logged instruments spaced from the surface to about 500m depth.
2. On the SAZ moorings, at the depths of the sediment traps and/or near the bottom as a contribution to the OceanSITES and Deep Ocean Observing System (DOOS) “Deep Heat Challenge”.

Data logging was in all cases internal to the instruments, and in general was only recovered when the moorings were recovered (except surface data telemetered from the SOFS moorings). The times of the mooring deployments are shown in Figure 2. SOTS mooring deployments covered in this report., and an overview of their temperature records prior to QC is provided in Figure 3. The individual temperature sensors are listed in Table 1.

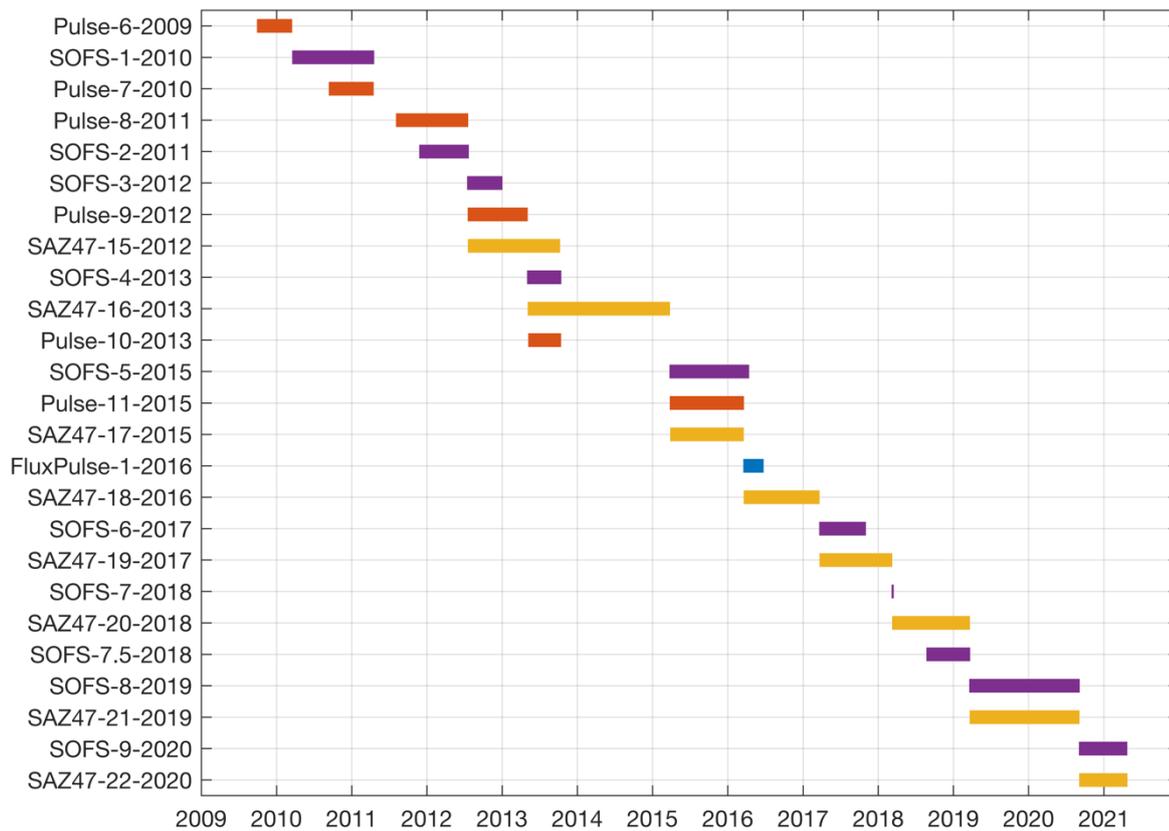


Figure 2. SOTS mooring deployments covered in this report.
SAZ in yellow, Pulse in orange, and SOFS in purple.

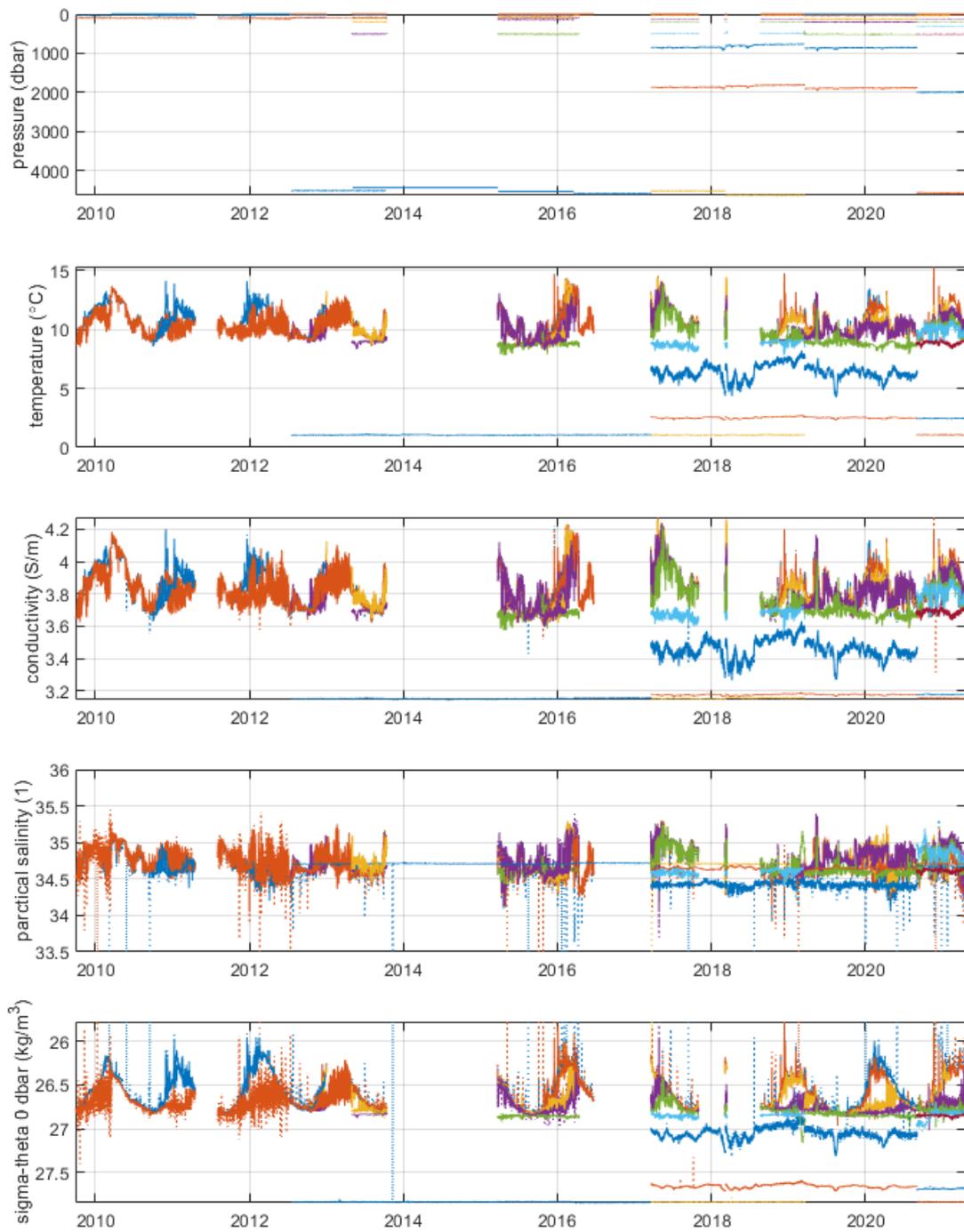


Figure 3. Overview of raw T, S, Sigma-theta (at pressure 0) results prior to QC.

Table 1. SOTS Salinity Sensors 2009-2020

Deployment	Depth*	Instrument: serial #	Pump/Press	Sampling (s)
Pulse-6-2009	37.5	SBE16plusV2: 6331	yes/yes	3600
Pulse-6-2009	100	SBE37SM: 6962	no/yes	60
SOFS-1-2010	0.66	SBE37SM: 7409	no/no	300
SOFS-1-2010	100	SBE37SM: 2971	no/yes	600
Pulse-7-2010	31.1	SBE16plusV2: 6331	yes/yes	3600
Pulse-7-2010	100	SBE37SM: 6962	no/yes	60
Pulse-8-2011	34	SBE16plusV2: 6330	yes/yes	3600
Pulse-8-2011	105	SBE37SM: 6962	no/yes	60
SOFS-2-2011	1.5	SBE37SM: 7409	no/no	300
SOFS-2-2011	100	SBE37SM: 2971	no/yes	600
Pulse-9-2012	38.5	SBE16plusV2: 6331	yes/yes	3600
Pulse-9-2012	100	SBE37SMP-ODO: 9515	yes/yes	1800
SAZ47-15-2012	4422	SBE37SM: 8597	no/yes	300
SOFS-3-2012	1	SBE37SM: 8764	no/no	300
SOFS-3-2012	1	SBE37SM: 8765	no/no	300
SOFS-3-2012	30	SBE37SMP-ODO: 9513	yes/yes	1800
SOFS-3-2012	100	SBE37SMP-ODO: 9514	yes/yes	1800
SOFS-4-2013	1.01	SBE37SM: 7408	no/no	300
SOFS-4-2013	1.01	SBE37SM: 7409	no/no	300
SOFS-4-2013	100	SBE37SM: 8985	no/no	60
SOFS-4-2013	500	SBE37SM: 9185	no/yes	300
SAZ47-16-2013	4300	SBE37SM: 1778	no/no	600
Pulse-10-2013	28	SBE16plusV2: 6330	yes/yes	3600
Pulse-10-2013	100	SBE37SMP-ODO: 9538	yes/yes	1800
Pulse-10-2013	200	SBE37SMP-ODO: 9513	yes/yes	1800
Pulse-11-2015	28	SBE16plusV2: 6330	yes/yes	3600
Pulse-11-2015	50	SBE37SMP-ODO: 9538	yes/yes	1800
Pulse-11-2015	100	SBE37SMP-ODO: 9513	yes/yes	1800
Pulse-11-2015	150	SBE37SMP-ODO: 9514	yes/yes	1800
SAZ47-17-2015	4250	SBE37SM: 8985	no/no	600
SOFS-5-2015	1.01	SBE37SM: 7409	no/no	300
SOFS-5-2015	1.1	SBE37SM: 7408	no/no	300
SOFS-5-2015	30	SBE37SM: 6962	no/no	600
SOFS-5-2015	100	SBE37SM: 4908	no/yes	600
SOFS-5-2015	500	SBE37SM: 4909	no/yes	600
FluxPulse-1-2016	1.01	SBE37SM: 10136	no/no	300
FluxPulse-1-2016	1.01	SBE37SM: 8764	no/no	300
SAZ47-18-2016	4500	SBE37SM: 8597	no/yes	600
SAZ47-19-2017	1000	SBE37SM: 7901	no/yes	600
SAZ47-19-2017	2000	SBE37SM: 7896	no/yes	600
SAZ47-19-2017	4500	SBE37SM: 2971	no/yes	600
SOFS-6-2017	1	SBE37SM: 10136	no/no	300
SOFS-6-2017	1	SBE37SM: 8764	no/no	300
SOFS-6-2017	30	SBE37SMP-ODO: 9538	yes/yes	1800
SOFS-6-2017	125	SBE37SMP-ODO: 9513	yes/yes	1800
SOFS-6-2017	200	SBE37SMP-ODO: 9514	yes/yes	1800

Deployment	Depth*	Instrument: serial #	Pump/Press	Sampling (s)
SOFS-6-2017	500	SBE37SMP-ODO: 14700	yes/yes	1800
SOFS-7-2018	1	SBE37SM: 7408	no/no	300
SOFS-7-2018	1	SBE37SM: 7409	no/no	300
SOFS-7-2018	30	SBE37SMP-ODO: 15969	yes/yes	1800
SOFS-7-2018	125	SBE37SMP-ODO: 15970	yes/yes	1800
SOFS-7-2018	200	SBE37SMP-ODO: 15971	yes/yes	1800
SOFS-7-2018	480	SBE37SMP-ODO: 15972	yes/yes	1800
SAZ47-20-2018	1000	SBE37SM: 1777	no/yes	600
SAZ47-20-2018	2000	SBE37SM: 3124	no/yes	600
SAZ47-20-2018	4500	SBE37SM: 2955	no/yes	600
SOFS-7.5-2018	1	SBE37SM: 7408	no/no	300
SOFS-7.5-2018	1	SBE37SM: 7409	no/no	300
SOFS-7.5-2018	30	SBE37SMP-ODO: 15969	yes/yes	1800
SOFS-7.5-2018	125	SBE37SMP-ODO: 15970	yes/yes	1800
SOFS-7.5-2018	200	SBE37SMP-ODO: 15971	yes/yes	1800
SOFS-7.5-2018	480	SBE37SMP-ODO: 15972	yes/yes	1800
SOFS-8-2019	1	SBE37SM: 15728	no/no	300
SOFS-8-2019	30	SBE37SMP-ODO: 20126	yes/yes	1800
SOFS-8-2019	125	SBE37SMP-ODO: 9513	yes/yes	1800
SOFS-8-2019	200	SBE37SMP-ODO: 9514	yes/yes	1800
SOFS-8-2019	510	SBE37SMP-ODO: 20127	yes/yes	1800
SAZ47-21-2019	1000	SBE37SM: 4906	no/yes	600
SAZ47-21-2019	2000	SBE37SM: 4907	no/yes	600
SOFS-9-2020	1	SBE37SM: 7408	no/no	300
SOFS-9-2020	1	SBE37SM: 7409	no/no	300
SOFS-9-2020	30	SBE37SMP-ODO: 15969	yes/yes	1800
SOFS-9-2020	125	SBE37SMP-ODO: 15970	yes/yes	1800
SOFS-9-2020	200	SBE37SMP-ODO: 14700	yes/yes	1800
SOFS-9-2020	300	SBE37SMP-ODO: 15971	yes/yes	1800
SOFS-9-2020	510	SBE37SMP-ODO: 15972	yes/yes	1800
SAZ47-22-2020	2000	SBE37SM: 3124	no/yes	60
SAZ47-22-2020	4500	SBE37SM: 2955	no/yes	60

Only recovered sensors with useful data are listed. **Depth in meters is nominal, as estimated from mooring designs and anchor positions. Sensor pressure measurements provide the best estimates of the actual time-varying sensor depths. These are detailed in the Annual SOTS Sensor Reports and provided in the NetCDF data files.*

4 Summary of Instrument Handling and Data Processing

Pre-deployment preparation

Instruments were prepared following manufacturer recommendations, including drying of pressure cases, greasing of seals, and insertion of new batteries. Instrument clocks were set to UTC via on-line synchronization. Instruments were mounted and measurement frequencies were scheduled as described for each instrument in the SOTS Annual Sensor reports. In general, mounting was via clamping to the mooring wires for SBE37 instruments and inside in-line instrument cages for other models, with the instruments downward-facing. Measurement frequency was at least hourly and as frequent as every 1 minute for some sensors – the details are shown in Table 1.

In some cases, batches of the instruments were operated either in a common water bath or on the CTD-Rosette at sea prior to deployment to provide an inter-comparison of their outputs. This data is sparse and has not been evaluated here; it will be examined during the production of an adjusted gridded product, in a forthcoming report.

Post-deployment evaluations

After recovery, the instruments were connected to a UTC time-synchronized computer and any clock drift was noted.

Instrument Calibrations

Pre- and post-deployment calibrations were carried out either by the manufacturer or the CSIRO Hydrochemistry Facility. Comparison of the results from pre- and post-calibration will be examined during the production of an adjusted gridded product, in a forthcoming report.

Common time scale product

In this report, sensor data is examined at its full temporal resolution, which varied from every minute to every two hours. No interpolation to a common grid is provided, but will be during the production of an adjusted gridded product in a forthcoming report.

5 QC Specifics

Our overall Quality Control philosophy is to remove no data, only to indicate probable data quality for each observation using a system of QC flags, as shown in Table 2. Flags 1 to 4 are standard in the US IOOS, QARTOD, and Argo programs (citations below). Flag 6 is added here to indicate data collected before or after mooring deployment, which has not been evaluated further.

Table 2. Flags used in salinity quality control

FLAG	DESCRIPTION
Pass, Good data = 1	Data have passed the highest level of quality control
Probably good = 2	Data were unable to be evaluated by at least one test, but were not flagged as suspect or fail by any other tests
Suspect or of high interest = 3	Data have failed one or more tests indicating suspicious values, however it is possible that sensor failure has not occurred
Fail = 4	Data have failed one or more tests indicating instrument or mooring failure
Sensor active but not deployed = 6	Data obtained when the sensor was out of water, or not at the assigned depth.

As the starting point for delayed mode quality control (DMQC) we adopted the hierarchy of tests, listed in Table 3 recommended by the Integrated Ocean Observing System (IOOS) for Quality Assurance of Real-Time Oceanographic Data (QARTOD; <https://ioos.noaa.gov/project/QARTOD>), using Version 2.1 of the Manual for Real-Time Quality Control of In-situ Temperature and Salinity Data (Bushnell and Worthington, 2020).

Each test was applied to all data points, including those that had been flagged as fail (flag=4) or suspect (flag=3) in previous tests. At the end of the sequence of tests, the highest flag produced by any test was assigned to each data point. At the end of the sequence of tests, the highest flag produced by any test was assigned to each data point.

Importantly, salinity is a derived product obtained by combining temperature and conductivity observations. For this purpose, we used only those temperatures that received QC flags of 1 or 2 in our previous examination of these sensors (Jansen et al., 2020). Notably, even these best temperature observations are not always sufficient to obtain accurate salinity estimates from the conductivity measurements, because of offsets between the temperatures observed by the external thermistors and the actual temperatures experienced within the conductivity cells. These offsets, which occur most prevalently when temperatures are changing rapidly in the ocean as water parcels pass the moorings, lead to spikes in the estimated salinities - just as they do for CTD casts, Argo floats, gliders, and other platforms (Alvarez, 2018; Garau et al., 2011; Morison et al., 1994). This issue is discussed further below.

Table 3. QC tests recommended by QARTOD

TEST GROUP	TEST NO.	TEST NAME	CONDUCTED
Group 1 <i>Required</i>	1	Timing/Gap Test	Yes, modified
	2	Syntax Test	Yes, modified
	3	Location Test	Yes
	4	Gross Range Test	Yes
	5	Climatology Test	Yes
Group 2 <i>Strongly Recommended</i>	6	Spike Test	Yes
	7	Rate of Change Test	Yes
	8	Flat Line Test	No
Group 3 <i>Suggested</i>	9	Multivariate Test	Yes
	10	Attenuated Signal Test	Via visualisation
	11	Neighbour Test	Via visualisation
	12	TS Curve/Space Test	Via visualisation
	13	Density Inversion Test	Via visualisation

5.1 Applied tests

5.1.1 Data visualization and identification of common problems

In working through the QARTOD tests, visualisation of the measured temperature and conductivity, and derived salinity and potential density (sigma-theta at 0 pressure) records and the flagging results made it clear that some tests functioned better than others, and many tests required compromises. Put simply, defining thresholds for flagging the data represents an optimal compromise between identifying too many false positives (i.e. data is accepted, even though it is bad) versus too many false negatives (i.e. data is rejected, even though it is good). To some degree, this optimal compromise depends on the use of the data. For example, if quantifying the annual salinity cycle is the target, then flagging occasional short-lived salinity excursions (which might be either instrumental spikes or rare events related to the passage of sub-tropical water parcels) as bad eliminates noise in the seasonal cycle and represents little loss of fidelity. However, if identification of the occasional presence of small subtropical water parcels which might bring in unusual organisms is the target, it is better not to exclude these results.

Ideally, the sensor records would unambiguously separate rare but real events from episodic sensor faults, but this can be very hard to assess, especially if there is only one sensor in the region of interest and if the full nature of the oceanic variability in the region is not yet known. The second of these problems is particularly problematic in the Southern Ocean at very shallow depths, because rough conditions generally mean that CTD casts sample the top 5m of the sea poorly if at all, and the large footprints of satellite sea surface measurements mean that spatially restricted high intensity events would not be visible.

Visualisation is an essential tool to define the nature of sensor problems and thus the selection of appropriate thresholds for the tests. Two problems were immediately evident:

1. many salinity records exhibit spikes, and these often exceed the presence of spikes in the conductivity records, as illustrated in Figure 4, Figure 5 and Figure 6.
2. comparison of adjacent sensors can suggest unstable potential density profiles (sigma-theta, at water pressure = 0), illustrated in Figure 5 and Figure 6, including as a result of the salinity spikes.

The issues informed the selection of thresholds for the QARTOD tests to flag 'bad' (flag 4) and 'suspect' (flag 3) data, as detailed for each test below. Our analysis to determine optimal thresholds for the tests focused in on the occurrence and origin of these salinity spikes, and we detail some of these results and considerations before presenting the selected set of QC thresholds.

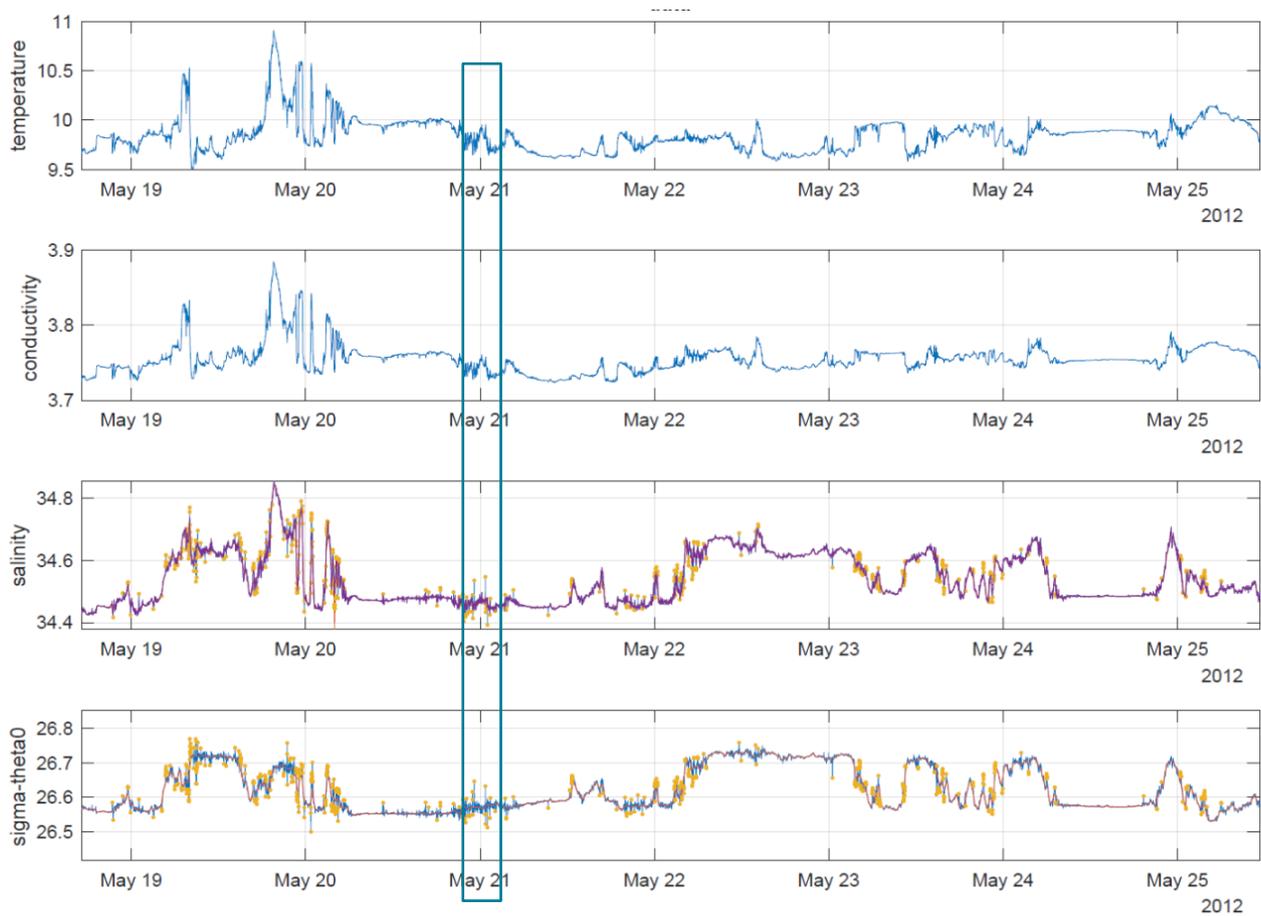


Figure 4. Pulse-8-2012 measured temperature and conductivity and calculated practical salinity and sigma-theta ($p=0$) records.
 The similarity of the temperature and conductivity records reflects the dominant thermal control of conductivity. The box on May 21 illustrates the presence of salinity spikes which are not present in either the temperature or conductivity records, and thus derive from ‘sensor mismatch’. The yellow dots mark the subset of salinity excursions which correspond to sigma-theta ($p=0$) excursions of more than 0.02. See text for discussion.

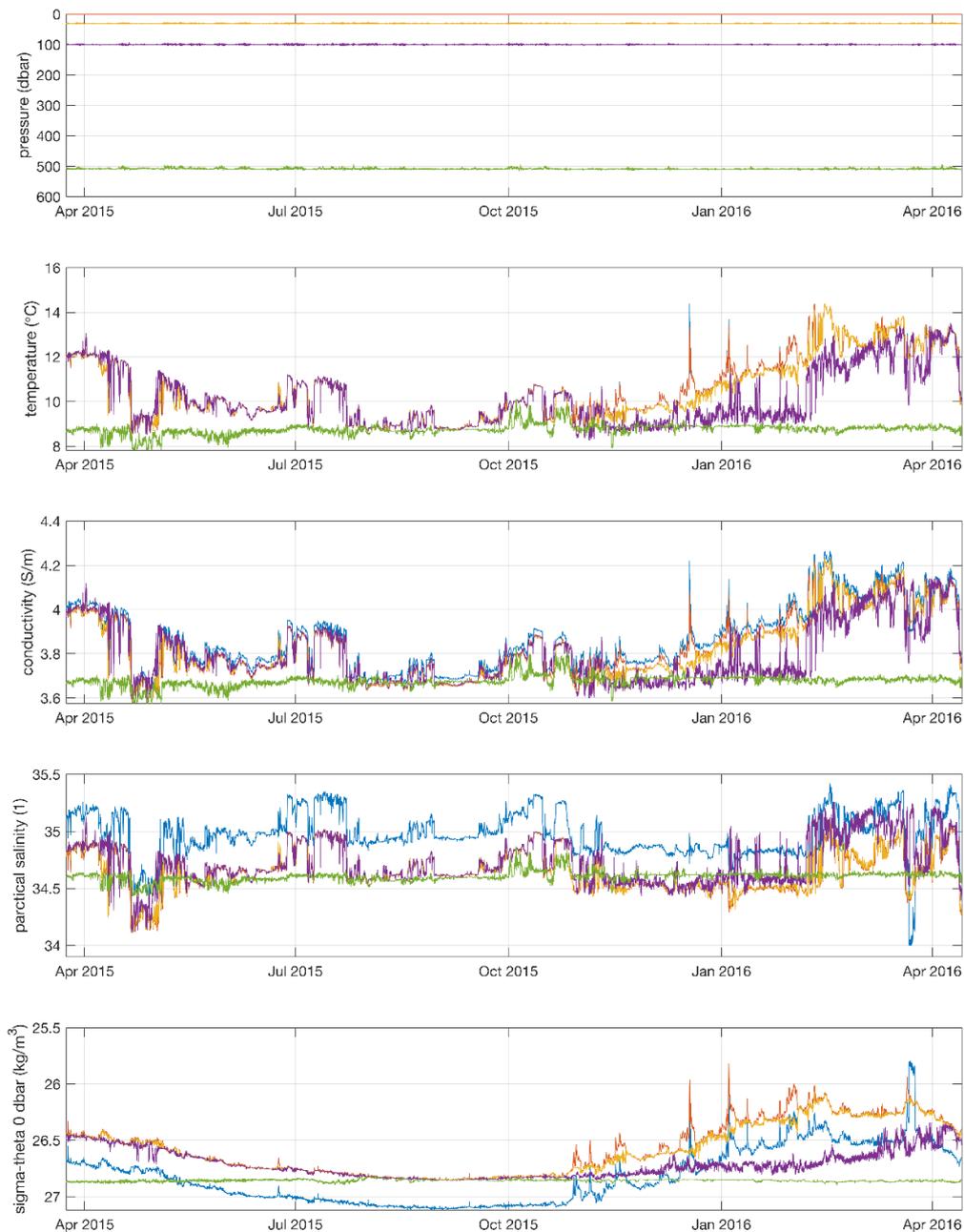


Figure 5. SOFS-5-2015 sensor pressures, temperatures, salinities, and sigma-theta values. 5 sensors are shown: overlapping blue and red lines at 1 m depth, yellow, purple, and green lines at 30, 100, and 500m.. The tightly overlapping temperature records at 1m revealed occasional pulses of very warm water exceeding 14 °C (this reproducibility was key to its verification; Jansen et al., 2020), but with slightly offset salinities. The sigma-theta records reveal that it is the blue salinity that is in error, because it suggests an unstable water column. Review of the 11-03-2015 calibration for this sensor found it to be in error, and use of the preceding 28-09-2012 calibration produced data that passed this stability test and is presented in the final data files.

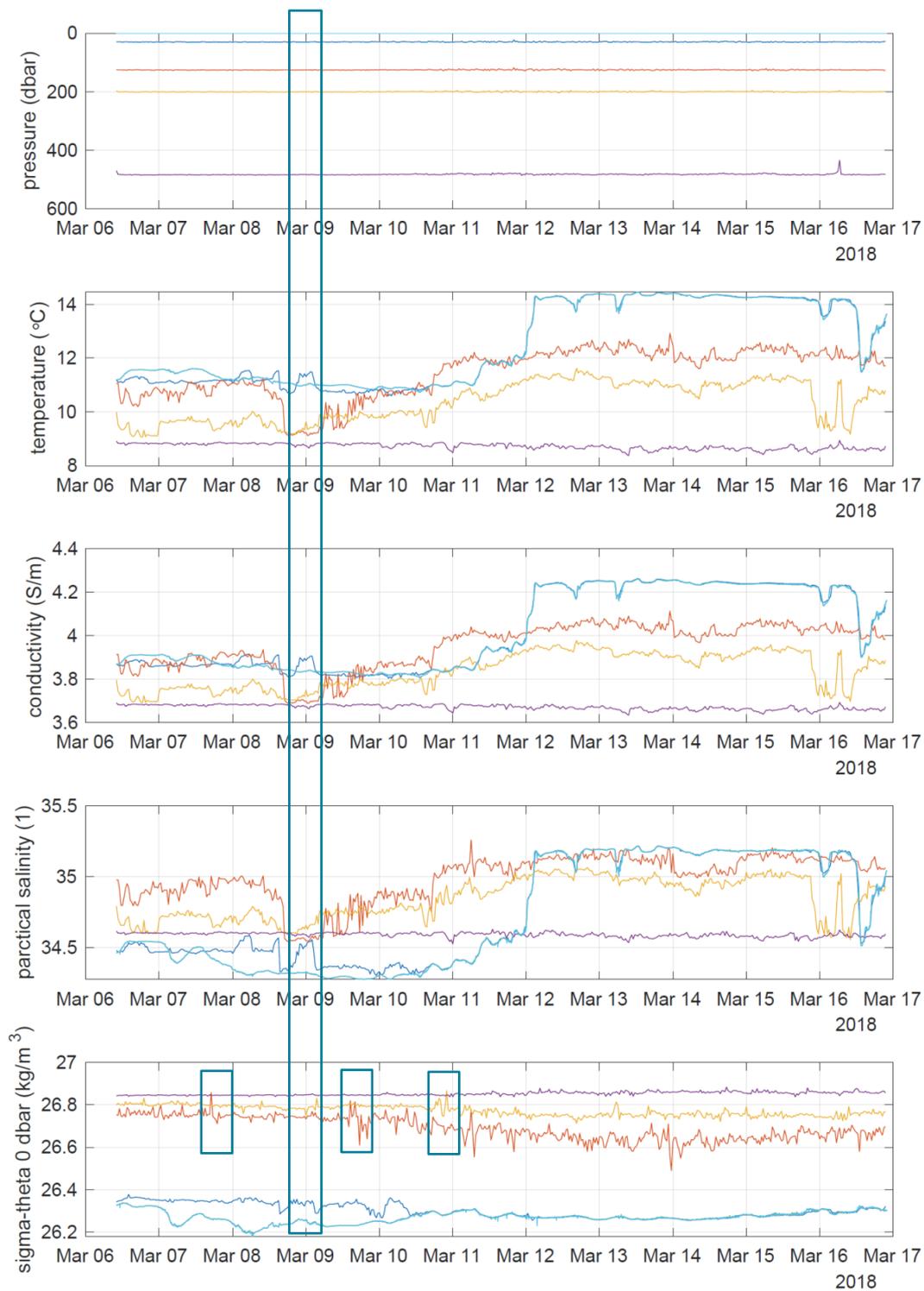


Figure 6. SOFS-7-2018 pressures, temperatures, conductivities, salinities, and potential densities. The long box marks when warmer water was present at 30m (dark blue line) than at the surface (light blue line), yet the water column remained stable because the subsurface was also salty. Quite cool water dropped the temperature at 125m (red trace) to slightly below that at 200m (yellow trace), accompanied by at most a small density inversion. Similar small inversions (smaller boxes) occurred when no unusual features in T or S occurred. These data make it clear that distinguishing small real oceanographic potential density inversions from spikes caused by T-S ‘sensor mismatch’ is challenging. See text for discussion.

5.1.2 Exploration of options for identification of salinity spikes from sensor mismatches

In the following paragraphs we explore two questions:

Is there a criterion that could be applied to identify salinity spikes (i.e. high frequency variability) caused by thermal versus conductivity sensor mismatch and separate them from ocean variability?

Could separation, even if imperfect, be achieved without introducing bias into the salinity time series?

Possibilities for this separation include spike amplitudes or their relationships to temperature, conductivity, or density variations. Below we examine these aspects in detail. We conclude that all approaches involve uncertainties and compromises, and that a method based on setting bounds on the magnitude of potential density ($\sigma\text{-}\theta$ at pressure 0) variations appears to be the most useful approach, and that it can be applied without bias.

The origin of sensor mismatch salinity spikes

Salinity spikes are a well-recognized problem for records determined from paired temperature and conductivity measurements, because of ‘sensor mismatch’, i.e. the temperature measurements do not accurately reflect the thermal conditions of the conductivity sensor. These mismatches arise for many reasons, including that the measurements are not in the same place, each sensor has a different response time, and a different thermal mass (see the Introduction for citations). The problems occur when ocean conditions are changing quickly. In particular, change in ocean temperature measured by an external thermistor tends to temporally lead the change in temperature within the conductivity cell, firstly because it takes time for the arriving water to flush through the cell and also because the cell has thermal mass that further lags the temperature change behind the thermistor.

Separation by comparison of different sensor types

Pumped conductivity cells reduce and standardize thermal lags (but do not eliminate them). Thus comparison of pumped and unpumped sensor salinity spikes offers one approach to setting thresholds for the generally higher spike levels of unpumped sensors. At SOTS, pairs of pumped and unpumped sensors have not been deployed at the same depth, and pumped sensors have generally sampled at much lower frequency because of their higher battery requirements. For these reasons, determining salinity spikes from pumped sensor mismatches at SOTS was not found to be a tightly useful criterion for flagging unpumped sensor errors. This is shown in Figure 7, which compares salinity spikes across pumped and unpumped sensors, and finds them to be similar in range.

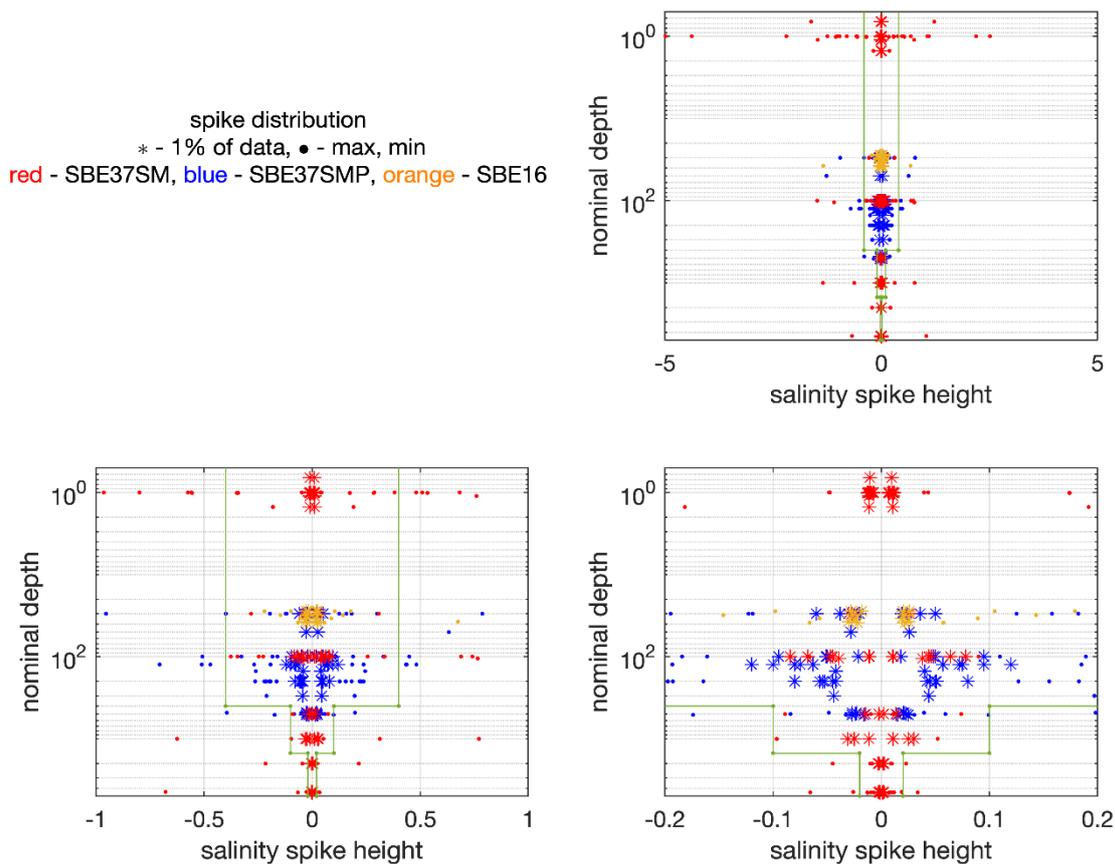


Figure 7. Distribution of salinity spike amplitudes with depth, comparing pumped (SMP) and unpumped (SM) sensors.

The 3 plots with different zoom in on the x-axis spike scale. Pumped sensors have similar spike ranges to unpumped sensors (except the SBE16 sensors used on Pulse moorings at ~30m depth, for which the spike range is narrowed in part by sparse sampling rates). Also shown as vertical green line segments are the depth-varying selected spike thresholds for the Climatology test.

Separation by comparison to temperature variability

Because salinity errors from sensor mismatches are proportional to the temperature difference between the conductivity cell and the thermistor (see citations in the Introduction), salinity spikes from this source should not exceed those that could be induced by oceanic temperature changes. Figure 8 shows that most salinity spikes could be explained by sensor mismatch, because they do not exceed this criterion. Unfortunately, this does not mean that they are derived from sensor mismatch, just that they could be. There are, however, some spikes that do exceed this criterion, and these must either be real or derived from other sources – in particular, salinity spikes that are matched with conductivity spikes which occur in the absence of strong temperature variations are likely to derive from the passage of objects through the cell. If these are large, they can be flagged based on their amplitude (using range and climatology tests), and if smaller may be flagged by density tests (as developed and discussed below).

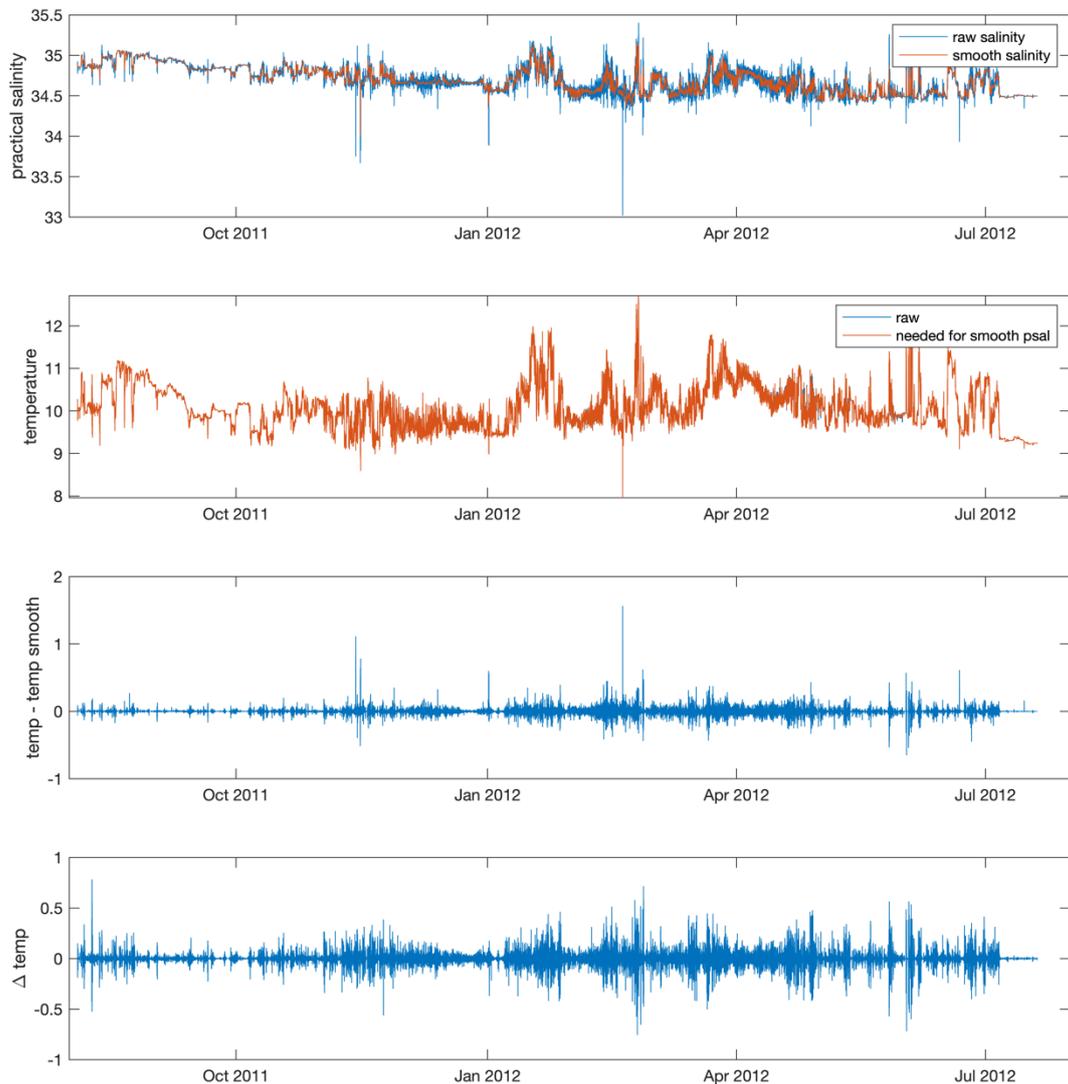


Figure 8. SOTS Pulse-8 mooring unpumped SBE37SM record at 105 m depth, every 60 seconds. Top plot shows raw and smoothed salinity time series (generated by a ‘lowess’ robust weighted linear regression using a 30 point window width, with initial weights based on cubic distance from the time of interest, and 3-fold iterative removal of outliers using Tukey’s bisquare weighting of residuals; (Cleveland, 1979)). Second plot shows that the temperatures required to obtain this smoothed salinity are very similar to those observed. The third plot details the differences, i.e. the thermal offsets between the thermistor and the conductivity cell that would be required to explain all the high frequency variability in the salinity record as resulting from sensor mismatch. The final plot shows that the minute by minute temperature variations in the ocean are larger than these thermal offsets, and thus sensor mismatch is a tenable explanation for the salinity variability (although oceanic contributions cannot be ruled out – see text for discussion).

Separation by comparison of salinity to conductivity

Sensor mismatch increases the noise in salinity records relative to the conductivity records from which they derive. This sensor behaviour can be understood by considering the arrival of a warm parcel (with unchanged salinity). The thermistor temperature will increase quickly, but the conductivity will increase more slowly as the new water flushes through the cell and some of its heat is absorbed by the device. Thus, the partitioning of the observed conductivity between its thermal and salinity contributions will over-estimate the thermal contribution to conductivity (because the thermistor is warmer than the conductivity cell) and under-estimate the actual salinity, leading to greater variance in the derived salinity than the measured, constant, conductivity (and negative slopes in T-S plots).

This suggests another path towards separating spikes from sensor mismatch, i.e. any salinity spikes that exceed those of conductivity could be discarded, provided that oceanic processes do not also increase salinity variations relative to conductivity variations. As shown in the example in Figure 9 and Figure 10, salinity variability is similar in magnitude to that of conductivity, sometimes higher (e.g. early April) and sometimes lower (e.g. late September). Could these variations be oceanic? This depends on the coupling of T-S variations that accompany oceanic processes. For mixing along isopycnal surfaces (which can occur with minimal change in T-S variance because there are no buoyancy forces to remove this 'spiciness'), conductivity (C) variance receives contributions from T variance and S variance with the same sign. Thus, the S variance will be smaller than the C variance. This 'density compensation' is common in the mixed layer at SOTS as can be seen by the passage of warm-salty waters which have little impact on sigma-theta (e.g. in early July 2015 in Figure 5). But for the case of deepening of the mixed layer, which at SOTS generally brings in saltier and colder water (as shown by the downward temperature, salinity, and density gradients in the ship CTD records in Figure 11, Figure 12 and Figure 13) the T variance and S variances contributions have opposite signs, so the S variance will exceed that of C. Air-sea fluxes can have either opposing or the same signs, depending on the details of the weather scale coupling of evaporation, precipitation, insolation, and air mass temperatures. Thus, it is not possible to limit 'good', i.e. 'oceanic' salinity variations to only those that do not exceed those of conductivity.

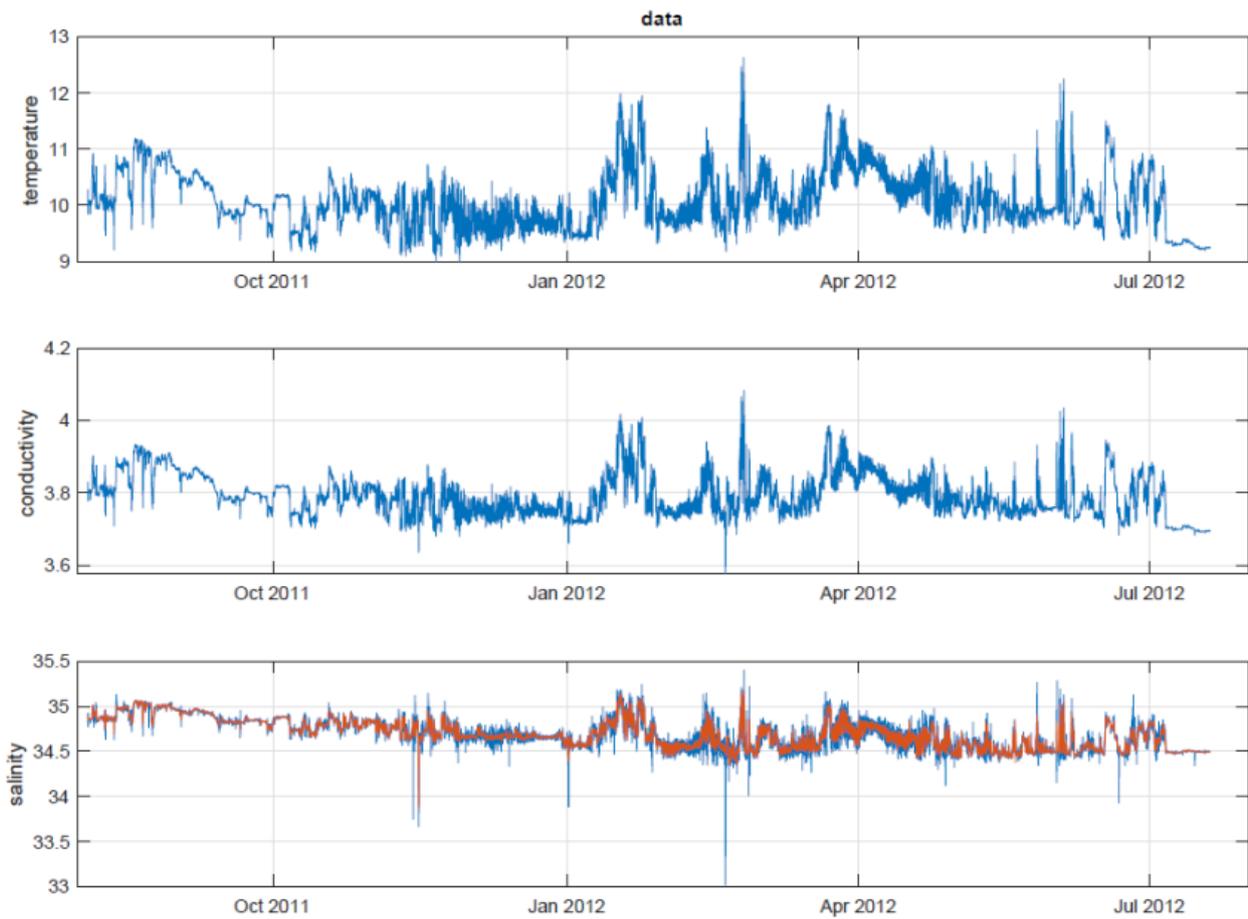


Figure 9. SOTS Pulse-8 mooring unpumped SBE37SM sensor records at 105 m depth, sampling every 60 seconds, for temperature, conductivity, and salinity. Note the dominance of the conductivity record by the temperature variations, i.e. the two records look very similar. The salinity panel also shows smoothed salinity, as described for Figure 8.

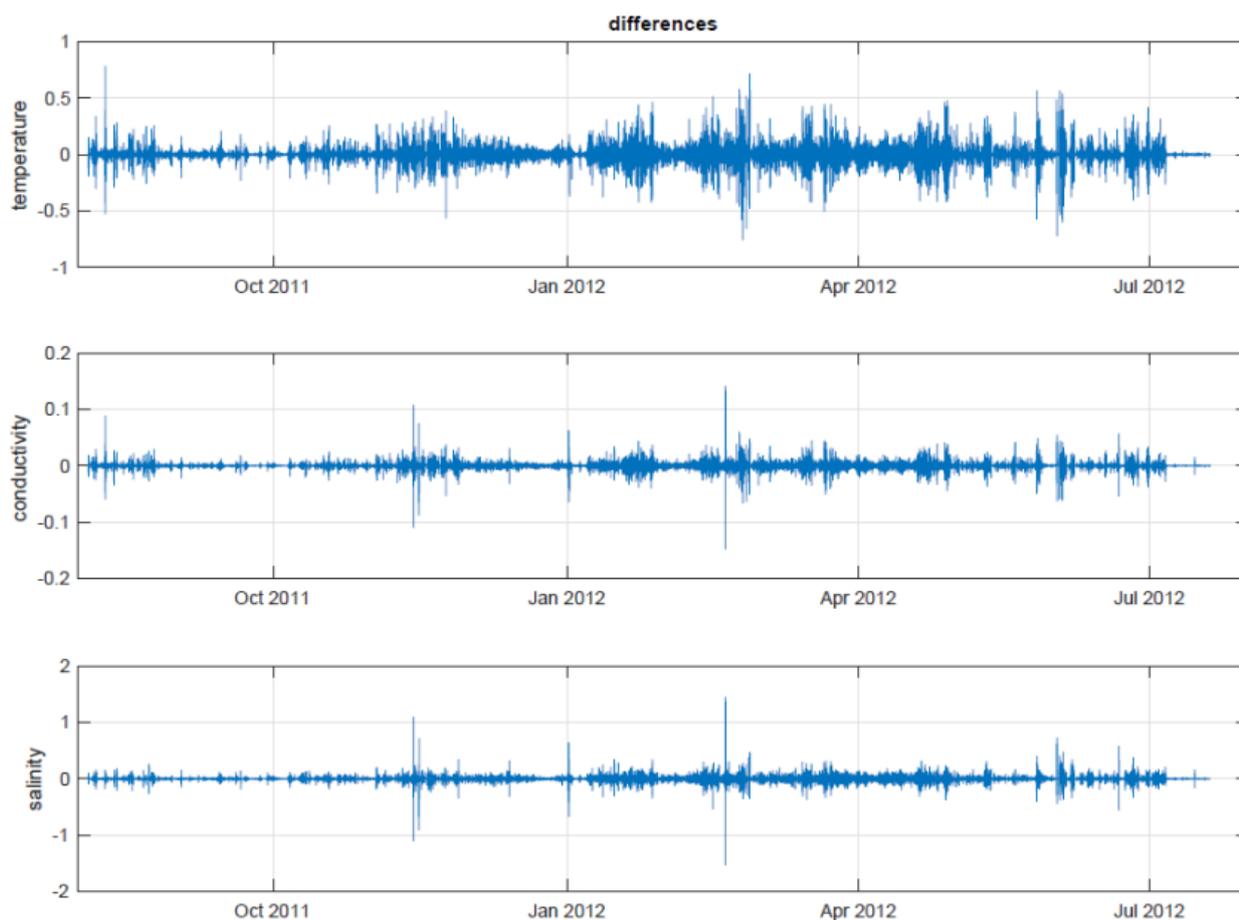


Figure 10. Differences between raw and smoothed time series for temperature, conductivity, and salinity for the sensor described in Figure 8 and Figure 9. The salinity variance is often smaller, but sometimes larger than that of conductivity (the salinity/conductivity scaling for this sensor pressure and temperature is very close to 10 so that the conductivity range of ± 0.1 is equivalent to salinity range of ± 1).

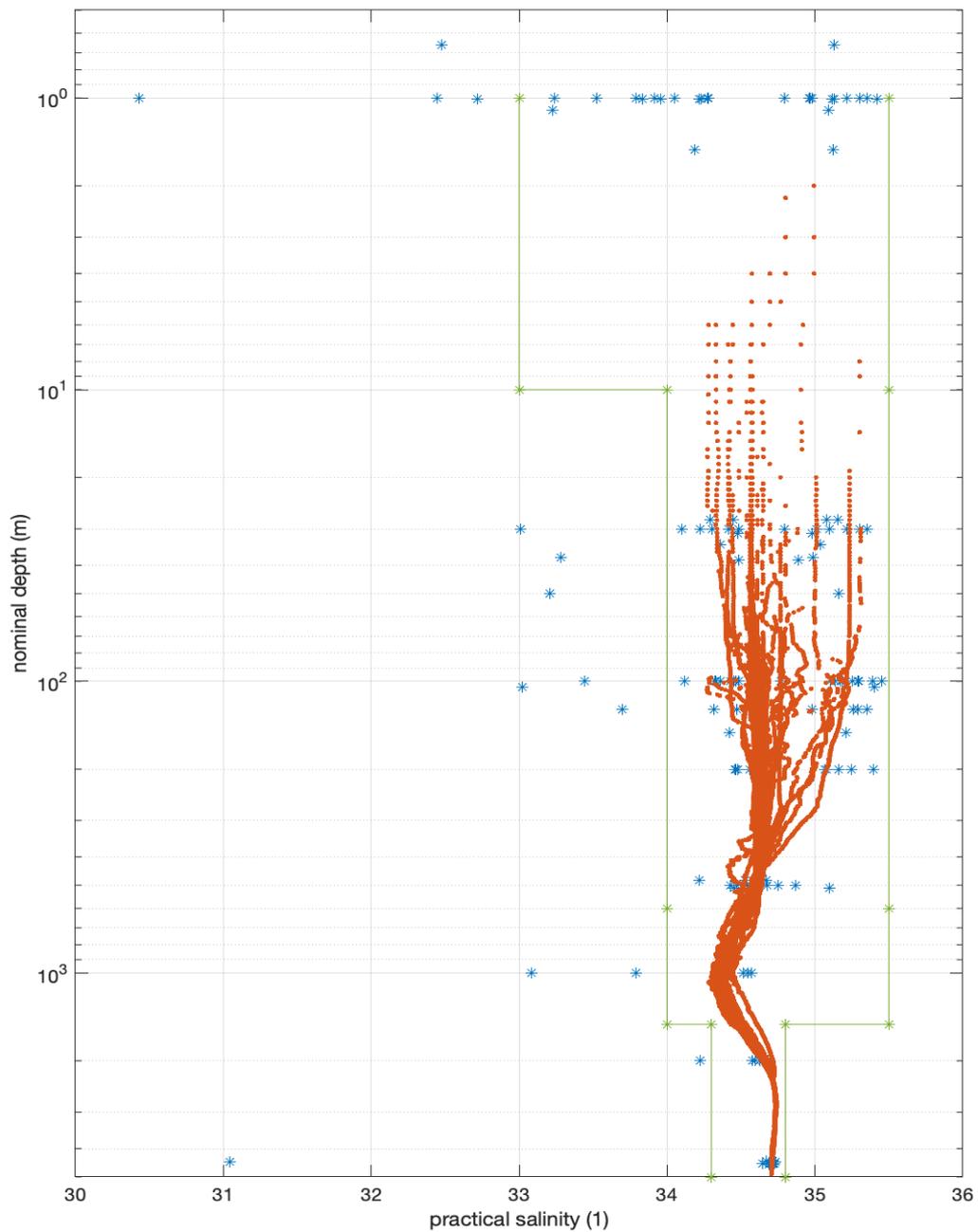


Figure 11. Ship CTD profiles and moored sensor extrema for salinity. Green line segments show bounds implemented in Climatology Test 5.

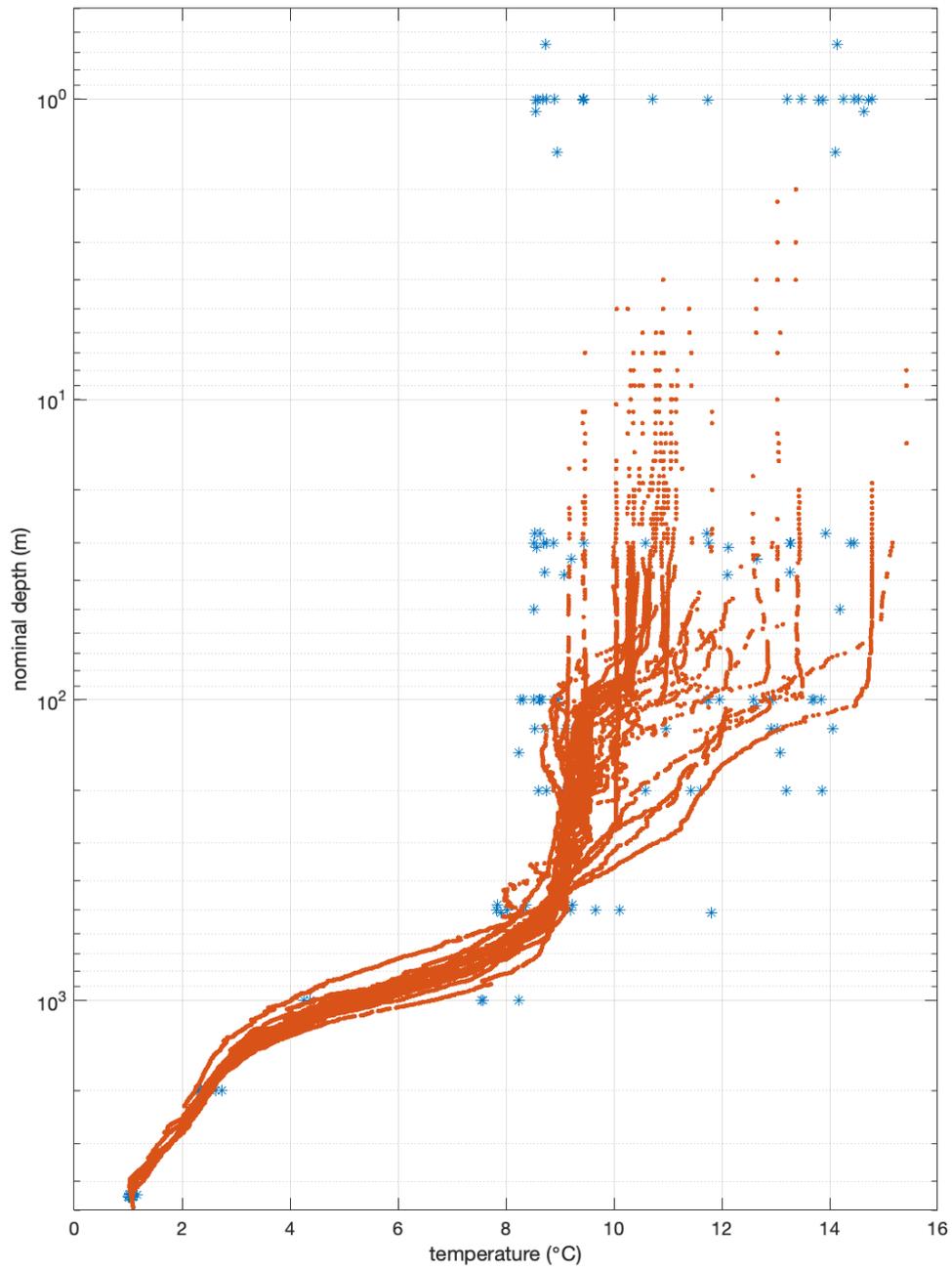


Figure 12. Ship CTD profiles and moored sensor extrema for temperature.

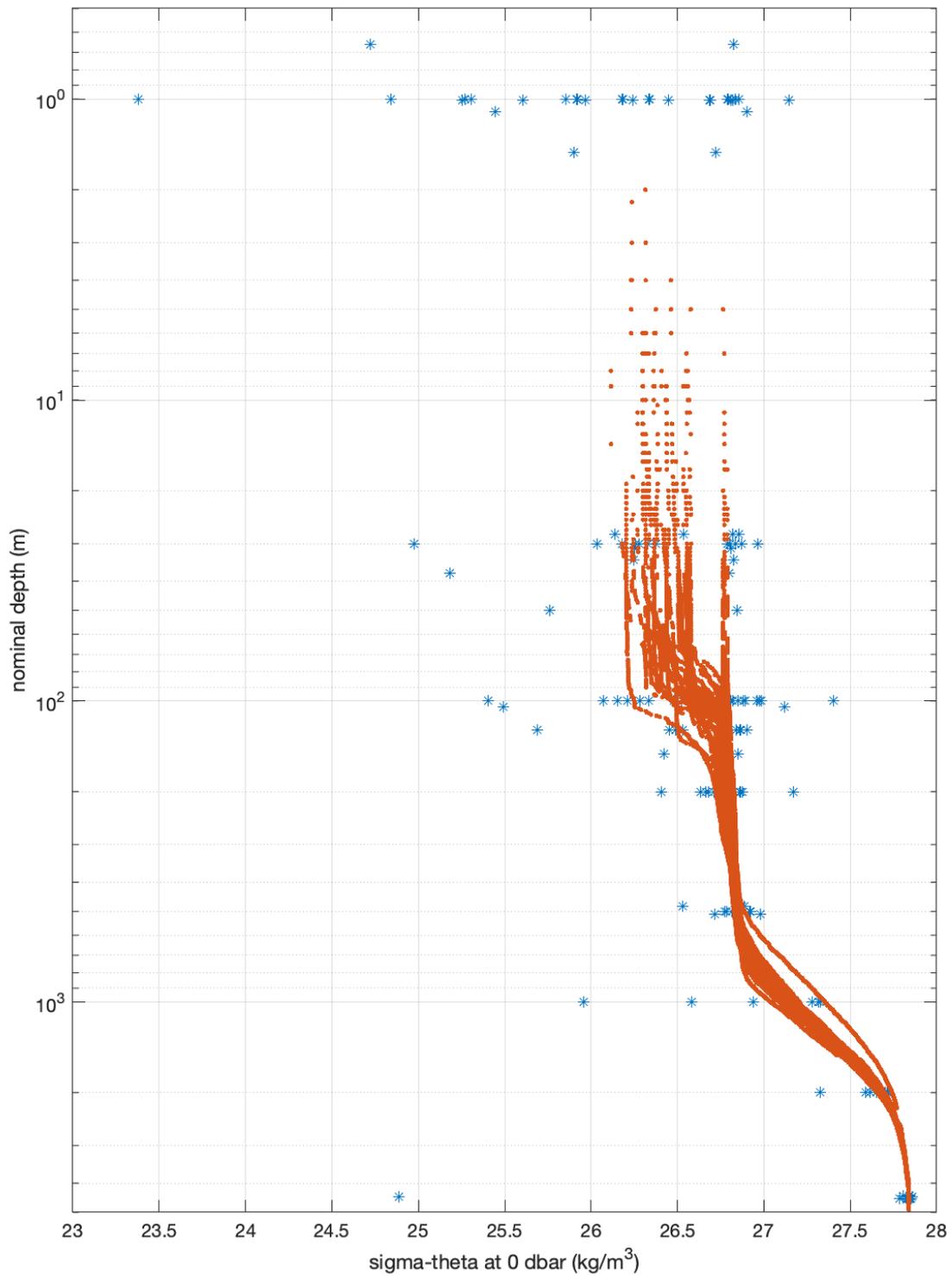


Figure 13. Ship CTD profiles and moored sensor extrema for potential density (sigma-theta at pressure 0).

Separation by a potential density threshold

The occurrence of ‘density compensation’ means that sigma-theta variations are generally smaller than those of either S or T, and thus using spikes in sigma-theta offers another approach to flag salinity estimates which are likely to be in error. Choosing a sigma-theta threshold for spikes is arbitrary, but at SOTS a value of 0.02 appears to work well. This value is less than the value of 0.03 often used to define mixed layer depth (de Boyer Montégut et al., 2004), and it appears likely to be larger than expected changes from oceanic processes, as can be seen by comparing this value to temperature variations observed in CTD casts in waters near SOTS as shown in Figure 11, especially over the short time scales that define spikes in the high frequency records. In this regard, perhaps the fastest expected density changes would occur for sensors at the base of the mixed layer, where sigma-theta increases by ~ 0.2 over 10 m depth so that vertical motions of the mooring or the ocean would need to exceed 1 m per minute to cause sigma-theta variations above the 0.02 threshold. This equates to 0.026 in S at a typical SOTS base of mixed layer temperature of 9.5 °C and 100 dbar pressure. Importantly, S spikes flagged using this criterion are distributed evenly with respect to the smoothed salinity, and thus their removal (e.g. as illustrated in Figure 14, Figure 15, Figure 16 and Figure 17) does not bias the salinity records. This symmetric behaviour occurs because sensor mismatch arises as oceanic T-S gradients both arrive and depart the sensor. Other sources of spikes are not symmetric, in particular the passage of objects (e.g. detritus or air bubbles) through the conductivity cell which tends to decrease conductivity and appear as fresh salinity spikes (Figure 18 shows an example).

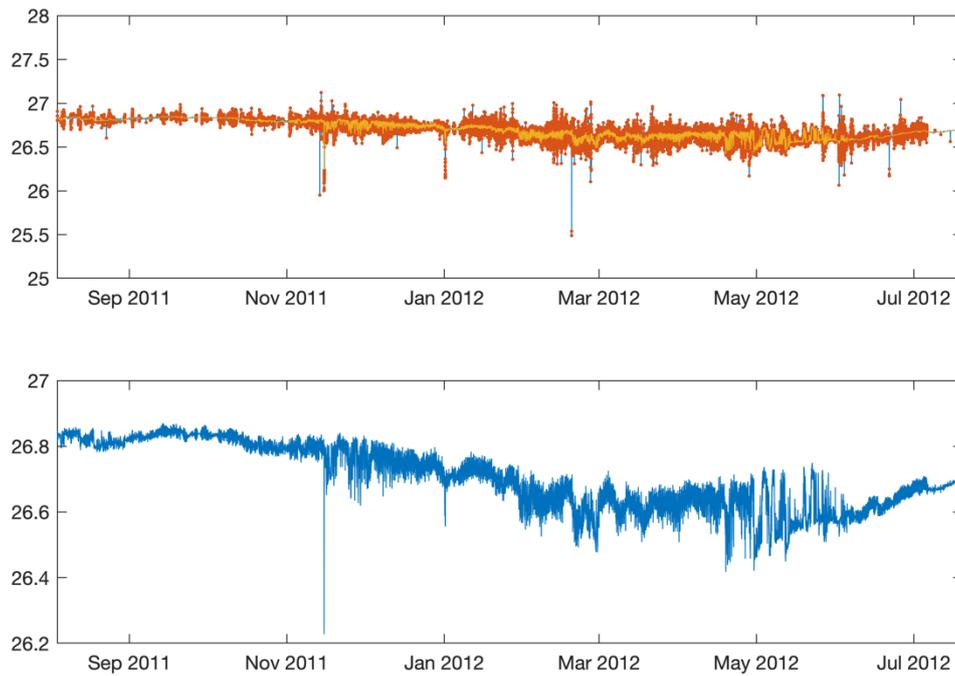


Figure 14. Potential density flagging for the SOTS Pulse-8 unpumped SBE37SM sensor at 105m. Top: thin blue line: raw temperature, orange dots: spikes based on 0.02 departure from smoothed record (yellow). Figure 8 caption has smoothing details. Bottom: Expanded view of potential density variations after removal of these spikes.

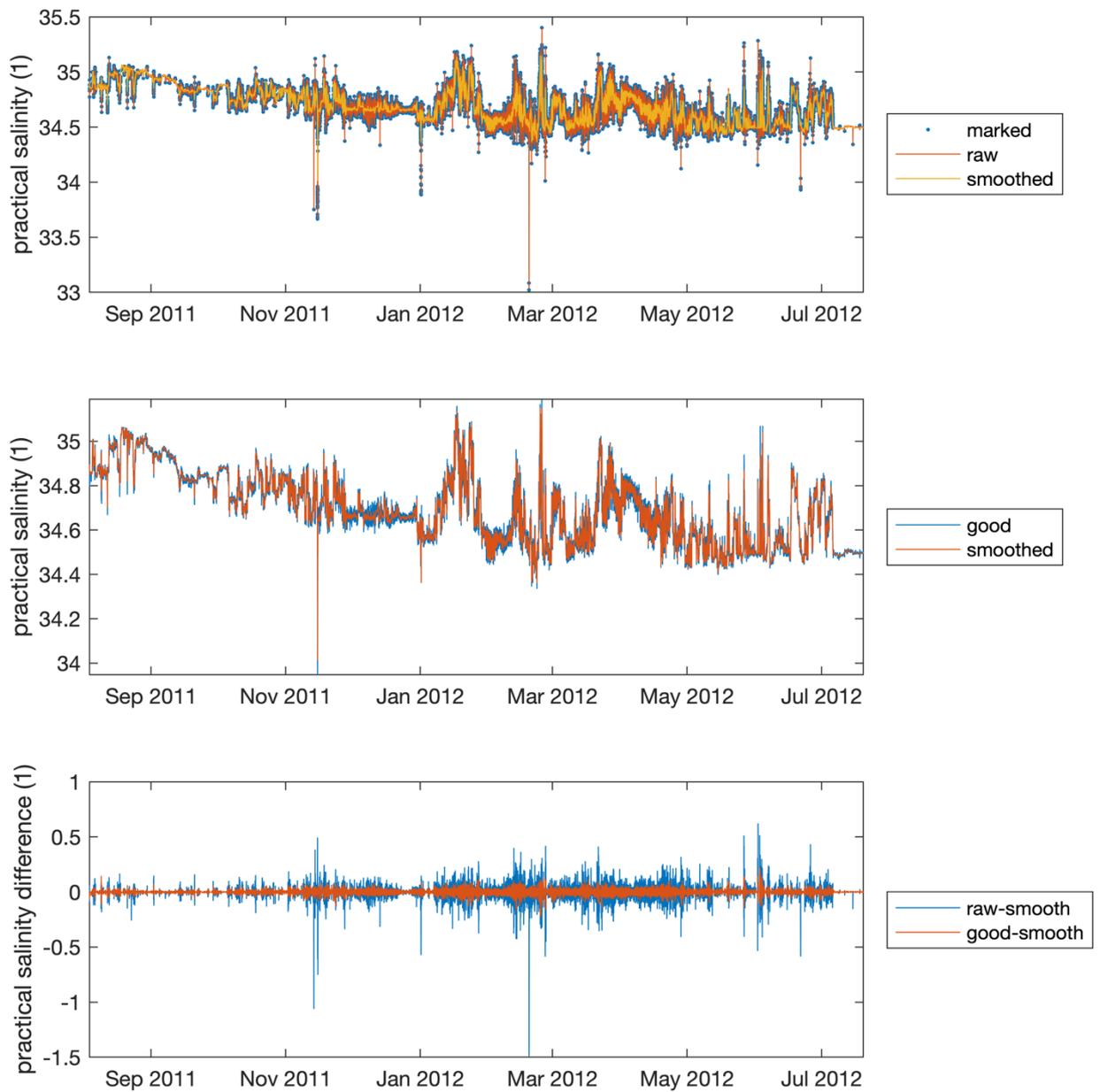


Figure 15. Visualization of salinity spikes identified from potential density spikes (see Figure 14 for spike removal details) Top: raw and smoothed salinity records and potential density flagged data; Middle: retained good salinity data compared to smoothed record; Bottom: comparison of raw-smoothed and good-smoothed data distributions.

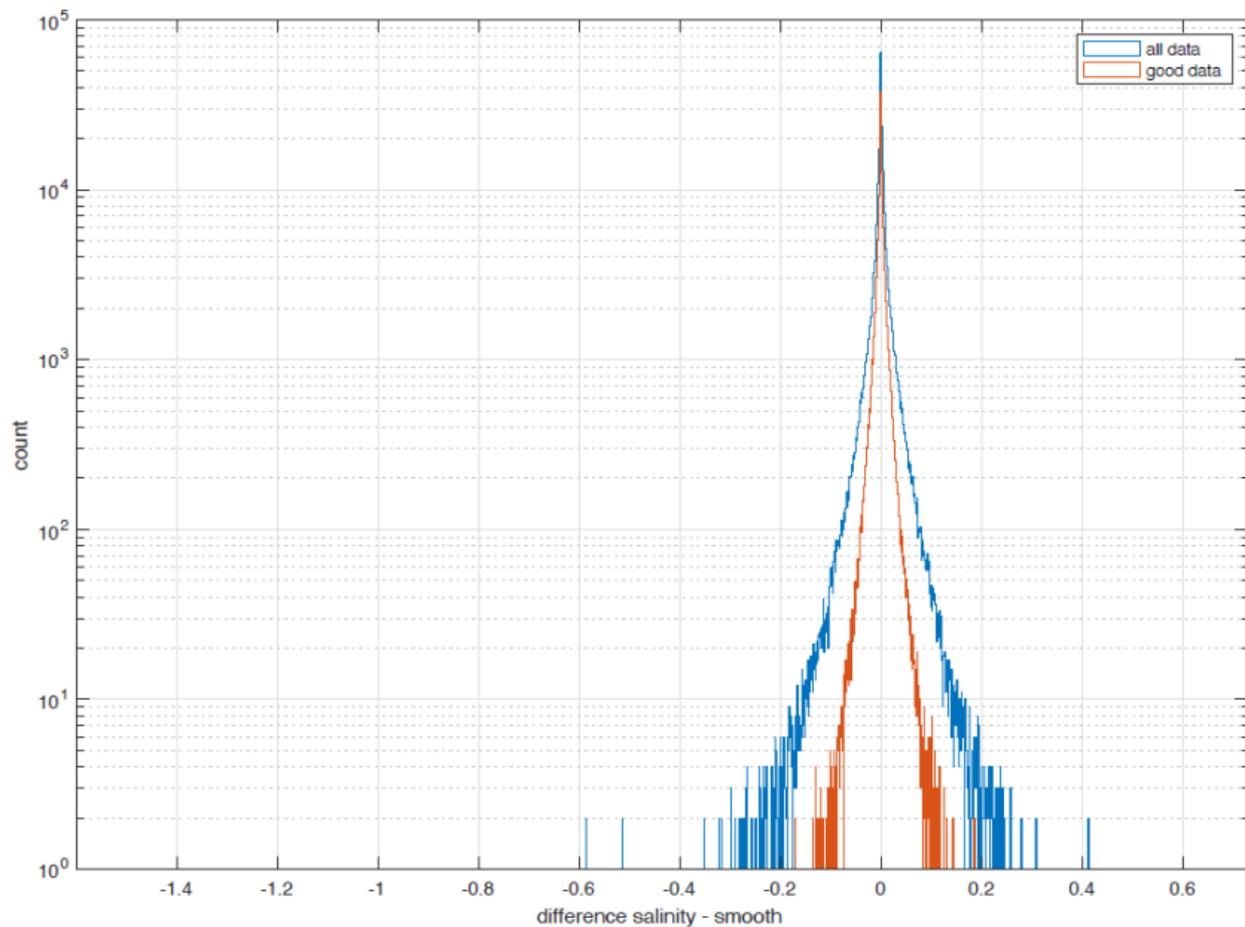


Figure 16. Distributions of raw and retained salinity data relative to smoothed salinity values for the record shown in Figure 14 using the potential density flagging criterion. Note that for salinity the residuals are symmetric around zero for the vast majority of results (with a few extreme exceptions) indicating that the smoothed record is not biased by this approach.

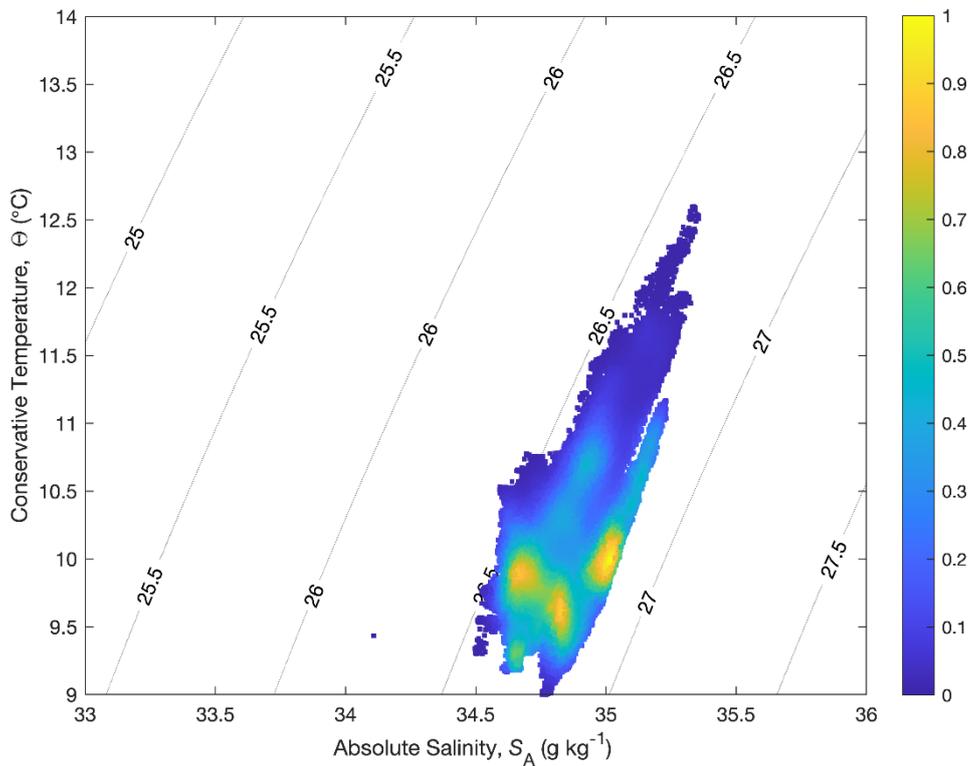
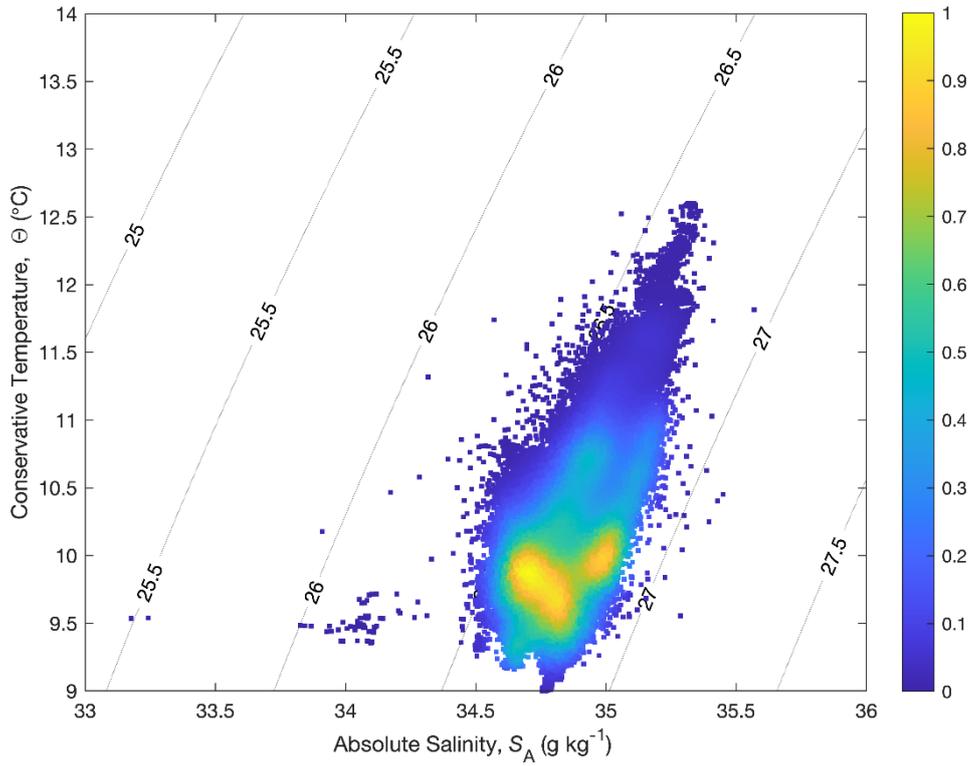


Figure 17. Conservative Temperature versus Absolute Salinity plots for Pulse-8-2011. Top: all the data, Bottom: data that passed the 0.02 kg m⁻³ potential density excursion criterion.



Figure 18. Salinity spikes identified from sigma-theta excursions for the SOFS-8 surface-float mounted CTD.

These spikes are generally toward fresh values (rather than being symmetrically distributed as observed for subsurface sensors, e.g. as illustrated in Figure 14) and are likely derived from breaking wave injected air bubbles.

5.1.3 Summary of perspectives and their application to salinity QC test formulation

Large spikes in S , which in general also occur in C , can be removed using S range and spike thresholds. These can be set to vary with depth via the Climatology test.

Moderate errors in S from calibration or other problems can be recognized using the water column stability criterion, i.e. that sigma-theta increases with depth.

Small spikes in S , some of which are not present or are smaller in C , are likely to derive from sensor mismatch. Their separation from oceanic variability is difficult, but appears to be achievable using thresholds for potential density (sigma-theta) departures from smoothed trends. This approach does not introduce bias, at least for the SOTS records examined here, which exhibit similar amounts and amplitudes of negative and positive spikes.

5.2 Detailed specifications and applications of the QARTOD tests

Test 1) Timing/Gap Test (Required)

Check for arrival of data.		
Test determines that the most recent data point has been measured and received within the expected time window (TIM_INC) and has the correct time stamp (TIM_STMP). Note: For those systems that do not update at regular intervals, a large value for TIM_STMP can be assigned. The gap check is not a solution for all timing errors. Data could be measured or received earlier than expected. This test does not address all clock drift/jump issues.		
Flags	Condition	Codable Instructions
Fail=4	Data have not arrived as expected.	If NOW – TIM_STMP > TIM_INC, flag = 4
Suspect=3	N/A	N/A
Pass=1	Applies for test pass condition.	N/A
Test Exception: None.		
Test specifications to be established locally by the operator.		
Example: TIM_INC = 1 hour		

Implementation for SOTS delayed mode QC was as follows:

This test is designed for real time data, and its application to delayed mode is very limited.

For SOTS instruments we retain all time-stamped data, and do not do any flagging or filling if a time point is missing. In other words, we accept missing intervals and expect the user to recognize that the time series may not be evenly spaced. Thus, calculations should always estimate the time interval when integrating values across adjacent data points, e.g. when calculating heat content changes.

For time stamps which are missing values of one or more variables (T, S, etc.), these are set to NaNs when the data is parsed from the instrument transmissions. These values are then flagged by Test 4) Gross Range Test (below).

Test 2) Syntax Test (Required)

Check to ensure that the message is structured properly		
<p>Received data message (full message) contains the proper structure without any indicators of flawed transmission such as parity errors. Possible tests are: a) the expected number of characters (NCHAR) for fixed length messages equals the number of characters received (REC_CHAR), or b) passes a standard parity bit check, cyclic redundancy check (CRC), etc. Many such syntax tests exist, and the operator should select the best criteria for one or more syntax tests.</p> <p>Capabilities for dealing with flawed messages vary among operators; some may have the ability to parse messages to extract data within the flawed message sentence before the flaw. A syntax check is performed only at the message level and not within the message content. In cases where a data record requires multiple messages, this check can be performed at the message level but is not used to check message content.</p>		
Flags	Condition	Codable Instructions
Fail=4	Data sentence cannot be parsed to provide a valid observation.	If REC_CHAR ≠ NCHAR, flag = 4
Suspect =3	N/A	N/A
Pass=1	Expected data sentence received; absence of parity errors.	
Test Exception: None.		
Test specifications to be established locally by the operator.		
Example: NCHAR = 128		

Implementation for SOTS delayed mode QC was as follows:

This test is designed for real time data, and its application to delayed mode is very limited.

If the message cannot be parsed, then the record will show a missing time stamp. No flagging is done.

Test 3) Location Test (Required)

Check for reasonable geographic location.		
Test checks that the reported present physical location (latitude/longitude) is within operator-determined limits. The location test(s) can vary from a simple impossible location to a more complex check for displacement (DISP) exceeding a distance limit (RANGEMAX) based upon a previous location and platform speed. Operators may also check for erroneous locations based upon other criteria, such as reported positions over land, as appropriate.		
Flags	Condition	Codable Instructions
Fail=4	Impossible location.	LAT > 90 or LONG > 180
Suspect=3	Unlikely platform displacement.	DISP > RANGEMAX
Pass=1	Applies for test pass condition.	N/A
Test Exception: Test does not apply to fixed deployments when no location is transmitted.		
Test specifications to be established locally by the operator.		
Example: Displacement DISP calculated between sequential position reports, RANGEMAX = 20 km		

Implementation for SOTS delayed mode QC was as follows:

The locations of the sensors were designated as being the locations of the mooring anchor positions (as estimated from the anchor drop position and/or acoustic triangulation - details are in the SOTS Annual Overview Reports). This location information is provided as a single pair of latitude and longitude values in the NetCDF files.

In addition, for the SOFS and Pulse surface floats, which collect and transmit GPS positions, this information is provided as time series of latitudes and longitudes, with flagging of:

Flag 4, QARTOD conventions for impossible latitudes and longitudes

Flag 3, latitude outside 30-60°; longitude outside 130-150 °E.

Note that this wide range does NOT flag data outside the mooring 'watch circles', that has at times been collected after surface portions of the moorings have broken free and drifted. Note also that the locations of the annual re-deployments of the SOTS moorings have typically varied by ~10 miles, and at times by as much as 60 miles.

Users who wish to limit data to within a watch circle, to some other restricted area, or to examine variations with location should use these time series of latitudes and longitudes, rather than the nominal positions provided by the anchor locations.

We also extended this test to include flagging the pressure records of the sensors (as an indication of their depth location). This allows us to flag data collected before and after the mooring has reached its resting place on the sea floor. This data can be useful for testing changes in calibrations, examining pressure effects on sensors, etc. After visualizing the mooring pressure records, we set a single pair of date/time stamps for the beginning and end of the moored period for all sensors on each mooring, and all data before and after these times is assigned Flag 6 to indicate that it was not collected as part of the 'moored observations' period. Note that the pressures of individual sensors may still vary in this period, and this should be assessed using those records (just as the locations may vary and must be assessed using the latitude and longitude variables as described above).

Test 4) Gross Range Test (Required)

Data point exceeds sensor or operator-selected min/max. Applies to T, SP, C and P.		
<p>All sensors have a limited output range, and this can form the most rudimentary gross range check. No values less than a minimum value or greater than the maximum value the sensor can output (T_SENSOR_MIN, T_SENSOR_MAX) are acceptable. Additionally, the operator can select a smaller span (T_USER_MIN, T_USER_MAX) based upon local knowledge or a desire to draw attention to extreme values.</p> <p>NOTE: Operators may choose to flag as suspect values that exceed the calibration span but not the hardware limits (e.g., a value that sensor is not capable of producing or negative conductivity).</p>		
Flags	Condition	Codable Instructions
Fail=4	Reported value is outside of sensor span.	If $T_n < T_SENSOR_MIN$, or $T_n > T_SENSOR_MAX$, flag = 4
Suspect=3	Reported value is outside of operator-selected span.	If $T_n < T_USER_MIN$, or $T_n > T_USER_MAX$, flag = 3
Pass=1	Applies for test pass condition.	
Test Exception: None.		
<p>Test specifications to be established locally by the operator.</p> <p>Examples: The following global range min/max are applied on some climate and forecast standard-names in the IMOS toolbox: depth: -5/12,000 m sea_water_pressure: -5/12,000 decibars (dbar) sea_water_pressure_due_to_sea_water: -15/12,000 dbar sea_water_salinity: 2/41 sea_water_temperature: -2.5/40 °C</p>		

Implementation for SOTS delayed mode QC was as follows:

Flag 4: Value outside of the following limits:

$$S_Sensor_Min = +2 \quad S_Sensor\ Max = +41$$

Flag 3: no thresholds or flags assigned

Test 5) Climatology Test (Required)

Test that data point falls within seasonal expectations. Applies to T and SP.		
<p>This test is a variation on the gross range check, where the thresholds T_Season_MAX and T_Season_MIN are adjusted monthly, seasonally, or at some other operator-selected time period (TIM_TST). Expertise of the operator is required to determine reasonable seasonal averages. Longer time series permit more refined identification of appropriate thresholds. The ranges should also vary with water depth, if the measurements are taken at sites that cover significant vertical extent and if climatological ranges are meaningfully different at different depths (e.g., narrower ranges at greater depth).</p>		
Flags	Condition	Codable Instructions
Fail=4	Because of the dynamic nature of T and S in some locations, no fail flag is identified for this test.	N/A
Suspect=3	Reported value is outside of operator-identified climatology window.	If $T_n < T_{Season_MIN}$ or $T_n > T_{Season_MAX}$, flag = 3
Pass=1	Applies for test pass condition.	N/A
Test Exception: None.		
Test specifications to be established locally by operator: A seasonal matrix of T_{max} and T_{min} values at all TIM_TST intervals.		
Examples: T_SPRING_MIN = 12 °C, T_SPRING_MAX = 18.0 °C		

Flag 4, none assigned

Flag 3, assigned as follows, based on CTD casts near SOTS (shown at Figure 11, Figure 12 and Figure 13), all mooring observations, and review of the World Ocean Atlas, depth-dependent thresholds were set as follows, in °C:

Depth (dbar)	S_Season_Min	S_Season_Max
0- 400	34	35.5
400-1500	34	35.5
>1500	34.3	34.8

Because mean seasonal salinity changes are small at SOTS (~1) and similar to short term changes driven by passage of water parcels or local vertical mixing, these thresholds were held constant throughout the year. These bounds are shown in Figure 11 relative to the maxima and minima observed in all the moored sensor records as well as CTD casts at the SOTS site.

Test 6) Spike Test (Strongly Recommended)

Data point $n-1$ exceeds a selected threshold relative to adjacent data points. Applies to T, SP, C, and P.

This check is for single value spikes, specifically the value at point $n-1$. Spikes consisting of more than one data point are difficult to capture, but their onset may be flagged by the rate of change test. The spike test consists of two operator-selected thresholds, THRESHLD_LOW and THRESHLD_HIGH. Adjacent data points ($n-2$ and n_0) are averaged to form a spike reference (SPK_REF). The absolute value of the spike is tested to capture positive and negative spikes. Large spikes are easier to identify as outliers and flag as failures. Smaller spikes may be real and are only flagged suspect. The thresholds may be fixed values or dynamically established (for example, a multiple of the standard deviation over an operator-selected period).

Flags	Condition	Codable Instructions
Fail=4	High spike threshold exceeded.	If $ T_{n-1} - SPK_REF > THRESHLD_HIGH$, flag = 4
Suspect=3	Low spike threshold exceeded.	If $ T_{n-1} - SPK_REF > THRESHLD_LOW$ and $ T_{n-1} - SPK_REF \leq THRESHLD_HIGH$, flag = 3
Pass=1	Applies for test pass condition.	N/A

Test Exception: None.

Test specifications to be established locally by the operator.

Examples: THRESHLD_LOW = 3 °C, THRESHLD_HIGH = 8 °C

Implementation for SOTS delayed mode QC was as follows:

Oceanographic variability tends to decrease with depth, and thus as for Test 5, we implemented depth dependent thresholds to assign Flag 4 (and did not assign Flag 3):

Depth (dbar)	Spike threshold psu
0- 400	0.4
400-1500	0.2
>1500	0.02

Comparison of these thresholds to observed spikes is provided in Figure 7.

Test 7) Rate of Change Test (Strongly Recommended)

Excessive rise/fall test. Applies to T, SP, C, and P.

This test inspects the time series for a time rate of change that exceeds a threshold value identified by the operator. T, SP, C, P values can change substantially over short periods in some locations, hindering the value of this test. A balance must be found between a threshold set too low, which triggers too many false alarms, and one set too high, making the test ineffective. Determining the excessive rate of change is left to the local operator.

The following shows two different examples of ways to select the thresholds provided by QARTOD VI participants. Implementation of this test can be challenging. Upon failure, it is unknown which of the points is bad. Further, upon failing a data point, it remains to be determined how the next iteration can be handled.

Example 1

The rate of change between temperature T_{n-1} and T_n must be less than three standard deviations ($3*SD$). The SD of the T time series is computed over the previous 25-hour period (operator-selected value) to accommodate cyclical diurnal and tidal fluctuations. Both the number of SDs (N_DEV) and the period over which the SDs (TIM_DEV) are calculated and determined by the local operator.

Example 2

The rate of change between temperature T_{n-1} and T_n must be less than $2\text{ }^\circ\text{C} + 2SD$.

$|T_{n-1} - T_{n-2}| + |T_{n-1} - T_n| \leq 2*N_DEV*SD$ (example provided by EuroGOOS).

Flags	Condition	Codable Instructions
Fail=4	No fail flag is identified for this test.	N/A
Suspect=3	The rate of change exceeds the selected threshold.	If $ T_n - T_{n-1} > N_DEV*SD$, flag = 3
Pass=1	Applies for test pass condition.	N/A

Test Exception: None.

Test specifications to be established locally by operator.

Example: $N_DEV = 3, TIM_DEV = 25$

Implementation for SOTS delayed mode QC was as follows:

We discussed the implementation of this test in some detail in Jansen et al., 2020, for several reasons, including that:

- i. the QARTOD test description has some internal inconsistencies
- ii. choosing thresholds for this test requires careful comparison of sampling frequency to oceanographic event frequencies and durations
- iii. the Australian IMOS Toolbox offers alternate algorithms which we examined but chose not to use

For ease of access, we repeat some of this discussion here, and add examples for salinity that complement those shown for temperature in the previous report.

i. QARTOD Inconsistencies

We note that the text and formula for Example 2 from the QARTOD manual are not in accord. The text suggests that the rate of change must be less than the sum of a constant threshold of 2°C plus 2 times the standard deviation over the previous TIM_DEV period, but the formula compares the average rate of change over the past 2 intervals (n vs $n-1$ and $n-1$ vs $n-2$) with the N standard deviations SD , without any constant threshold. The formula as written also fails to include consideration of the sampling interval. An appropriate formula for a variable V including a constant threshold rate, V_t ,

with augmentation when the signal is noisy (as represented by N_DEV times the standard deviation SD calculated over the past time period TIM_DEV) would read:

Flag 3 if $[|V_n - V_{n-1}|] / [t_n - t_{n-1}] > V_t + N_DEV * SD$

Note that this formulation means that R_t should be selected as the threshold change in the rate of change variable V_t over the time period TIM_DEV , and that TIM_DEV should be selected to cover a reasonable number of prior observations so that its SD is well behaved. This formulation would avoid excessive flagging of records with low variability, by setting a minimum rate of change V_t .

ii. Examples of observed rates of change at SOTS and their influence on threshold choices

An example S time series illustrates the challenges of determining whether data should be flagged as bad or suspect based on rate of change. For the SOFS surface float, SBE37 unpumped CTDs sampling at high temporal frequency occasionally exhibit rapid salinity changes, e.g. the fresh excursion (labelled as episode 1) and salty excursion (labelled as episode 2) in Figure 19. Both events have durations too long for them to be identified as spikes. The first event is not present as a low conductivity excursion and thus results from conductivity dropping less than expected from the coincident temperature excursions. Their rapidity and the fact that this salinity event is only present in one sensor suggest they arise from sensor mismatch and thus should be flagged as suspect. In contrast, episode 2 which shows similar rates of change is coincident with clear conductivity variations and occurred in multiple sensors and is thus likely real.

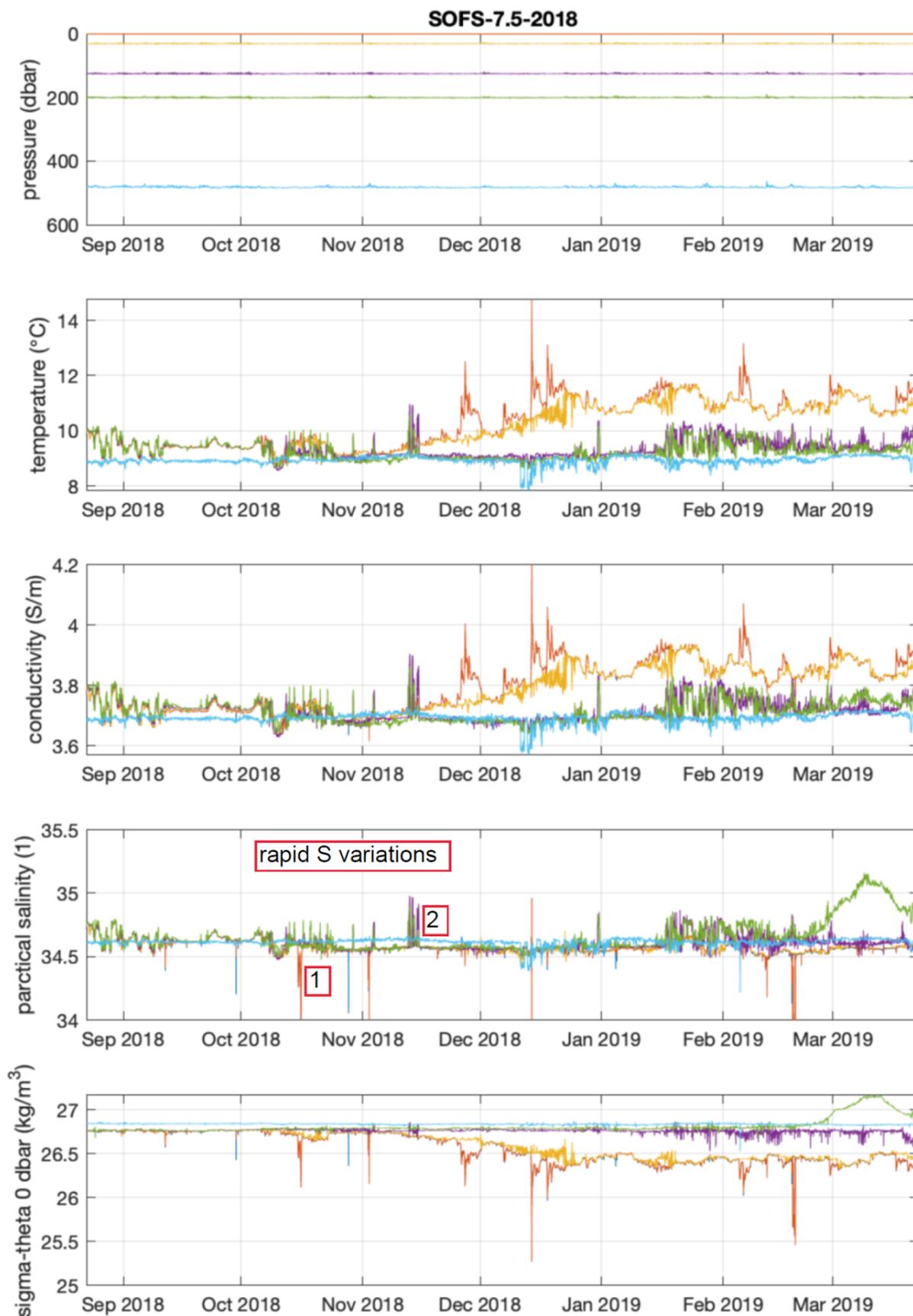


Figure 19. SOFS-7.5 salinity variations relative to other properties including episodes [1] with high rates of change for salinity that likely result from sensor mismatch, and others [2] which are oceanic in origin.

The observable rate-of-change clearly depends on the sampling frequency, and most sensors at SOTS sample more slowly. Thus, a single rate-of-change threshold for all sensors can be difficult to define. For simplicity, and to avoid flagging good data as bad, we have chosen a high rate of change threshold for all sensors. This approach could inappropriately miss flagging rapid changes in lower frequency records, but in practice we found that those problems are often detected by the Test 6 spike algorithm. As with Tests 5 and 6, we implemented depth dependent thresholds (assigning only Flag 3):

Depth (dbar)	Rate of Change Threshold psu hour^{-1}
0- 400	30
400-1500	10
>1500	1.2

This depth dependence scales the thresholds to the observed variability, an aspect which the use of the measurement standard deviation was intended to do in the QARTOD formulation (with or without the addition of a minimum threshold V_t), but importantly without the problem that the standard deviation increases as the proportion of bad data increases. In other words, bootstrapping thresholds from standard deviations can only be successful when the variability is actually oceanographic and data is both infrequent and intermittent, and thus it is better to choose thresholds from the best performing sensors and apply them across all sensors, rather than setting thresholds from individual records. Figure 20 compares the rate of change thresholds and moored observations.

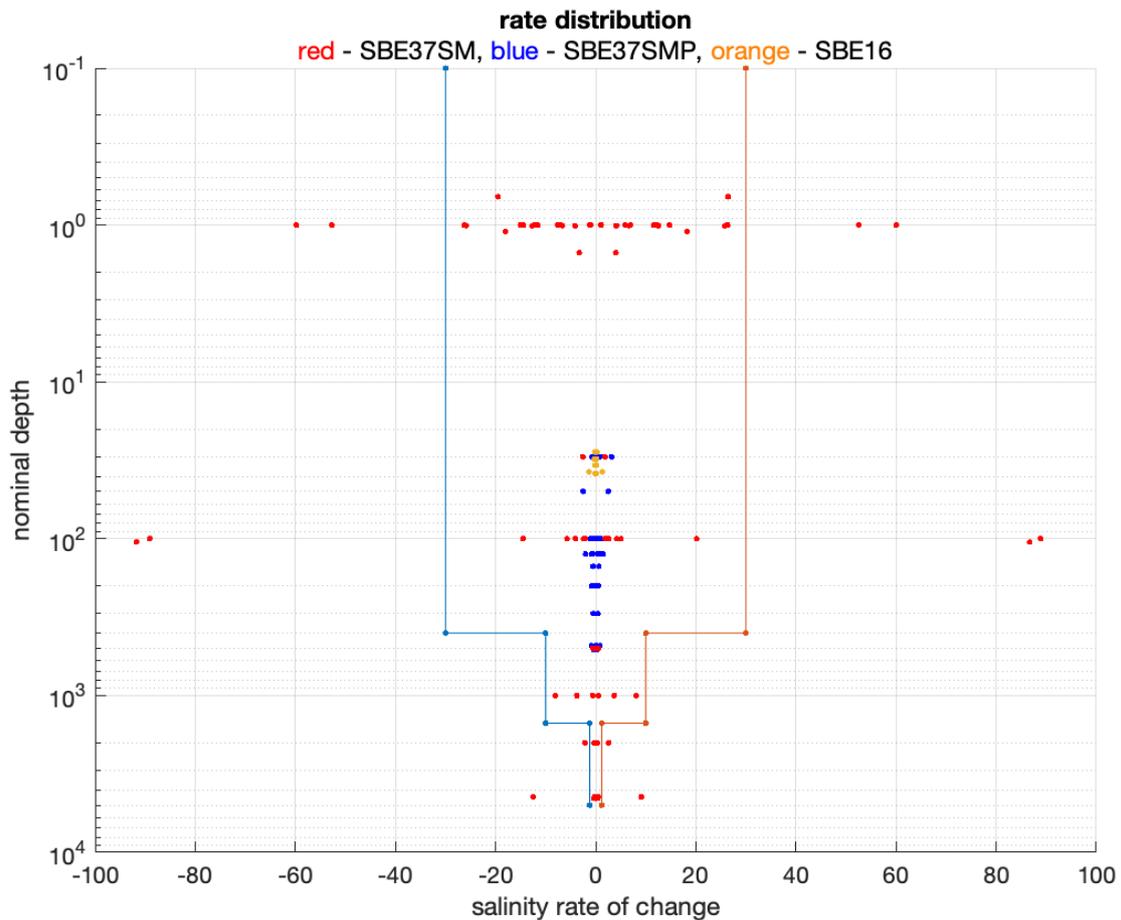


Figure 20. Comparison of Test 7 rate of change thresholds and observed rate of change maxima.

iii. consideration of IMOS Toolbox Spike / Rate of Change tests

The IMOS Toolbox offers two interesting algorithms, known as Hampel and Otsu in reference to the early works that introduced the concepts (Hampel, 1974; Otsu, 1979).

The Hampel algorithm is very similar to the QARTOD rate of change test – in that it uses a window (e.g. 25 hours) over which variability is determined to derive a threshold that is then used to throw out spikes. It differs from the QARTOD rate of change only in that the variability measure is linear (rather than squared, i.e. standard deviation). Because the window can be much wider than the measurement interval (up to the whole record length), it effectively separates the spikes from the unaffected data based on whether short-duration amplitudes are larger than long duration average variability amplitudes. Thus, it suffers from the same general problem as discussed above for the QARTOD algorithm – it drives thresholds from compromised data, and specifically if high rates of change from sensor errors are frequent, they determine the variability and thus cannot be distinguished from good data.

The Otsu algorithm, as developed for image recognition, is more interesting. It makes a histogram of the rate of change amplitudes between adjacent points (so it is sort of an estimate of the probability distribution of all the variability), and then divides this into two classes – acceptable variability and unacceptable variability - in a way that maximizes the difference between the two

classes. This works as long as the spikes are steeper than the data. In its simplest form it uses the full record to define the histogram, but of course that can be chopped into bits. Again, it can only work when some of the record is good, so that there is a portion that defines the acceptable variability. In practice, this same goal was achieved by our setting of thresholds via visualisation of the SOTS records, including comparison of Neighbour records. Future work to pursue quantitative examination of the variability probability distribution functions of good records may well prove useful, but was beyond the scope of this report.

Test 8) Flat Line Test (Strongly Recommended)

Invariant value. Applies to T, SP, C, and P.		
When some sensors and/or data collection platforms fail, the result can be a continuously repeated observation of the same value. This test compares the present observation n to a number (REP_CNT_FAIL or REP_CNT_SUSPECT) of previous observations. Observation n is flagged if it has the same value as previous observations within a tolerance value, EPS, to allow for numerical round-off error. Note that historical flags are not changed.		
Flags	Condition	Codable Instructions
Fail=4	When the five most recent observations are equal, T_n is flagged fail.	CNT = 0 For $l = 1, \text{REP_CNT_FAIL}$ If $ T_n - T_{n-l} < \text{EPS}$, CNT = CNT+1 If CNT = REP_CNT_FAIL, flag = 4
Suspect=3	It is possible but unlikely that the present observation and the two previous observations would be equal. When the three most recent observations are equal, T_n is flagged suspect.	CNT = 0 For $l = 1, \text{REP_CNT_SUSPECT}$ If $ T_n - T_{n-l} < \text{EPS}$, CNT = CNT+1 If CNT = REP_CNT_SUSPECT, flag = 3
Pass=1	Applies for test pass condition.	N/A
Test Exception: None.		
Test specifications to be established locally by the operator.		
Examples: REP_CNT_FAIL = 5, REP_CNT_SUSPECT= 3, EPS = 0.05°		

NOT Implemented for SOTS delayed mode QC of salinity

The choice of tolerance value for this test is very important, and testing with SOTS data found that for these sensors, which have high digital-analog resolution (SBE37, SBE16, etc.), five repeated values were not observed. Therefore, the test was not implemented. [See also the discussion in Jansen et al., 2020 for low analog-digital resolution sensors where repeat values are common but do not indicate errors.]

Test 9) Multi-Variate Test (Suggested)

Comparison to other variables. Applies to T, SP, and P.		
<p>This is an advanced family of tests, starting with the simpler test described here and anticipating growth towards full co-variance testing in the future. It is doubtful that anyone is conducting tests such as these in real time. As these tests are developed and implemented, they should be documented and standardized in later versions of this manual.</p> <p>This example pairs rate of change tests as described in test 7. The T (or SP or P) rate of change test is conducted with a more restrictive threshold (N_T_DEV). If this test fails, a second rate of change test operating on a second variable (salinity or conductivity would be the most probable) is conducted. The absolute value rate of change should be tested, since the relationship between T and variable two is indeterminate. If the rate of change test on the second variable fails to exceed a threshold (e.g., an anomalous step is found in T and is lacking in salinity), then the T_n value is flagged.</p> <p>Note that Test 12, TS Curve/Space Test is a well-known example of the multi-variate test.</p>		
Flags	Condition	Codable Instructions
Fail=4	No fail flag is identified for this test.	N/A
Suspect=3	T_n fails the rate of change and the second variable does not exceed the rate of change.	$\text{If } T_n - T_{n-1} > N_T_DEV * SD_T$ <p style="text-align: center;">AND</p> $ SP_n - SP_{n-1} < N_SP_DEV * SD_SP, \text{ flag} = 3$
Pass=1	N/A	N/A
Test Exception: None.		
Test specifications to be established locally by the operator.		
Examples: N_T_DEV = 2, N_TEMP_DEV = 2, TIM_DEV = 25 hours		

Implementation for SOTS delayed mode QC of salinity was as follows, as developed and discussed in detail above.

Potential density (sigma-theta at pressure 0) was calculated for each T-S-P instrument. Spikes in sigma-theta, relative to its smoothed time series, were used to assign flags to salinity:

Flag 3 sigma-theta spikes >0.02

Test 10) Attenuated Signal Test (Suggested)

A test for inadequate variation of the time series. Applies to T, SP, C, and P.		
A common sensor failure mode can provide a data series that is nearly but not exactly a flat line (e.g., if the sensor head were to become wrapped in debris). This test inspects for an SD value or a range variation (MAX-MIN) value that fails to exceed threshold values (MIN_VAR_WARN, MIN_VAR_FAIL) over a selected time period (TST_TIM).		
Flags	Condition	Codable Instructions
Fail=4	Variation fails to meet the minimum threshold MIN_VAR_FAIL.	If During TST_TIM, SD <MIN_VAR_FAIL, or During TST_TIM, MAX-MIN <MIN_VAR_FAIL, flag = 4
Suspect=3	Variation fails to meet the minimum threshold MIN_VAR_WARN.	If During TST_TIM, SD <MIN_VAR_WARN, or During TST_TIM, MAX-MIN <MIN_VAR_WARN, flag = 3
Pass=1	Applies for test pass condition.	N/A
Test Exception: None.		
Test specifications to be established locally by the operator.		
Examples: TST_TIM = 12 hours MIN_VAR_WARN = 0.5 °C, MIN_VAR_FAIL = 0.1 °C		

Implementation for SOTS delayed mode QC was as follows:

The definition of the minimum variability thresholds (MIN_VAR_FAIL/WARN) requires precise understanding of the oceanographic expectation, and will vary strongly with depth. In this sense it has overlaps with Tests 6 and 7 for spikes and rates of change. Also, as noted in the introduction, such expectations of minimum variability are still under development for the Southern Ocean owing to the sparse history of temporally resolved observations. In practice, the best estimate of the expectation comes from sensors at SOTS that are considered to have functioned without attenuation, and thus are equivalent to an aspect of Neighbour tests. *For this reason, we did not perform Test 10 separately; rather its information was captured by our implementation of Test 11.* In future, as knowledge of minimum variability is obtained, separate implementation of Test 10 may become useful.

Test 11) Neighbor Test (Suggested)

Comparison to nearby sensors. Applies to T, SP, C, and P.		
<p>This test is potentially the most useful when a nearby sensor has a similar response. Ideally, redundant sensors using different technology would be co-located and alternately serviced at different intervals. This close neighbor would provide the ultimate QC check, but cost often prohibits such a deployment</p> <p>However, there are few instances where a second sensor is sufficiently proximate to provide a useful QC check. Just a few hundred meters in the horizontal and less than 10 m vertical separation can often yield greatly different results. Nevertheless, the test should not be overlooked where it may have application.</p> <p>This test is the same as Test 9), <i>Multi-variate Check – comparison to other variables</i> where the second variable is the second sensor. The selected thresholds depend entirely upon the relationship between the two sensors as determined by the local knowledge of the operator.</p> <p>In the instructions and examples below, data from one site (T1) are compared to a second site (T2). The standard deviation for each site (SD1, SD2) is calculated over the period (TIM_DEV) and multiplied as appropriate (N_T1_DEV for site T1) to calculate the rate of change threshold. Note that an operator could also choose to use the same threshold for each site, since they are presumed to be similar.</p>		
Flags	Condition	Codable Instructions
Fail=4	No fail flag is identified for this test.	N/A
Suspect=3	T1 _n fails the rate of change and the second sensor T2 _n does not exceed the rate of change.	$ T1_n - T1_{n-1} > N_T1_DEV * SD1$ AND $ T2_n - T2_{n-1} < N_T2_DEV * SD2, \text{ flag} = 3$
Pass=1	N/A	N/A
<p>Test Exception: There is no adequate neighbor.</p>		
<p>Test specifications to be established locally by the operator.</p> <p>Examples: N_T1_DEV = 2, N_T2_DEV=2, TIM_DEV = 25 hours</p>		

Implementation for SOTS delayed mode QC was as follows:

In principle, this is a powerful test, particularly when sensors are mounted in pairs and thus either they reinforce the fidelity of the data when they are indistinguishable or emphasize that at least one of the sensors has failed when they differ. Obviously, examination of all neighbouring sensors provides the most powerful approach. Moreover, other aspects than the standard deviation need examination– for example two sensors may have the same standard deviation but may drift relative to each other. For these reasons, we did not codify paired tests, but instead used parallel visualization of all salinity sensors on each mooring to search for problems. The sparse vertical distribution of sensors made this less useful than for temperature (which revealed offsets between some sensor types; Jansen et al., 2020). The visualization approach and results are detailed in the next section, after implementation of the remaining QARTOD tests is described.

Test 12) TS Curve/Space Test (Suggested)

Comparison to expected TS relationship. Applies to T, SP.		
The TS curve is a classic tool used to evaluate observations, especially in the open ocean below the thermocline. Site-specific TS curve characteristics are used to identify outliers. The curve could be either a fitted equation or numerical table. For a given T_n , SP_n is expected to be within $SP_{fit} \pm SP_{fit_warn}$ or SP_{fit_fail} , operator-provided values. The value SP_{fit} is obtained from the equation or table.		
Flags	Condition	Codable Instructions
Fail=4	For a given temperature, the observed salinity falls outside the TS curve failure threshold.	If $ SP_n - SP_{fit} > SP_{fit_fail}$, flag = 4
Suspect=3	For a given temperature, the observed salinity falls outside the TS curve warning threshold.	If $ SP_n - SP_{fit} \leq SP_{fit_fail}$ and $ SP_n - SP_{fit} > SP_{fit_warn}$, flag = 3
Pass=1	N/A	N/A
Test Exception: The test will probably not be useful in estuaries or ocean surface waters.		
Test specifications to be established locally by the operator.		
Examples: At the Bermuda Atlantic Time Series site, for a temperature of 18 °C, $SP_{fit} = 36.5$ $SP_{fit_fail} = 0.05$, $SP_{fit_warn} = 0.02$		

Implemented for SOTS delayed mode QC of salinity as follows:

Limited ship CTD data make the definition of expected T-S relationships difficult, especially below 2000m. Comparison of the SOTS moored CTD data to ship data is shown in Figure 21. This reveals that most data that lies well outside the ship-CTD results has failed other QC tests. The moored data is far more abundant than the ship-CTD data, and thus the larger moored data variability may be real. On this basis, no further flagging of data was implemented. It may be possible to refine this approach in future as more ship-CTD data becomes available.

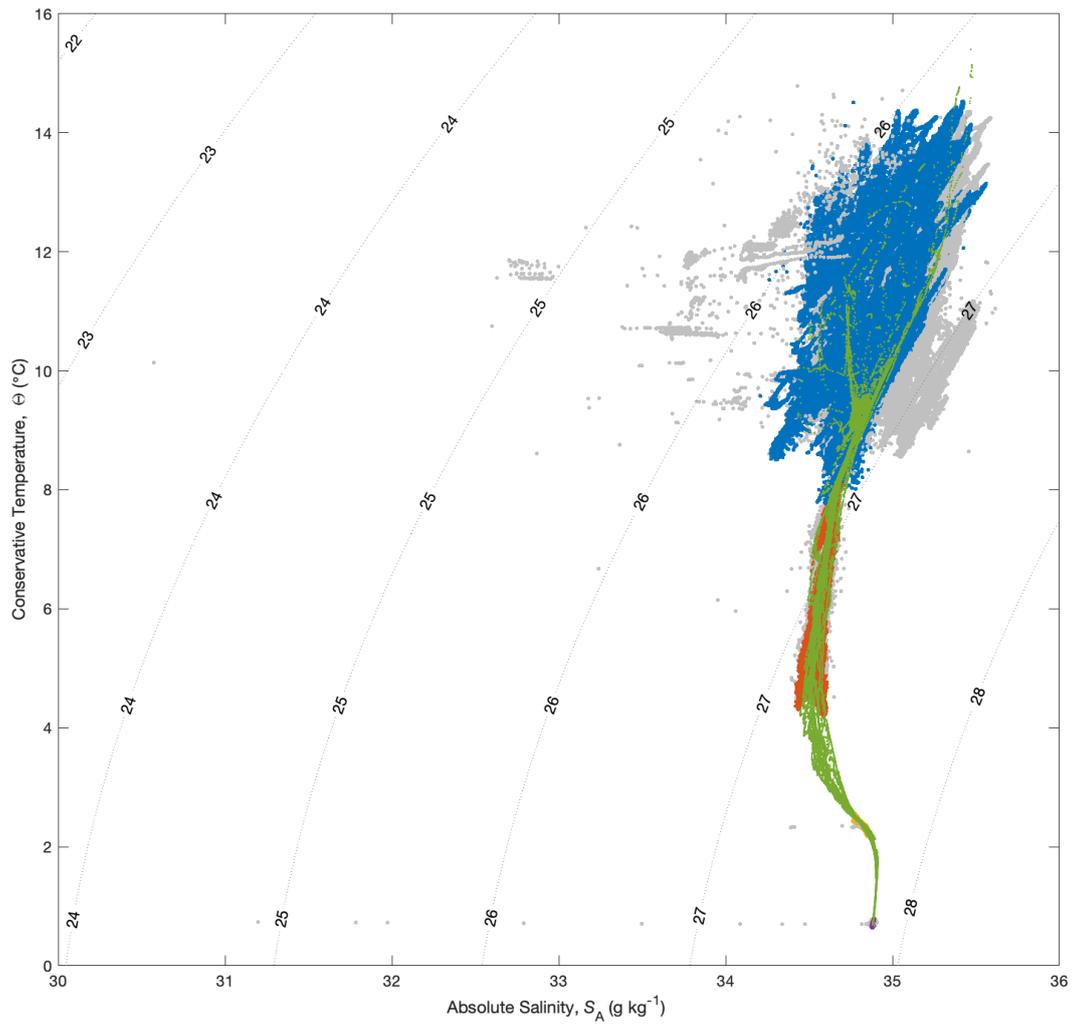


Figure 21. T-S diagram for ship-CTD (green) and all moored CTD observations at SOTS. (blue indicates data < 600 m, red 600-1500 m, yellow 1500-4000 m, purple > 4000 m). Grey indicates data has failed a QC test.

Test 13) Density Inversion Test (Suggested)

Checks that density increases with pressure (depth).		
<p>With few exceptions, potential water density σ_θ will increase with increasing pressure. When vertical profile data are obtained, this test is used to flag as failed T, C, and SP observations, which yield densities that do not sufficiently increase with pressure. A small, operator-selected density threshold (DT) allows for micro-turbulent exceptions. Here, $\sigma_{\theta n}$ is defined as one sample increment deeper than $\sigma_{\theta n-1}$. With proper consideration, the test can be run on downcasts, upcasts, or down/up cast results produced in real-time.</p> <p>From a computational point of view, this test is similar to the rate of change test (test 7), except that the time axis is replaced by depth. The same code can be used for both, using different variables and thresholds. As with the rate of change test, it is not known which side of the step is good versus bad.</p> <p>An example of the software to compute sigma-theta is available at http://www.teos-10.org/software.htm.</p>		
Flags	Condition	Codable Instructions
Fail=4	Potential density does not sufficiently increase with increasing depth.	If $\sigma_{\theta n-1} + DT > \sigma_{\theta n}$, flag = 4
Suspect=3	No suspect flag is identified for this test.	N/A
Pass=1	Potential density sufficiently increases with increasing depth.	If $\sigma_{\theta n-1} + DT \leq \sigma_{\theta n}$, flag = 1
Test Exception: None.		
Test specifications to be established locally by the operator.		
Examples: DT = 0.03 kg/m ³		

Implemented for SOTS delayed mode QC of salinity, via visualization, as follows:

Sigma-theta at pressure = 0 was calculated for all T,S,P sensors on each mooring, and the criterion that this should increase monotonically downwards was used to identify potential problems. Departures from this criterion were uncommon, but some did occur and these are annotated in these plots for each sensor in Appendix C, and listed in Table 4. Importantly, this test depends on the relative accuracy of the temperature and salinity measurements for sensor pairs and not just their precision. For example, in one case, use of the most recent conductivity cell calibration for a sensor suggested an unstable water column when it is compared to adjacent sensors, but this problem disappeared if an earlier calibration was used (see Figure 5 example). Thus it is not reasonable to reject data as definitively bad if the water column instability is within the uncertainty of the calibrations.

5.3 Manual Flagging via Neighbouring sensor visualizations

After extensive exploration, we settled on 2 plot types to visualize possible sensor problems (and provide these for all deployments below, with annotation of sensor errors that they revealed):

1. Stacked time series for each deployment for all its salinity sensors, showing sensor pressures, temperatures, conductivities, salinities, and potential densities (sigma-theta at pressure 0).
2. Correlation plots of Potential Temperature vs. Absolute Salinity which include contours of constant in-situ density.

Using these plots, several problematic sensor records were identified and flagged as annotated on the plots shown in Appendix C and listed in Table 4.

These visualizations also reveal that the salinity variations are fascinating in their diversity, rapidity, and origins. In particular: i. very rapid temporal variations occurred synchronously at all depths indicating very sharp and vertical boundaries between water parcels ii. vertical movements (from both heave and mooring dynamics) causes mirror imaging of rapid salinity (and temperature) fluctuations for sensors above and below the seasonal pycnocline, and iii. thermal inversions below the wind-mixed surface layer were in general density compensated by salinity increases.

Table 4. Manual flag assignments from Neighbour and Multi-variate test visualizations

Mooring	Feature identified	Flag assignment
SOFS-7.5 SN 15971	Density inversion, after 2019-02-09	4
SAZ47-15-2012 SN 8597	drop in salinity, cell contamination 2013-02-19 to 2013-03-06	4
SAZ47-16-2013 SN 1778	drop in salinity, cell contamination 2014-01-20 to 2014-01-24	4
SAZ47-17-2015 SN 8985	drop in salinity, cell contamination 2015-05-01 to 2015-05-03	4
SAZ47-18-2016 SN 8597	drop in salinity, cell contamination 2017-01-12 to 2017-01-23	4
SOFS-9 SN 15971	Density inversion, before 2020-10-25	4

Table 5. Summary of flag statistics from the automated and manual QC efforts

[Note that the sigma-theta salinity sensor-mismatch QC approach was only applied to sensors with sufficiently high temporal resolution for effective smoothing.]

Deploy.	Instrument	Serial_#	Depth	flag	flag 1	flag 2	flag 3	flag 4	flag 6	% flag 3 or 4
Pulse-6-2009	SBE16plusV2	1606331	38	final flags	4058		1		169	0.02
				location (test 3)	4059			169	0	
				range (test 4-5)		1			0.02	
				spike (test 6)					0	
				rate-of-change (test 7)					0	
	SBE37SM-RS232	6962	100	final flags	215634		30730		15733	12.47
				location (test 3)	246364			15733	0	
				range (test 4-5)		2			0	
				spike (test 6)		5			0	
				rate-of-change (test 7)		2			0	
				sigma-theta0 (test 9)			30721			12.47
				final flags	114154		508		16092	0.44
				location (test 3)	114662			16092	0	
				range (test 4-5)		95			0.08	
				spike (test 6)					0	
SOFS-1-2010	SBE37SM-RS485	3707409	1	rate-of-change (test 7)						0
				sigma-theta0 (test 9)			413			0.36
				final flags	53417		3919		4674	6.84
				location (test 3)	57336			4674	0	
				range (test 4-5)					0	
	SBE37-SM	2971	100	spike (test 6)						0
				rate-of-change (test 7)					0	
				sigma-theta0 (test 9)			3919			6.84
				final flags	5228			690	0	
				location (test 3)	5228			690	0	
Pulse-7-2010	SBE16plus	1606331	31	range (test 4-5)						0
				spike (test 6)					0	
				rate-of-change (test 7)					0	
				final flags	19633		62		6971	0.31
				location (test 3)	19695			6971	0	
	SBE37SM-RS232	3706962	100	range (test 4-5)						0
				spike (test 6)					0	
				rate-of-change (test 7)					0	
				rate-of-change (test 7)					0	
				rate-of-change (test 7)					0	

Deploy.	Instrument	Serial_#	Depth	flag	flag 1	flag 2	flag 3	flag 4	flag 6	% flag 3 or 4
				sigma-theta0 (test 9)			62			0.31
Pulse-8-2011	SBE16plus	1606330	34	final flags	4311			985	139	18.6
				location (test 3)	5296				139	0
				range (test 4-5)			393			7.42
				spike (test 6)			7			0.13
				rate-of-change (test 7)						0
				manual (test 10-13)				985		18.6
	SBE37SM-RS232	6962	105	final flags	464933		40313		9011	7.98
				location (test 3)	505246				9011	0
				range (test 4-5)			61			0.01
				spike (test 6)			5			0
				rate-of-change (test 7)			2			0
				sigma-theta0 (test 9)			40245			7.97
SOFS-2-2011	SBE37SM-RS485	3707409	2	final flags	69070		326		10358	0.47
				location (test 3)	69396				10358	0
				range (test 4-5)						0
				spike (test 6)						0
				rate-of-change (test 7)						0
				sigma-theta0 (test 9)			326			0.47
	SBE37-SM	2971	100	final flags	28867		5831		2302	16.81
				location (test 3)	34698				2302	0
				range (test 4-5)						0
				spike (test 6)						0
				rate-of-change (test 7)						0
				sigma-theta0 (test 9)			5831			16.81
SOFS-3-2012	SBE37SM-RS485	3708764	1	final flags	49379		61		11854	0.12
				location (test 3)	49440				11854	0
				range (test 4-5)			1			0
				spike (test 6)			1			0
				rate-of-change (test 7)						0
				sigma-theta0 (test 9)			59			0.12
	SBE37SM-RS485	3708765	1	final flags	49332		89		11637	0.18
				location (test 3)	49421				11637	0
				range (test 4-5)			1			0
				spike (test 6)			2			0
				rate-of-change (test 7)						0

Deploy.	Instrument	Serial_#	Depth	flag	flag 1	flag 2	flag 3	flag 4	flag 6	% flag 3 or 4
				sigma-theta0 (test 9)			86			0.17
	SBE37SMP-ODO-RS232	9513	30	final flags	8239		1		1154	0.01
				location (test 3)	8240				1154	0
				range (test 4-5)						0
				spike (test 6)			1			0.01
				rate-of-change (test 7)						0
	SBE37SMP-ODO-RS232	9514	100	final flags	8239		1		1157	0.01
				location (test 3)	8240				1157	0
				range (test 4-5)						0
				spike (test 6)			1			0.01
				rate-of-change (test 7)						0
Pulse-9-2012	SBE16plusV2	1606331	38	final flags	3966			687	776	14.76
				location (test 3)	4653				776	0
				range (test 4-5)			190			4.08
				spike (test 6)						0
				rate-of-change (test 7)						0
				manual (test 10-13)				687		14.76
	SBE37SMP-ODO-RS232	3709515	100	final flags	14002		3		999	0.02
				location (test 3)	14005				999	0
				range (test 4-5)						0
				spike (test 6)			3			0.02
				rate-of-change (test 7)						0
SAZ47-15-2012	SBE37SM-RS232	3708597	4422	final flags	122186		2410	4320	3308	5.22
				location (test 3)	128916				3308	0
				range (test 4-5)						0
				spike (test 6)			1			0
				rate-of-change (test 7)						0
				sigma-theta0 (test 9)			3289			2.55
				manual (test 10-13)				4320		3.35
SOFS-4-2013	SBE37SM-RS485	3707408	1	final flags	47869		70		11983	0.15
				location (test 3)	47939				11983	0
				range (test 4-5)						0
				spike (test 6)						0
				rate-of-change (test 7)						0
				sigma-theta0 (test 9)			70			0.15
	SBE37SM-RS485	3707409	1	final flags	47870		69		13705	0.14

Deploy.	Instrument	Serial_#	Depth	flag	flag 1	flag 2	flag 3	flag 4	flag 6	% flag 3 or 4
				location (test 3)	47939				13705	0
				range (test 4-5)			1			0
				spike (test 6)						0
				rate-of-change (test 7)						0
				sigma-theta0 (test 9)			68			0.14
	SBE37SM-RS232	3708985	100	final flags	238275		1420		9353	0.59
				location (test 3)	239695				9353	0
				range (test 4-5)						0
				spike (test 6)						0
				rate-of-change (test 7)						0
				sigma-theta0 (test 9)			1420			0.59
	SBE37SM-RS232	3709185	500	final flags	47939				1654	0
				location (test 3)	47939				1654	0
				range (test 4-5)						0
				spike (test 6)						0
				rate-of-change (test 7)						0
				sigma-theta0 (test 9)						0
SAZ47-16-2013	SBE37-SM	1778	4428	final flags	91264		7478	576	3466	8.11
				location (test 3)	99318				3466	0
				range (test 4-5)			7			0.01
				spike (test 6)			6			0.01
				rate-of-change (test 7)						0
				sigma-theta0 (test 9)			7544			7.6
				manual (test 10-13)				576		0.58
Pulse-10-2013	SBE16plus	1606330	28	final flags	3828				28	0
				location (test 3)	3828				28	0
				range (test 4-5)						0
				spike (test 6)						0
				rate-of-change (test 7)						0
	SBE37SMP-ODO-RS232	3709538	100	final flags	7654		1		516	0.01
				location (test 3)	7655				516	0
				range (test 4-5)						0
				spike (test 6)			1			0.01
				rate-of-change (test 7)						0
	SBE37SMP-ODO-RS232	3709513	200	final flags	7655				518	0
				location (test 3)	7655				518	0

Deploy.	Instrument	Serial_#	Depth	flag	flag 1	flag 2	flag 3	flag 4	flag 6	% flag 3 or 4
				range (test 4-5)						0
				spike (test 6)						0
				rate-of-change (test 7)						0
SOFS-5-2015	SBE37SM-RS485	3707409	1	final flags	109915		1466		5266	1.32
				location (test 3)	111381				5266	0
				range (test 4-5)			776			0.7
				spike (test 6)			4			0
				rate-of-change (test 7)						0
				sigma-theta0 (test 9)			686			0.62
	SBE37SM-RS485	3707408	1	final flags	110798		583		5247	0.52
				location (test 3)	111381				5247	0
				range (test 4-5)			3			0
				spike (test 6)			2			0
				rate-of-change (test 7)						0
				sigma-theta0 (test 9)			578			0.52
	SBE37SM-RS232	3706962	30	final flags	54364		1326		1356	2.38
				location (test 3)	55690				1356	0
				range (test 4-5)						0
				spike (test 6)						0
				rate-of-change (test 7)						0
				sigma-theta0 (test 9)			1326			2.38
	SBE37-SM	4908	100	final flags	49486		6204		1196	11.14
				location (test 3)	55690				1196	0
				range (test 4-5)						0
				spike (test 6)			4			0.01
				rate-of-change (test 7)						0
				sigma-theta0 (test 9)			6200			11.13
	SBE37-SM	4909	500	final flags	55640		50		2076	0.09
				location (test 3)	55690				2076	0
				range (test 4-5)						0
				spike (test 6)						0
				rate-of-change (test 7)						0
				sigma-theta0 (test 9)			50			0.09
Pulse-11-2015	SBE16plus	1606330	28	final flags	8613		1		242	0.01
				location (test 3)	8614				242	0
				range (test 4-5)						0
				spike (test 6)			1			0.01

Deploy.	Instrument	Serial_#	Depth	flag	flag 1	flag 2	flag 3	flag 4	flag 6	% flag 3 or 4
				rate-of-change (test 7)						0
	SBE37SMP-ODO-RS232	3709538	50	final flags	17300		1		900	0.01
				location (test 3)	17301				900	0
				range (test 4-5)			1			0.01
				spike (test 6)						0
				rate-of-change (test 7)						0
	SBE37SMP-ODO-RS232	3709513	100	final flags	17300		1		903	0.01
				location (test 3)	17301				903	0
				range (test 4-5)						0
				spike (test 6)			1			0.01
				rate-of-change (test 7)						0
	SBE37SMP-ODO-RS232	3709514	150	final flags	17300		1		904	0.01
				location (test 3)	17301				904	0
				range (test 4-5)						0
				spike (test 6)			1			0.01
				rate-of-change (test 7)						0
SAZ47-17-2015	SBE37SM-RS232	3708985	4526	final flags	50485		700	288	1394	1.92
				location (test 3)	51473				1394	0
				range (test 4-5)						0
				spike (test 6)			1			0
				rate-of-change (test 7)						0
				sigma-theta0 (test 9)			751			1.46
				manual (test 10-13)				288		0.56
FluxPulse-1-2016	SBE37SM-RS485	3708764	1	final flags	28264		103		8736	0.36
				location (test 3)	28367				8736	0
				range (test 4-5)			2			0.01
				spike (test 6)			1			0
				rate-of-change (test 7)						0
				sigma-theta0 (test 9)			100			0.35
	SBE37SM-RS485	3710136	1	final flags	28255		113		8732	0.4
				location (test 3)	28368				8732	0
				range (test 4-5)						0
				spike (test 6)						0
				rate-of-change (test 7)						0
				sigma-theta0 (test 9)			113			0.4
SAZ47-18-2016	SBE37SM-RS232	3708597	4500	final flags	50430		1057	1584	784	4.98

Deploy.	Instrument	Serial_#	Depth	flag	flag 1	flag 2	flag 3	flag 4	flag 6	% flag 3 or 4
				location (test 3)	53071				784	0
				range (test 4-5)						0
				spike (test 6)						0
				rate-of-change (test 7)						0
				sigma-theta0 (test 9)			1063			2
				manual (test 10-13)				1584		2.98
SOFS-6-2017	SBE37SM-RS485	3708764	1	final flags	65232		144		29640	0.22
				location (test 3)	65376				29640	0
				range (test 4-5)			1			0
				spike (test 6)			4			0.01
				rate-of-change (test 7)						0
				sigma-theta0 (test 9)			139			0.21
	SBE37SM-RS485	3710136	1	final flags	65226		129		29618	0.2
				location (test 3)	65355				29618	0
				range (test 4-5)						0
				spike (test 6)			4			0.01
				rate-of-change (test 7)						0
				sigma-theta0 (test 9)			125			0.19
	SBE37SMP-ODO-RS232	3709538	30	final flags	10894		2		823	0.02
				location (test 3)	10896				823	0
				range (test 4-5)			2			0.02
				spike (test 6)						0
				rate-of-change (test 7)						0
	SBE37SMP-ODO-RS232	3709513	125	final flags	10889		7		823	0.06
				location (test 3)	10896				823	0
				range (test 4-5)			4			0.04
				spike (test 6)			3			0.03
				rate-of-change (test 7)						0
	SBE37SMP-ODO-RS232	3709514	200	final flags	10895		1		823	0.01
				location (test 3)	10896				823	0
				range (test 4-5)						0
				spike (test 6)			1			0.01
				rate-of-change (test 7)						0
	SBE37SMP-ODO-RS232	3714700	500	final flags	10895		1		824	0.01
				location (test 3)	10896				824	0
				range (test 4-5)						0

Deploy.	Instrument	Serial_#	Depth	flag	flag 1	flag 2	flag 3	flag 4	flag 6	% flag 3 or 4
				spike (test 6)			1			0.01
				rate-of-change (test 7)						0
SAZ47-19-2017	SBE37SM-RS232	3707901	1000	final flags	50870		45		807	0.09
				location (test 3)	50915				807	0
				range (test 4-5)						0
				spike (test 6)						0
				rate-of-change (test 7)						0
				sigma-theta0 (test 9)			45			0.09
	SBE37SM-RS232	3707896	2000	final flags	50881		34		809	0.07
				location (test 3)	50915				809	0
				range (test 4-5)			5			0.01
				spike (test 6)			7			0.01
				rate-of-change (test 7)						0
				sigma-theta0 (test 9)			22			0.04
	SBE37-SM	2971	4500	final flags	49615		1300		803	2.55
				location (test 3)	50915				803	0
				range (test 4-5)						0
				spike (test 6)			1			0
				rate-of-change (test 7)						0
				sigma-theta0 (test 9)			1299			2.55
SOFS-7-2018	SBE37SM-RS485	3707408	1	final flags	3025				5907	0
				location (test 3)	3025				5907	0
				range (test 4-5)						0
				spike (test 6)						0
				rate-of-change (test 7)						0
				sigma-theta0 (test 9)						0
	SBE37SM-RS485	3707409	1	final flags	3024		1		5902	0.03
				location (test 3)	3025				5902	0
				range (test 4-5)						0
				spike (test 6)						0
				rate-of-change (test 7)						0
				sigma-theta0 (test 9)			1			0.03
	SBE37SMP-ODO-RS232	3715969	30	final flags	504				2340	0
				location (test 3)	504				2340	0
				range (test 4-5)						0
				spike (test 6)						0

Deploy.	Instrument	Serial_#	Depth	flag	flag 1	flag 2	flag 3	flag 4	flag 6	% flag 3 or 4
				rate-of-change (test 7)						0
	SBE37SMP-ODO-RS232	3715970	125	final flags	504				981	0
				location (test 3)	504				981	0
				range (test 4-5)						0
				spike (test 6)						0
				rate-of-change (test 7)						0
	SBE37SMP-ODO-RS232	3715971	200	final flags	504				983	0
				location (test 3)	504				983	0
				range (test 4-5)						0
				spike (test 6)						0
				rate-of-change (test 7)						0
	SBE37SMP-ODO-RS232	3715972	480	final flags	504				983	0
				location (test 3)	504				983	0
				range (test 4-5)						0
				spike (test 6)						0
				rate-of-change (test 7)						0
SAZ47-20-2018	SBE37-SM	1777	1000	final flags	52250		2154		1322	3.96
				location (test 3)	54404				1322	0
				range (test 4-5)			1			0
				spike (test 6)						0
				rate-of-change (test 7)						0
				sigma-theta0 (test 9)			2153			3.96
	SBE37-SM	3124	2000	final flags	54403		1		1313	0
				location (test 3)	54404				1313	0
				range (test 4-5)						0
				spike (test 6)			1			0
				rate-of-change (test 7)						0
				sigma-theta0 (test 9)						0
	SBE37-SM	2955	4500	final flags	52879		1524		929	2.8
				location (test 3)	54403				929	0
				range (test 4-5)						0
				spike (test 6)			4			0.01
				rate-of-change (test 7)						0
				sigma-theta0 (test 9)			1520			2.79
SOFS-7.5-2018	SBE37SM-RS485	3707408	1	final flags	60639		483		8224	0.79
				location (test 3)	61122				8224	0

Deploy.	Instrument	Serial_#	Depth	flag	flag 1	flag 2	flag 3	flag 4	flag 6	% flag 3 or 4
				range (test 4-5)			6			0.01
				spike (test 6)			2			0
				rate-of-change (test 7)						0
				sigma-theta0 (test 9)			475			0.78
	SBE37SM-RS485	3707409	1	final flags	60425		732		8227	1.2
				location (test 3)	61157				8227	0
				range (test 4-5)			201			0.33
				spike (test 6)			5			0.01
				rate-of-change (test 7)						0
				sigma-theta0 (test 9)			526			0.86
	SBE37SMP-ODO-RS232	3715969	30	final flags	10193				1266	0
				location (test 3)	10193				1266	0
				range (test 4-5)						0
				spike (test 6)						0
				rate-of-change (test 7)						0
	SBE37SMP-ODO-RS232	3715970	125	final flags	10193				1131	0
				location (test 3)	10193				1131	0
				range (test 4-5)						0
				spike (test 6)						0
				rate-of-change (test 7)						0
	SBE37SMP-ODO-RS232	3715971	200	final flags		8181		2012	1131	19.74
				location (test 3)	10193				1131	0
				range (test 4-5)						0
				spike (test 6)						0
				rate-of-change (test 7)						0
				manual (test 10-13)		8181		2012		19.74
	SBE37SMP-ODO-RS232	3715972	480	final flags	10191		2		1131	0.02
				location (test 3)	10193				1131	0
				range (test 4-5)						0
				spike (test 6)			2			0.02
				rate-of-change (test 7)						0
SOFS-8-2019	SBE37SM-RS485	3715728	1	final flags	154123		314		10552	0.2
				location (test 3)	154437				10552	0
				range (test 4-5)			2			0
				spike (test 6)			2			0
				rate-of-change (test 7)						0

Deploy.	Instrument	Serial_#	Depth	flag	flag 1	flag 2	flag 3	flag 4	flag 6	% flag 3 or 4
				sigma-theta0 (test 9)			310			0.2
	SBE37SMP-ODO-RS232	3720126	30	final flags	25753				1984	0
				location (test 3)	25753				1984	0
				range (test 4-5)						0
				spike (test 6)						0
				rate-of-change (test 7)						0
	SBE37SMP-ODO-RS232	3709513	125	final flags	25749		4		1986	0.02
				location (test 3)	25753				1986	0
				range (test 4-5)						0
				spike (test 6)			4			0.02
				rate-of-change (test 7)						0
	SBE37SMP-ODO-RS232	3709514	200	final flags	25753				1997	0
				location (test 3)	25753				1997	0
				range (test 4-5)						0
				spike (test 6)						0
				rate-of-change (test 7)						0
	SBE37SMP-ODO-RS232	3720127	510	final flags	22970				1991	0
				location (test 3)	22970				1991	0
				range (test 4-5)						0
				spike (test 6)						0
				rate-of-change (test 7)						0
SAZ47-21-2019	SBE37	4906	1000	final flags	74950		1880		1423	2.45
				location (test 3)	76830				1423	0
				range (test 4-5)			2			0
				spike (test 6)			1			0
				rate-of-change (test 7)						0
				sigma-theta0 (test 9)			1877			2.44
	SBE37-SM	4907	2000	final flags	76826		4		1412	0.01
				location (test 3)	76830				1412	0
				range (test 4-5)						0
				spike (test 6)						0
				rate-of-change (test 7)						0
				sigma-theta0 (test 9)			4			0.01
SOF5-9-2020	SBE37SM-RS485	3707408	1	final flags	67062		543		50764	0.8
				location (test 3)	67605				50764	0
				range (test 4-5)			3			0

Deploy.	Instrument	Serial_#	Depth	flag	flag 1	flag 2	flag 3	flag 4	flag 6	% flag 3 or 4
				spike (test 6)			2			0
				rate-of-change (test 7)						0
				sigma-theta0 (test 9)			538			0.8
	SBE37SM-RS485	3707409	1	final flags	67210		426		47860	0.63
				location (test 3)	67636				47860	0
				range (test 4-5)			4			0.01
				spike (test 6)			1			0
				rate-of-change (test 7)						0
				sigma-theta0 (test 9)			421			0.62
	SeaFETv1	1001	30	final flags	90197		1319		820	1.44
				location (test 3)	91516				820	0
				range (test 4-5)						0
				spike (test 6)			1			0
				rate-of-change (test 7)			1092			1.19
				sigma-theta0 (test 9)			226			0.25
	SBE37SMP-ODO-RS232	3715970	125	final flags	11270		2		1596	0.02
				location (test 3)	11272				1596	0
				range (test 4-5)						0
				spike (test 6)			2			0.02
				rate-of-change (test 7)						0
	SBE37SMP-ODO-RS232	3714700	200	final flags	11272				5167	0
				location (test 3)	11272				5167	0
				range (test 4-5)						0
				spike (test 6)						0
				rate-of-change (test 7)						0
	SBE37SMP-ODO-RS232	3715971	300	final flags		8688		2584	4178	22.92
				location (test 3)	11272				4178	0
				range (test 4-5)						0
				spike (test 6)						0
				rate-of-change (test 7)						0
				manual (test 10-13)		8688		2584		22.92
	SBE37SMP-ODO-RS232	3715972	510	final flags	11272				5023	0
				location (test 3)	11272				5023	0
				range (test 4-5)						0
				spike (test 6)						0
				rate-of-change (test 7)						0

Deploy.	Instrument	Serial_#	Depth	flag	flag 1	flag 2	flag 3	flag 4	flag 6	% flag 3 or 4
SAZ47-22-2020	SBE37-SM	3124	2000	final flags	33765		5		1566	0.01
				location (test 3)	33770				1566	0
				range (test 4-5)						0
				spike (test 6)			4			0.01
				rate-of-change (test 7)						0
				sigma-theta0 (test 9)			1			0
	SBE37-SM	2955	4500	final flags	32874		896		942	2.65
				location (test 3)	33770				942	0
				range (test 4-5)						0
				spike (test 6)						0
				rate-of-change (test 7)						0
				sigma-theta0 (test 9)				896		2.65

6 Discussion and recommendations

6.1 QARTOD tests that were not performed:

Some of the recommended QARTOD tests were deemed not applicable, specifically Tests 8 and 10. However, their intent, was captured by other approaches. See Section 5.1 for full details.

6.2 Main causes for data flagging

The most common reasons for data concern identified by the QARTOD automated procedures were from the spikes and rate of change tests, and the multi-variate and neighbour visualisations. These were of two broad classes – objects passing through the conductivity cells that led to large errors, and smaller spikes from temperature-conductivity sensor mismatches as identified and flagged from sigma-theta variations. In addition, some sensors exhibited unexplained and relatively long duration (days to weeks to months) departures from reasonable conductivity values

6.3 Did the QC tests work and how good are the data?

Evaluating the success of the tests requires determining whether they correctly identified and flagged only and all *truly* bad data (flag 4) and possibly bad data (flag 3) and retained only and all *truly* good (flag 1) and *probably* good (flag 2) data. This requires some independent understanding of which data is good. We examined this briefly in several ways:

6.3.1 Assessment of offsets between sensors when the upper water column appears to have been well mixed in late winter

These periods are annotated in Appendix C. They suggest that in general, sensor salinity offsets were less than 0.02, during a single mooring deployment. However, offsets between subsequent moorings appear likely to have been larger at least for the very deep (>4000m) SAZ sensor as a result of uncertainties in its pressure measurement (this issue will be detailed in the forthcoming multi-year gridded product report).

6.3.2 Comparison to ship CTD profiles

The visualisations in T-S plots showed that most but not all data that fell outside the bounds of CTD salinity profiles was flagged as bad (Flag 4) or requiring caution (Flag 3), while also revealing that oceanographic variability as observed by the moored sensors exceeds that captured by the sparse CTD sampling (see Figure 13 and Appendix C).

6.3.3 Comparison of pre- and post-deployment sensor calibrations

Changes in calibrations were generally very small but occasionally sufficient to alter sigma-theta values by ~ 0.02 , and thus sufficient to affect visualization of water column stability. Selecting

optimal calibrations on this basis is not appropriate, because it would be biased towards errors that happened to reduce stability and not be recognized for errors that increased stability. Calibration uncertainties are not evaluated further here. They will be re-examined during the production of a gridded common time product, in a forthcoming report.

6.4 Could the QC tests be improved? What are the implications for QA?

In future years, it may be possible for an improved climatology based in part on the SOTS observations to improve the QARTOD test thresholds, and/or to implement more sophisticated filters (e.g. using probability density functions as discussed at Test 7).

A few overall recommendations for Quality Assurance have emerged from the QC:

1. Check all sensor calibrations against the growing record of calibrations to verify that none are unusual and thus potentially suspect.
2. Favour pumped sensors over unpumped sensors (this is especially important for salinity because of associated thermal mass and lag problems – see discussions above)
3. Pair sensors whenever possible, and favour deploying pairs of sensors at a few depths over single sensors at more depths.
4. Compare all sensors against each other before and after deployment, either in the laboratory or via a common deployment on the CTD or both.

6.5 Which data should you use, and what are the associated uncertainties?

We recommend that you use all data with flag values of 2 or less. This is because none of this data has failed a QC test (the only reason that a flag value of 2 has been assigned is that one or more of the tests could not be performed). Users interested in rapid surface events may also wish to consider use of Flag 3 data.

Our comparisons to CTD data and calibrations provide some insights into possible errors that may remain after data flagging, and thus the overall uncertainty of the records. Our selection of thresholds optimizes retention of data unless it can clearly be flagged as bad (Flag 4) or suspect (Flag 3), and thus the thresholds will allow some bad data to pass these filters (as discussed in the Introduction). The Sigma-theta smoothness criterion of 0.02 restricts most errors to $< \sim 0.03$ salinity, unless the error persists long enough to not be recognized as a spike. Therefore, after flagging, an individual or set of data could still be in error by as much as any of the thresholds used for the climatology, spike, and rate of change, T-S, inversion and other tests, which are quite large in surface waters (see the specific Tests for these values). Indeed, these bounds generally greatly exceed the standard deviation of any particular time series, because while large variations may occur in the

ocean they happen rarely. Thus, the standard deviation of a record also provides an estimate of the uncertainty in the quality-controlled data, especially when taken over short sub-sets of the data that avoid the predominantly seasonal changes. Using running median filter to emphasize the typical rather than rare behaviour is thus also a useful approach to obtain a low uncertainty time series, but as described in the Introduction, the oceanographic feature(s) of interest must determine the appropriate smoothing and this is thus left to data users to select to fit their purposes.

7 Accessing the Data

Data are provided on-line from the Australian Ocean Data Network in CF compliant netcdf format files, with one file per deployment. We recommend using all data with flags of 1 or 2.

The URL for data access is:

<https://portal.aodn.org.au/>

Data file structure

```
netcdf IMOS_DWM-SOTS_COPST_20120627_SOFS_FV01_Pulse-9-2012-SBE37SMP-ODO-RS232-03709515-100m_END-20130507_C-20210811 {
dimensions:
    TIME = 15004 ;
variables:
    double TIME(TIME) ;
        TIME:long_name = "time" ;
        TIME:units = "days since 1950-01-01 00:00:00 UTC" ;
        TIME:calendar = "gregorian" ;
        TIME:axis = "T" ;
        TIME:standard_name = "time" ;
        TIME:valid_max = 90000. ;
        TIME:valid_min = 0. ;
    float TEMP(TIME) ;
        TEMP:_FillValue = NaNf ;
        TEMP:comment = "Temperature [ITS-90, deg C]" ;
        TEMP:units = "degrees_Celsius" ;
        TEMP:calibration_SerialNumber = "9515" ;
        TEMP:calibration_CalibrationDate = "10-May-12" ;
        TEMP:calibration_A0 = -7.638603e-05 ;
        TEMP:calibration_A1 = 0.0002987087 ;
        TEMP:calibration_A2 = -3.73475e-06 ;
        TEMP:calibration_A3 = 1.818577e-07 ;
        TEMP:calibration_Slope = 1. ;
        TEMP:calibration_Offset = 0. ;
        TEMP:coordinates = "TIME LATITUDE LONGITUDE NOMINAL_DEPTH" ;
        TEMP:long_name = "sea_water_temperature" ;
        TEMP:standard_name = "sea_water_temperature" ;
        TEMP:valid_max = 40.f ;
        TEMP:valid_min = -2.5f ;
        TEMP:ancillary_variables = "TEMP_quality_control TEMP_quality_control_loc
TEMP_quality_control_gr TEMP_quality_control_spk TEMP_quality_control_roc" ;
    float CNDC(TIME) ;
        CNDC:_FillValue = NaNf ;
        CNDC:comment = "Conductivity [S/m]" ;
        CNDC:units = "S/m" ;
        CNDC:calibration_SerialNumber = "9515" ;
        CNDC:calibration_CalibrationDate = "10-May-12" ;
        CNDC:calibration_UseG_J = 1. ;
        CNDC:calibration_G = -0.9923906 ;
        CNDC:calibration_H = 0.1248248 ;
        CNDC:calibration_I = -0.000376197 ;
        CNDC:calibration_J = 4.100898e-05 ;
        CNDC:calibration_CPcor = -9.57e-08 ;
        CNDC:calibration_CTcor = 3.25e-06 ;
        CNDC:calibration_WBOTC = 3.241293e-07 ;
        CNDC:calibration_Slope = 1. ;
        CNDC:calibration_Offset = 0. ;
        CNDC:coordinates = "TIME LATITUDE LONGITUDE NOMINAL_DEPTH" ;
        CNDC:long_name = "sea_water_electrical_conductivity" ;
        CNDC:standard_name = "sea_water_electrical_conductivity" ;
        CNDC:valid_max = 50000.f ;
        CNDC:valid_min = 0.f ;
        CNDC:ancillary_variables = "CNDC_quality_control CNDC_quality_control_loc" ;
    float PSAL(TIME) ;
        PSAL:_FillValue = NaNf ;
```

```

PSAL:comment = "Salinity, Practical [PSU]" ;
PSAL:units = "1" ;
PSAL:coordinates = "TIME LATITUDE LONGITUDE NOMINAL_DEPTH" ;
PSAL:long_name = "sea_water_practical_salinity" ;
PSAL:standard_name = "sea_water_practical_salinity" ;
PSAL:valid_max = 41.f ;
PSAL:valid_min = 2.f ;
PSAL:ancillary_variables = "PSAL_quality_control PSAL_quality_control_loc
PSAL_quality_control_gr PSAL_quality_control_spk PSAL_quality_control_roc" ;
float PRES(TIME) ;
PRES:_FillValue = NaNf ;
PRES:Comment = "Pressure, Strain Gauge [db]" ;
PRES:units = "dbar" ;
PRES:calibration_SerialNumber = "3537453" ;
PRES:calibration_CalibrationDate = "07-May-12" ;
PRES:calibration_PA0 = 0.09658488 ;
PRES:calibration_PA1 = 0.001611054 ;
PRES:calibration_PA2 = 3.322273e-12 ;
PRES:calibration_PTEMPA0 = -61.83441 ;
PRES:calibration_PTEMPA1 = 0.05481579 ;
PRES:calibration_PTEMPA2 = -7.526737e-07 ;
PRES:calibration_PTCA0 = 525385. ;
PRES:calibration_PTCA1 = 4.731493 ;
PRES:calibration_PTCA2 = -0.09109347 ;
PRES:calibration_PTCB0 = 25.06012 ;
PRES:calibration_PTCB1 = -0.000175 ;
PRES:calibration_PTCB2 = 0. ;
PRES:calibration_Offset = 0. ;
PRES:applied_offset = -10.1353f ;
PRES:coordinates = "TIME LATITUDE LONGITUDE NOMINAL_DEPTH" ;
PRES:long_name = "sea_water_pressure_due_to_sea_water" ;
PRES:standard_name = "sea_water_pressure_due_to_sea_water" ;
PRES:valid_max = 12000.f ;
PRES:valid_min = -15.f ;
PRES:ancillary_variables = "PRES_quality_control PRES_quality_control_loc" ;
float DENSITY(TIME) ;
DENSITY:_FillValue = NaNf ;
DENSITY:comment = "calculated using gsw-python https://teos-10.github.io/GSW-
Python/index.html" ;
DENSITY:units = "kg/m^3" ;
DENSITY:long_name = "sea_water_density" ;
DENSITY:standard_name = "sea_water_density" ;
DENSITY:valid_max = 1100.f ;
DENSITY:valid_min = 1000.f ;
DENSITY:ancillary_variables = "DENSITY_quality_control DENSITY_quality_control_loc"
;

float DOX2(TIME) ;
DOX2:_FillValue = NaNf ;
DOX2:comment = "Oxygen, SBE 63 [umol/kg]" ;
DOX2:units = "umol/kg" ;
DOX2:calibration_SerialNumber = "0146" ;
DOX2:calibration_CalibrationDate = "16-May-12" ;
DOX2:calibration_A0 = 1.0513 ;
DOX2:calibration_A1 = -0.0015 ;
DOX2:calibration_A2 = 0.3902 ;
DOX2:calibration_B0 = -0.24434 ;
DOX2:calibration_B1 = 1.6217 ;
DOX2:calibration_C0 = 0.1066 ;
DOX2:calibration_C1 = 0.004597001 ;
DOX2:calibration_C2 = 6.332e-05 ;
DOX2:calibration_TA0 = 0.000667473 ;
DOX2:calibration_TA1 = 0.0002487965 ;
DOX2:calibration_TA2 = 7.2637e-07 ;
DOX2:calibration_TA3 = 9.623948e-08 ;
DOX2:calibration_pcor = 0.011 ;
DOX2:calibration_Slope = 1. ;
DOX2:calibration_Offset = 0. ;
DOX2:ancillary_variables = "DOX2_quality_control DOX2_quality_control_loc" ;
float OXSOL(TIME) ;
OXSOL:_FillValue = NaNf ;
OXSOL:comment = "Oxygen Saturation, Garcia & Gordon [umol/kg]" ;
OXSOL:units = "umol/kg" ;
OXSOL:ancillary_variables = "OXSOL_quality_control OXSOL_quality_control_loc" ;
float DOX_TEMP(TIME) ;
DOX_TEMP:_FillValue = NaNf ;
DOX_TEMP:comment = "Oxygen Temperature, SBE 63 [ITS-90, deg C]" ;
DOX_TEMP:units = "degrees_Celsius" ;

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        DOX_TEMP:ancillary_variables = "DOX_TEMP_quality_control
DOX_TEMP_quality_control_loc" ;
    double LATITUDE ;
        LATITUDE:axis = "Y" ;
        LATITUDE:long_name = "latitude" ;
        LATITUDE:reference_datum = "WGS84 geographic coordinate system" ;
        LATITUDE:standard_name = "latitude" ;
        LATITUDE:units = "degrees_north" ;
        LATITUDE:valid_max = 90. ;
        LATITUDE:valid_min = -90. ;
    double LONGITUDE ;
        LONGITUDE:axis = "X" ;
        LONGITUDE:long_name = "longitude" ;
        LONGITUDE:reference_datum = "WGS84 geographic coordinate system" ;
        LONGITUDE:standard_name = "longitude" ;
        LONGITUDE:units = "degrees_east" ;
        LONGITUDE:valid_max = 180. ;
        LONGITUDE:valid_min = -180. ;
    double NOMINAL_DEPTH ;
        NOMINAL_DEPTH:axis = "Z" ;
        NOMINAL_DEPTH:long_name = "nominal depth" ;
        NOMINAL_DEPTH:positive = "down" ;
        NOMINAL_DEPTH:reference_datum = "sea surface" ;
        NOMINAL_DEPTH:standard_name = "depth" ;
        NOMINAL_DEPTH:units = "m" ;
        NOMINAL_DEPTH:valid_max = 12000. ;
        NOMINAL_DEPTH:valid_min = -5. ;
    float SIGMA_T0(TIME) ;
        SIGMA_T0: FillValue = NaNf ;
        SIGMA_T0:units = "kg/m^3" ;
        SIGMA_T0:long_name = "sea water sigma_theta" ;
        SIGMA_T0:standard_name = "sea_water_sigma_theta" ;
        SIGMA_T0:reference_pressure = "0 dbar" ;
        SIGMA_T0:valid_max = 100.f ;
        SIGMA_T0:valid_min = 0.f ;
        SIGMA_T0:comment = "calculated using gsw-python https://teos-10.github.io/GSW-
Python/index.html" ;
        SIGMA_T0:ancillary_variables = "SIGMA_T0_quality_control
SIGMA_T0_quality_control_loc" ;
    byte TEMP_quality_control(TIME) ;
        TEMP_quality_control: FillValue = 99b ;
        TEMP_quality_control:long_name = "quality flag for sea water temperature" ;
        TEMP_quality_control:standard_name = "sea_water_temperature_status_flag" ;
        TEMP_quality_control:quality_control_conventions = "IMOS standard flags" ;
        TEMP_quality_control:flag_values = 0b, 1b, 2b, 3b, 4b, 6b, 7b, 9b ;
        TEMP_quality_control:flag_meanings = "unknown good_data probably_good_data
probably_bad_data bad_data not_deployed interpolated missing_value" ;
        TEMP_quality_control:comment = "maximum of all flags" ;
    byte CNDC_quality_control(TIME) ;
        CNDC_quality_control: FillValue = 99b ;
        CNDC_quality_control:long_name = "quality flag for
sea_water_electrical_conductivity" ;
        CNDC_quality_control:standard_name = "sea_water_electrical_conductivity_status_flag"
;
        CNDC_quality_control:quality_control_conventions = "IMOS standard flags" ;
        CNDC_quality_control:flag_values = 0b, 1b, 2b, 3b, 4b, 6b, 7b, 9b ;
        CNDC_quality_control:flag_meanings = "unknown good_data probably_good_data
probably_bad_data bad_data not_deployed interpolated missing_value" ;
        CNDC_quality_control:comment = "maximum of all flags" ;
    byte PSAL_quality_control(TIME) ;
        PSAL_quality_control: FillValue = 99b ;
        PSAL_quality_control:long_name = "quality flag for sea water practical salinity" ;
        PSAL_quality_control:standard_name = "sea_water_practical_salinity_status_flag" ;
        PSAL_quality_control:quality_control_conventions = "IMOS standard flags" ;
        PSAL_quality_control:flag_values = 0b, 1b, 2b, 3b, 4b, 6b, 7b, 9b ;
        PSAL_quality_control:flag_meanings = "unknown good_data probably_good_data
probably_bad_data bad_data not_deployed interpolated missing_value" ;
        PSAL_quality_control:comment = "maximum of all flags" ;
    byte PRES_quality_control(TIME) ;
        PRES_quality_control: FillValue = 99b ;
        PRES_quality_control:long_name = "quality flag for
sea_water_pressure_due_to_sea_water" ;
        PRES_quality_control:standard_name = "sea_water_pressure_due_to_sea_water
status_flag" ;
        PRES_quality_control:quality_control_conventions = "IMOS standard flags" ;
        PRES_quality_control:flag_values = 0b, 1b, 2b, 3b, 4b, 6b, 7b, 9b ;
        PRES_quality_control:flag_meanings = "unknown good_data probably_good_data
probably_bad_data bad_data not_deployed interpolated missing_value" ;

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PRES_quality_control:comment = "maximum of all flags" ;
byte DENSITY_quality_control(TIME) ;
    DENSITY_quality_control: FillValue = 99b ;
    DENSITY_quality_control:long_name = "quality flag for sea_water_density" ;
    DENSITY_quality_control:standard_name = "sea_water_density_status_flag" ;
    DENSITY_quality_control:quality_control_conventions = "IMOS standard flags" ;
    DENSITY_quality_control:flag_values = 0b, 1b, 2b, 3b, 4b, 6b, 7b, 9b ;
    DENSITY_quality_control:flag_meanings = "unknown good_data probably_good_data
probably_bad_data bad_data not_deployed interpolated missing_value" ;
    DENSITY_quality_control:comment = "maximum of all flags" ;
byte DOX2_quality_control(TIME) ;
    DOX2_quality_control: FillValue = 99b ;
    DOX2_quality_control:quality_control_conventions = "IMOS standard flags" ;
    DOX2_quality_control:flag_values = 0b, 1b, 2b, 3b, 4b, 6b, 7b, 9b ;
    DOX2_quality_control:flag_meanings = "unknown good_data probably_good_data
probably_bad_data bad_data not_deployed interpolated missing_value" ;
    DOX2_quality_control:comment = "maximum of all flags" ;
byte OXSOL_quality_control(TIME) ;
    OXSOL_quality_control: FillValue = 99b ;
    OXSOL_quality_control:quality_control_conventions = "IMOS standard flags" ;
    OXSOL_quality_control:flag_values = 0b, 1b, 2b, 3b, 4b, 6b, 7b, 9b ;
    OXSOL_quality_control:flag_meanings = "unknown good_data probably_good_data
probably_bad_data bad_data not_deployed interpolated missing_value" ;
    OXSOL_quality_control:comment = "maximum of all flags" ;
byte DOX_TEMP_quality_control(TIME) ;
    DOX_TEMP_quality_control: FillValue = 99b ;
    DOX_TEMP_quality_control:quality_control_conventions = "IMOS standard flags" ;
    DOX_TEMP_quality_control:flag_values = 0b, 1b, 2b, 3b, 4b, 6b, 7b, 9b ;
    DOX_TEMP_quality_control:flag_meanings = "unknown good_data probably_good_data
probably_bad_data bad_data not_deployed interpolated missing_value" ;
    DOX_TEMP_quality_control:comment = "maximum of all flags" ;
byte SIGMA_T0_quality_control(TIME) ;
    SIGMA_T0_quality_control: FillValue = 99b ;
    SIGMA_T0_quality_control:long_name = "quality flag for sea_water_sigma_theta" ;
    SIGMA_T0_quality_control:standard_name = "sea_water_sigma_theta_status_flag" ;
    SIGMA_T0_quality_control:quality_control_conventions = "IMOS standard flags" ;
    SIGMA_T0_quality_control:flag_values = 0b, 1b, 2b, 3b, 4b, 6b, 7b, 9b ;
    SIGMA_T0_quality_control:flag_meanings = "unknown good_data probably_good_data
probably_bad_data bad_data not_deployed interpolated missing_value" ;
    SIGMA_T0_quality_control:comment = "maximum of all flags" ;
byte TEMP_quality_control_loc(TIME) ;
    TEMP_quality_control_loc: FillValue = 99b ;
    TEMP_quality_control_loc:long_name = "in/out of water flag for
sea_water_temperature" ;
    TEMP_quality_control_loc:units = "1" ;
    TEMP_quality_control_loc:comment = "data flagged not deployed (6) when out of water"
;
byte CNDC_quality_control_loc(TIME) ;
    CNDC_quality_control_loc: FillValue = 99b ;
    CNDC_quality_control_loc:long_name = "in/out of water flag for
sea_water_electrical_conductivity" ;
    CNDC_quality_control_loc:units = "1" ;
    CNDC_quality_control_loc:comment = "data flagged not deployed (6) when out of water"
;
byte PSAL_quality_control_loc(TIME) ;
    PSAL_quality_control_loc: FillValue = 99b ;
    PSAL_quality_control_loc:long_name = "in/out of water flag for
sea_water_practical_salinity" ;
    PSAL_quality_control_loc:units = "1" ;
    PSAL_quality_control_loc:comment = "data flagged not deployed (6) when out of water"
;
byte PRES_quality_control_loc(TIME) ;
    PRES_quality_control_loc: FillValue = 99b ;
    PRES_quality_control_loc:long_name = "in/out of water flag for
sea_water_pressure_due_to_sea_water" ;
    PRES_quality_control_loc:units = "1" ;
    PRES_quality_control_loc:comment = "data flagged not deployed (6) when out of water"
;
byte DENSITY_quality_control_loc(TIME) ;
    DENSITY_quality_control_loc: FillValue = 99b ;
    DENSITY_quality_control_loc:long_name = "in/out of water flag for sea_water_density"
;
    DENSITY_quality_control_loc:units = "1" ;
    DENSITY_quality_control_loc:comment = "data flagged not deployed (6) when out of
water" ;
byte DOX2_quality_control_loc(TIME) ;
    DOX2_quality_control_loc: FillValue = 99b ;
    DOX2_quality_control_loc:units = "1" ;

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DOX2_quality_control_loc:comment = "data flagged not deployed (6) when out of water"
;
byte OXSOL_quality_control_loc(TIME) ;
OXSOL_quality_control_loc: FillValue = 99b ;
OXSOL_quality_control_loc:units = "1" ;
OXSOL_quality_control_loc:comment = "data flagged not deployed (6) when out of
water" ;
byte DOX_TEMP_quality_control_loc(TIME) ;
DOX_TEMP_quality_control_loc: FillValue = 99b ;
DOX_TEMP_quality_control_loc:units = "1" ;
DOX_TEMP_quality_control_loc:comment = "data flagged not deployed (6) when out of
water" ;
byte SIGMA_T0_quality_control_loc(TIME) ;
SIGMA_T0_quality_control_loc: FillValue = 99b ;
SIGMA_T0_quality_control_loc:long_name = "in/out of water flag for
sea_water_sigma_theta" ;
SIGMA_T0_quality_control_loc:units = "1" ;
SIGMA_T0_quality_control_loc:comment = "data flagged not deployed (6) when out of
water" ;
byte TEMP_quality_control_gr(TIME) ;
TEMP_quality_control_gr: FillValue = 99b ;
TEMP_quality_control_gr:long_name = "global_range flag for sea_water_temperature" ;
TEMP_quality_control_gr:units = "1" ;
TEMP_quality_control_gr:comment = "Test 4. gross range test" ;
byte TEMP_quality_control_spk(TIME) ;
TEMP_quality_control_spk: FillValue = 99b ;
TEMP_quality_control_spk:long_name = "spike flag for sea_water_temperature" ;
TEMP_quality_control_spk:units = "1" ;
TEMP_quality_control_spk:comment = "Test 6. spike test" ;
byte TEMP_quality_control_roc(TIME) ;
TEMP_quality_control_roc: FillValue = 99b ;
TEMP_quality_control_roc:long_name = "rate_of_change flag for sea_water_temperature"
;
TEMP_quality_control_roc:units = "1" ;
TEMP_quality_control_roc:comment = "Test 7. rate of change test" ;
byte PSAL_quality_control_gr(TIME) ;
PSAL_quality_control_gr: FillValue = 99b ;
PSAL_quality_control_gr:long_name = "global_range flag for
sea_water_practical_salinity" ;
PSAL_quality_control_gr:units = "1" ;
PSAL_quality_control_gr:comment = "Test 4. gross range test" ;
byte PSAL_quality_control_spk(TIME) ;
PSAL_quality_control_spk: FillValue = 99b ;
PSAL_quality_control_spk:long_name = "spike flag for sea_water_practical_salinity" ;
PSAL_quality_control_spk:units = "1" ;
PSAL_quality_control_spk:comment = "Test 6. spike test" ;
byte PSAL_quality_control_roc(TIME) ;
PSAL_quality_control_roc: FillValue = 99b ;
PSAL_quality_control_roc:long_name = "rate_of_change flag for
sea_water_practical_salinity" ;
PSAL_quality_control_roc:units = "1" ;
PSAL_quality_control_roc:comment = "Test 7. rate of change test" ;

// global attributes:
:abstract = "Oceanographic and meteorological data from the Southern Ocean Time
Series observatory in the Southern Ocean southwest of Tasmania" ;
:acknowledgement = "Any users of IMOS data are required to clearly acknowledge the
source of the material derived from IMOS in the format: \"Data was sourced from the Integrated
Marine Observing System (IMOS) - IMOS is a national collaborative research infrastructure, supported
by the Australian Government.\" If relevant, also credit other organisations involved in collection
of this particular datastream (as listed in 'credit' in the metadata record).\" ;
:author = "Jansen, Peter" ;
:author_email = "peter.jansen@csiro.au" ;
:citation = "The citation in a list of references is: 'IMOS [year-of-data-
download], [Title], [data-access-URL], accessed [date-of-access]\'." ;
:comment = "Geospatial vertical min/max information has been filled using the
NOMINAL_DEPTH." ;
:Conventions = "CF-1.6,IMOS-1.4" ;
:data_centre = "Australian Ocean Data Network (AODN)" ;
:data_centre_email = "info@aodn.org.au" ;
:date_created = "2021-08-11T07:24:55Z" ;
:deployment_code = "Pulse-9-2012" ;
:disclaimer = "Data, products and services from IMOS are provided \"as is\" without
any warranty as to fitness for a particular purpose." ;
:featureType = "timeSeries" ;
:file_version_quality_control = "Raw data is defined as unprocessed data and data
products that have not undergone quality control. The data may be in engineering physical units,

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time and location details can be in relative units and values can be pre-calibration measurements."
;
:geospatial_lat_max = -46.84932 ;
:geospatial_lat_min = -46.84932 ;
:geospatial_lat_units = "degrees_north" ;
:geospatial_lon_max = 142.39855 ;
:geospatial_lon_min = 142.39855 ;
:geospatial_lon_units = "degrees_east" ;
:geospatial_vertical_max = 100. ;
:geospatial_vertical_min = 100. ;
:geospatial_vertical_positive = "down" ;
:institution = "DWM-SOTS" ;
:institution_references = "http://www.imos.org.au/aodn.html" ;
:instrument = "Sea-Bird Electronics ; SBE37SMP-ODO-RS232" ;
:instrument_model = "SBE37SMP-ODO-RS232" ;
:instrument_nominal_depth = 100. ;
:instrument_serial_number = "03709515" ;
:keywords_vocabulary = "IMOS parameter names. See https://github.com/aodn/imos-
toolbox/blob/master/IMOS/imosParameters.txt" ;
:license = "http://creativecommons.org/licenses/by/4.0/" ;
:naming_authority = "IMOS" ;
:platform_code = "SOFS" ;
:principal_investigator = "Trull, Tom" ;
:principal_investigator_email = "tom.trull@csiro.au" ;
:project = "Integrated Marine Observing System (IMOS)" ;
:site_code = "SOTS" ;
:site_nominal_depth = 4300. ;
:standard_name_vocabulary = "NetCDF Climate and Forecast (CF) Metadata Convention
Standard Name Table 67" ;
:time_coverage_end = "2013-05-07T22:30:24Z" ;
:time_coverage_start = "2012-06-27T05:28:40Z" ;
:time_deployment_end = "2013-05-05T01:15:00Z" ;
:time_deployment_start = "2012-07-17T07:00:00Z" ;
:title = "Oceanographic mooring data deployment of SOFS at latitude -46.8 longitude
142.4 depth 100 (m) instrument Sea-Bird Electronics ; SBE37SMP-ODO-RS232 serial 03709515" ;
:voyage_deployment =
"http://www.cmar.csiro.au/data/trawler/survey_details.cfm?survey=SS2012_V03" ;
:voyage_recovery =
"http://www.cmar.csiro.au/data/trawler/survey_details.cfm?survey=SS2013_V03" ;
:file_version = "Level 1 - Quality Controlled Data" ;
:history = "2020-07-15 created from file SBE37SMP-ODO-
RS232_03709515_2013_05_07.cnv\n2020-07-15 : attributes added from file(s) [metadata/pulse-saz-sofs-
flux.metadata.csv, metadata/imos.metadata.csv, metadata/sots.metadata.csv,
metadata/sofs.metadata.csv, metadata/variable.metadata.csv]\n2021-07-30 : added DENSITY and SIGMA-
THETA0 from TEMP, PSAL, PRES, LAT, LON\n2021-08-11 : quality_control variables added.\n2021-08-11 :
in/out marked 999\n2021-08-11 TEMP global range min = -2 max = 30 marked 0.0\n2021-08-11 TEMP global
range min = 5 max = 16 marked 0.0\n2021-08-11 TEMP spike height = 2 marked 3\n2021-08-11 TEMP max
rate = 80 marked 0\n2021-08-11 PSAL global range min = 2 max = 41 marked 0.0\n2021-08-11 PSAL global
range min = 34 max = 35.5 marked 0.0\n2021-08-11 PSAL spike height = 0.4 marked 3\n2021-08-11 PSAL
max rate = 30 marked 0" ;
:references = "http://www.imos.org.au; Jansen P, Weeding B, Shadwick EH and Trull TW
(2020). Southern Ocean Time Series (SOTS) Quality Assessment and Control Report Temperature Records
Version 1.0. CSIRO, Australia. DOI: 10.26198/gfgr-fq47 (https://doi.org/10.26198/gfgr-fq47)" ;

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References

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Appendix A Python files used for processing

Please refer to the following link for access to the Python files involved in performing the QC tests described in this report:

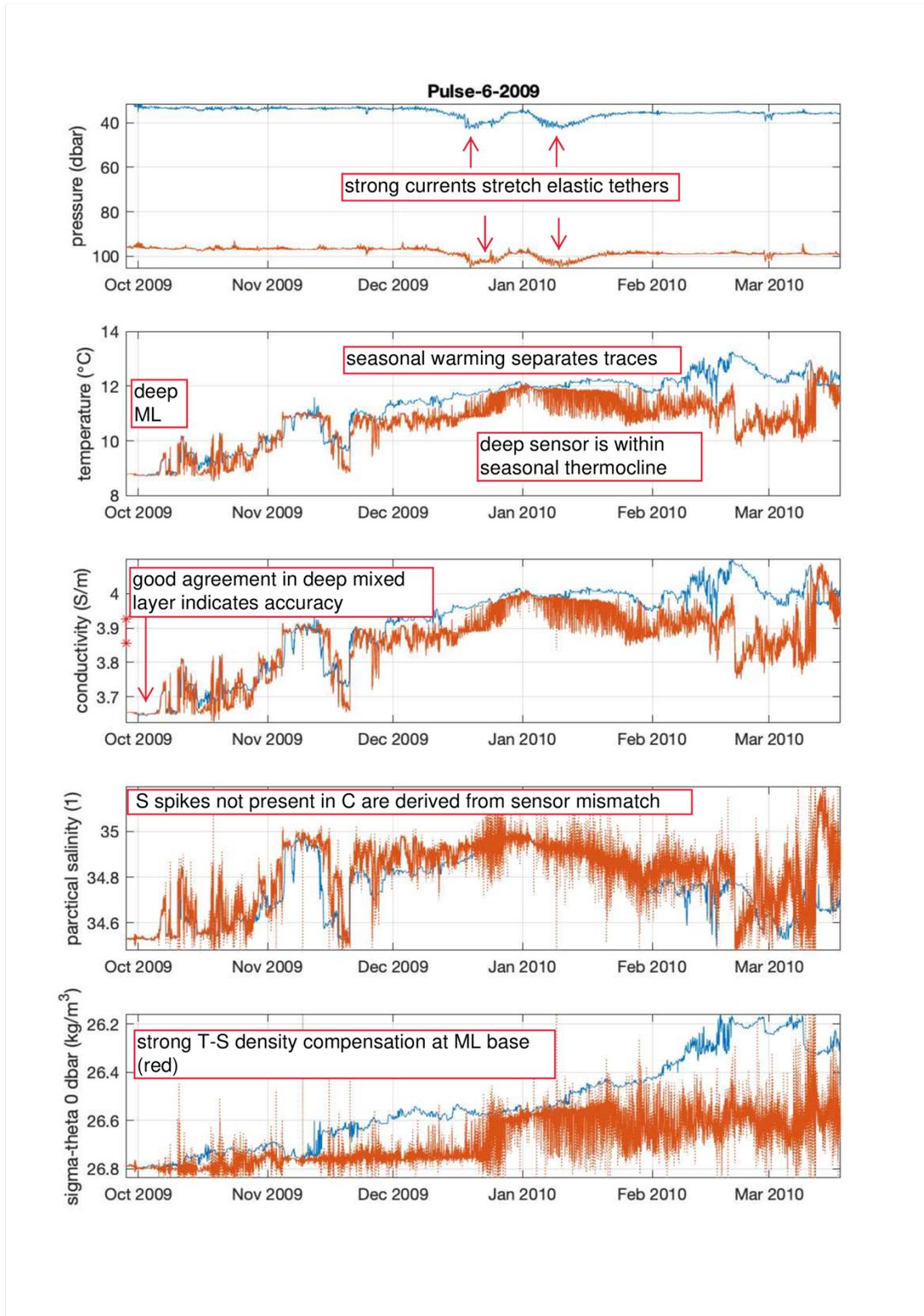
<https://github.com/petejan/imos-tools>

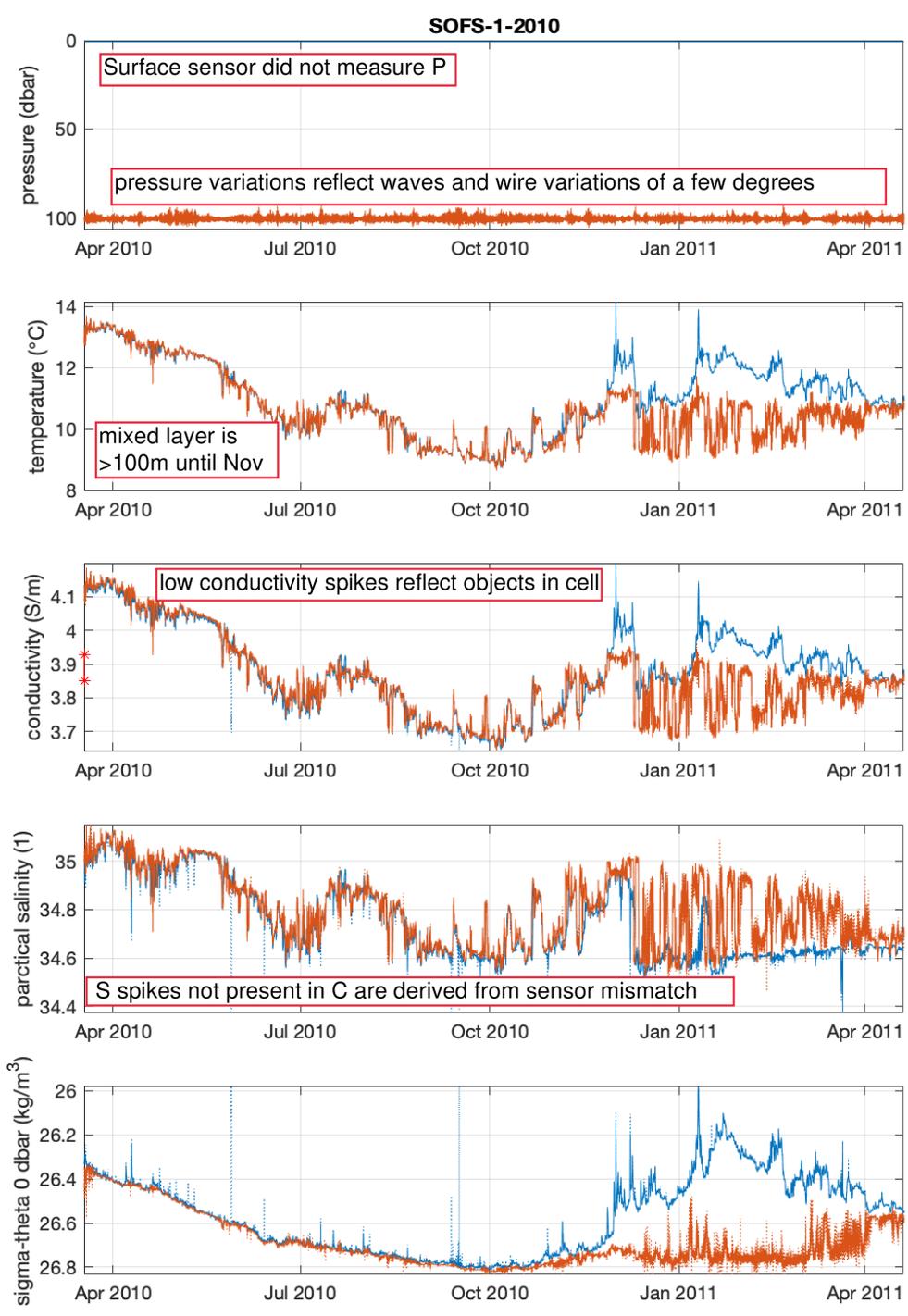
Appendix B Sensor Calibration Sheets

Calibration sheets for all T and S sensors deployed at the SOTS site are available at:

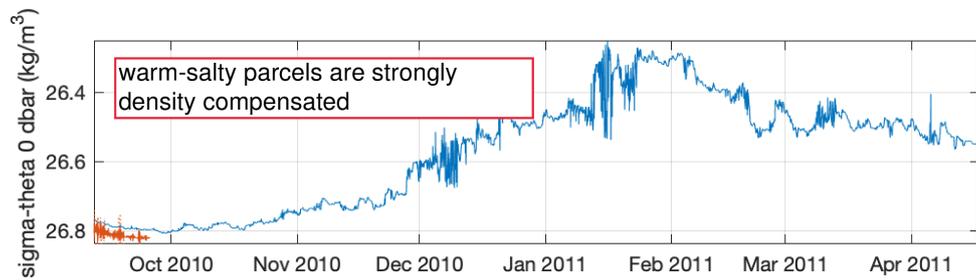
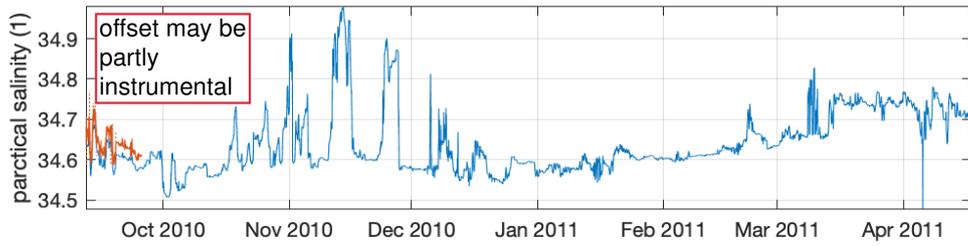
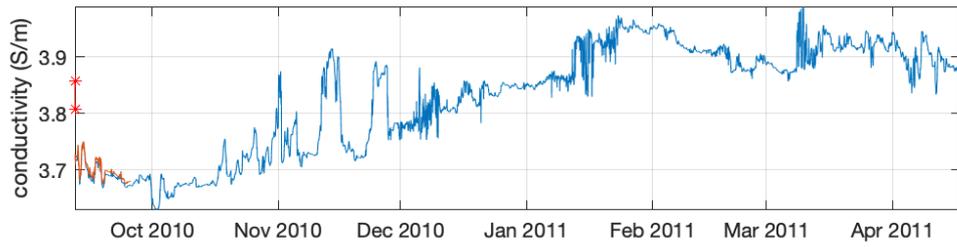
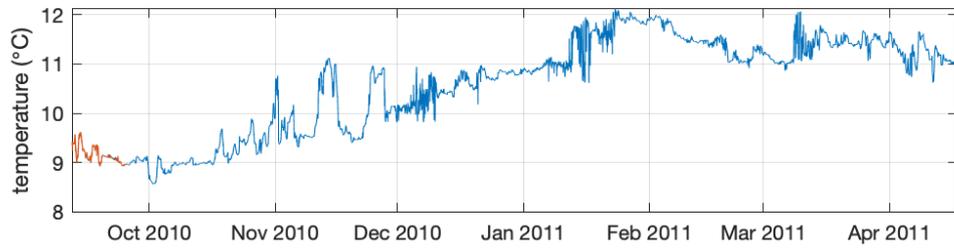
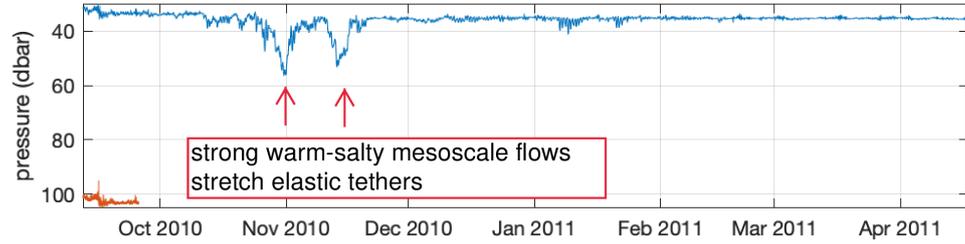
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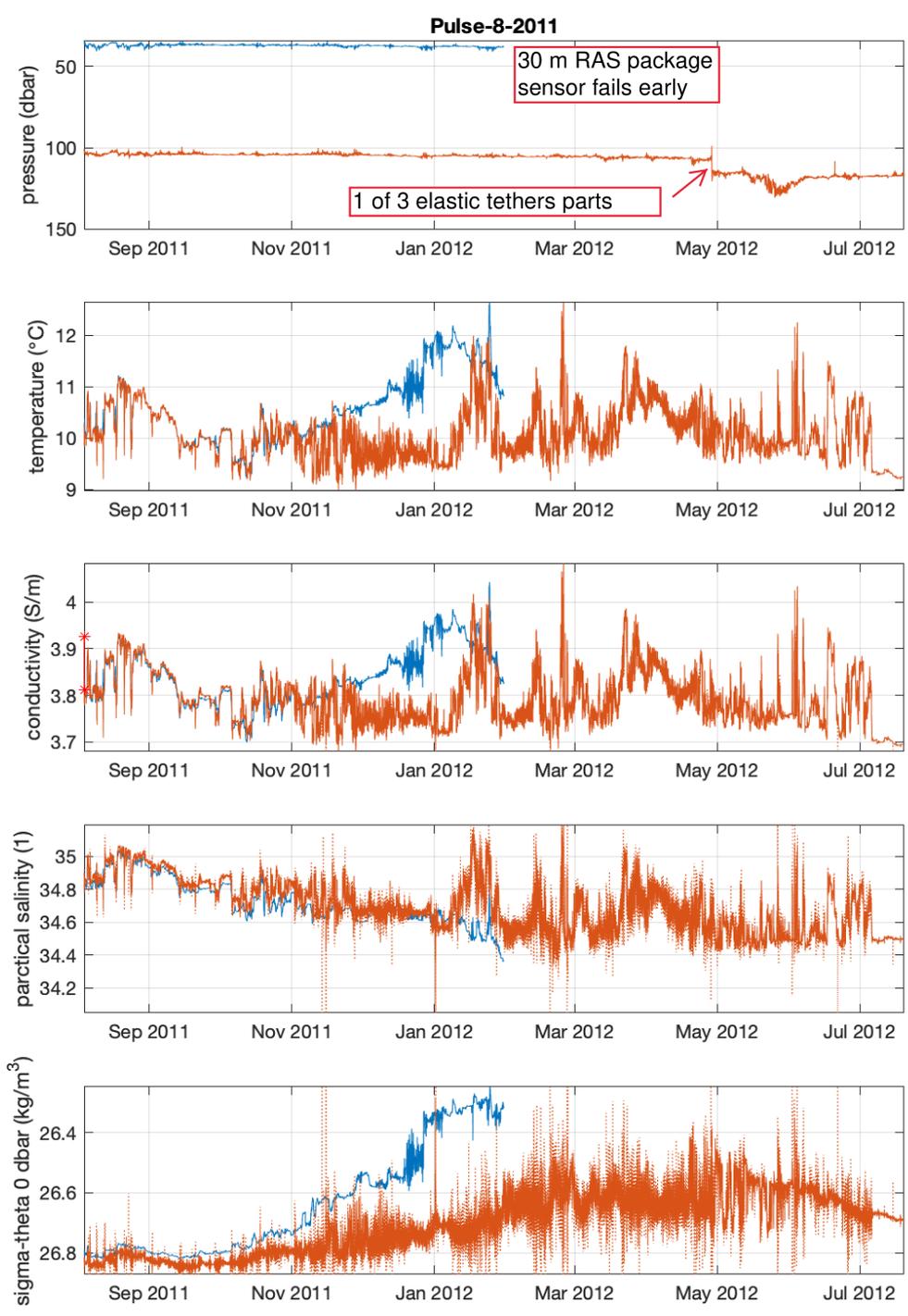
Appendix C Annotated QC plots for all deployments

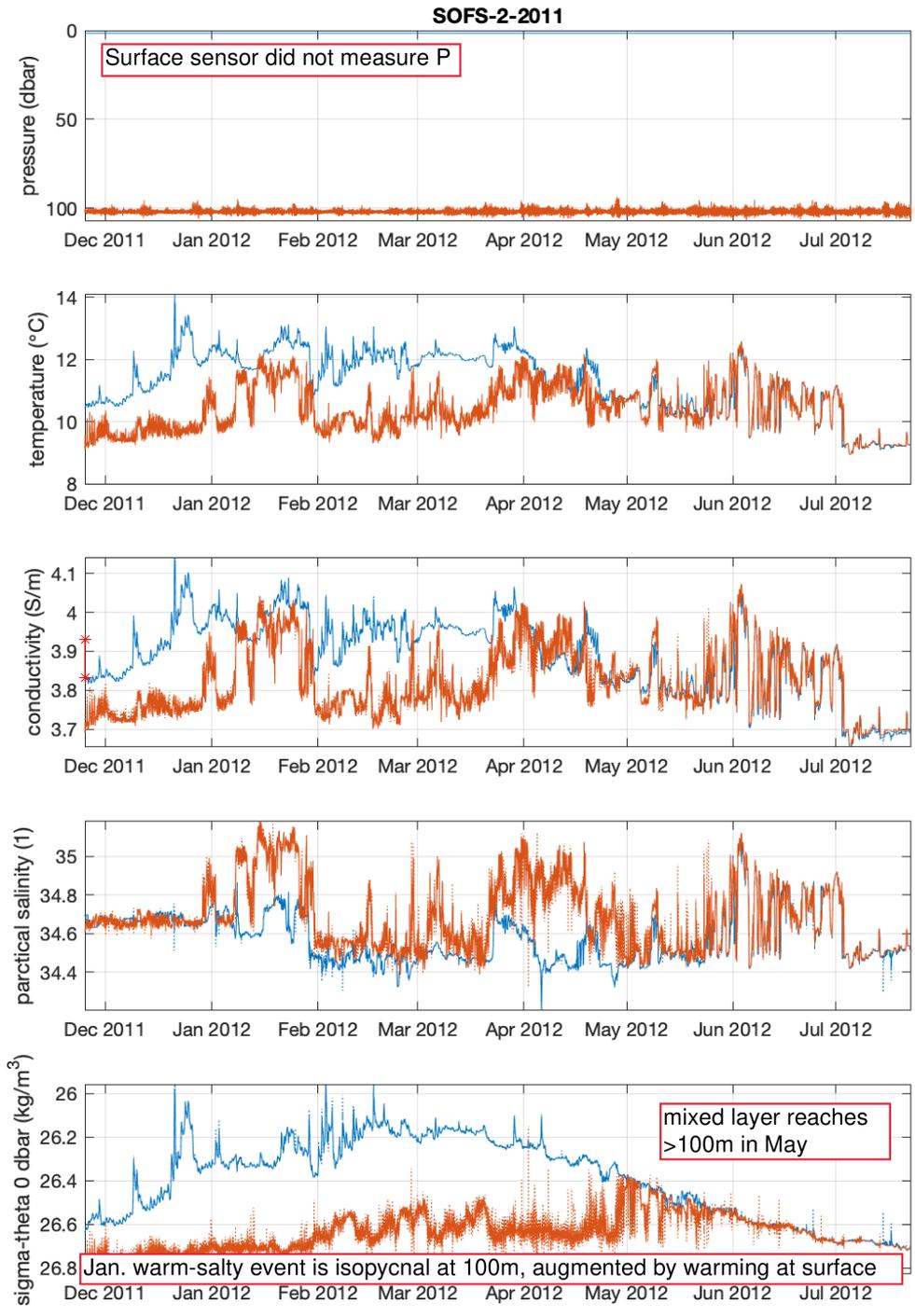


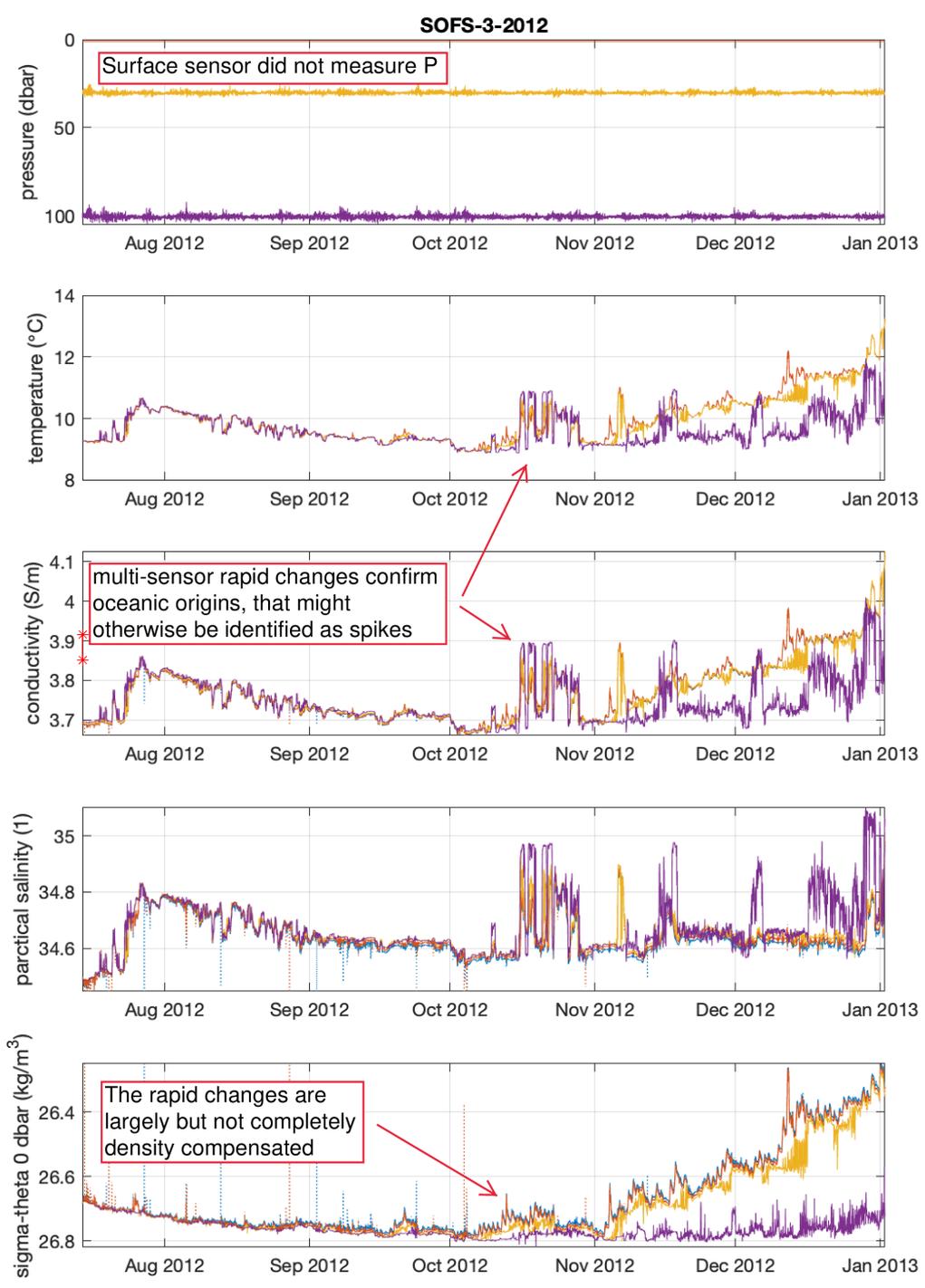


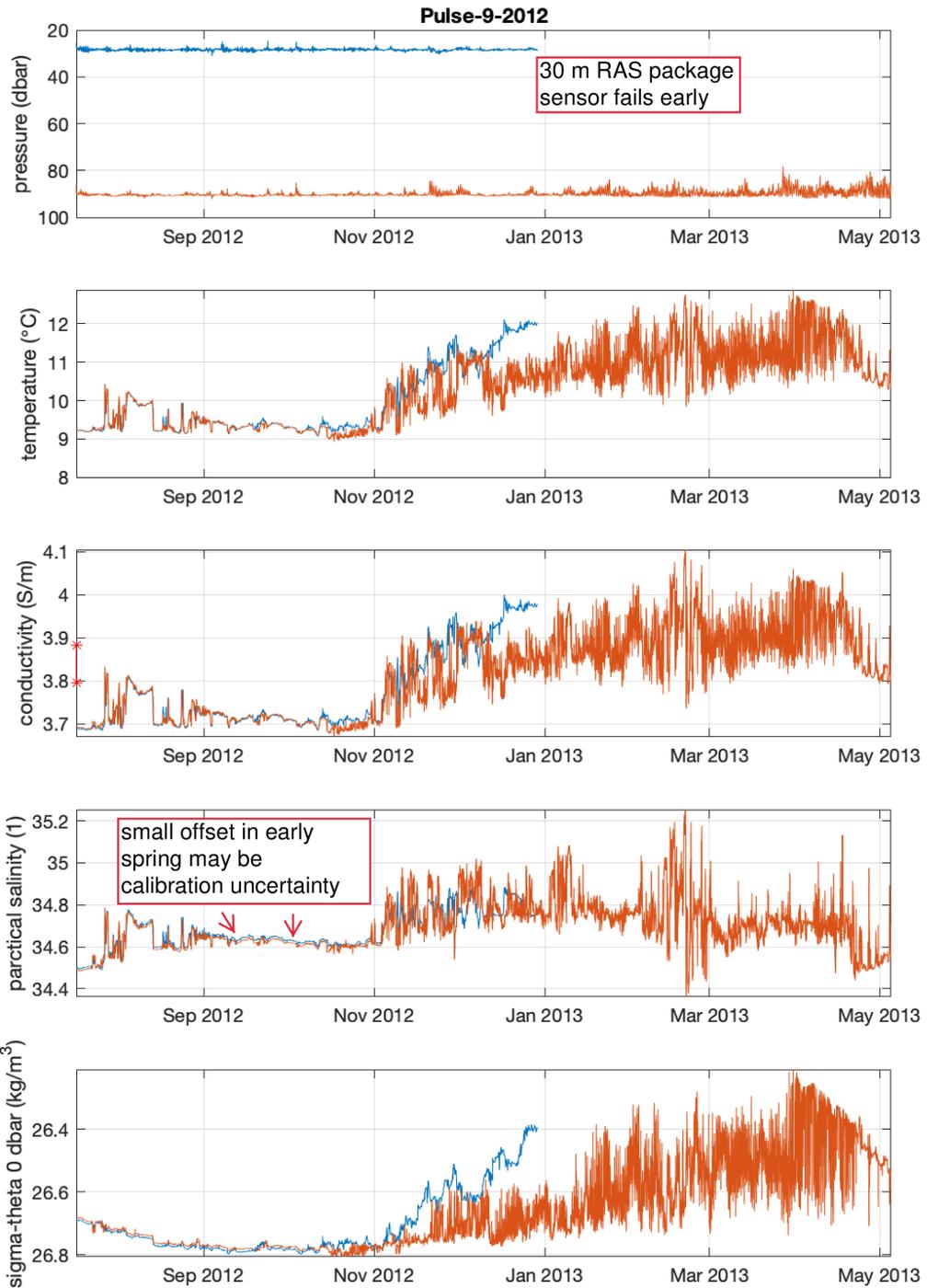
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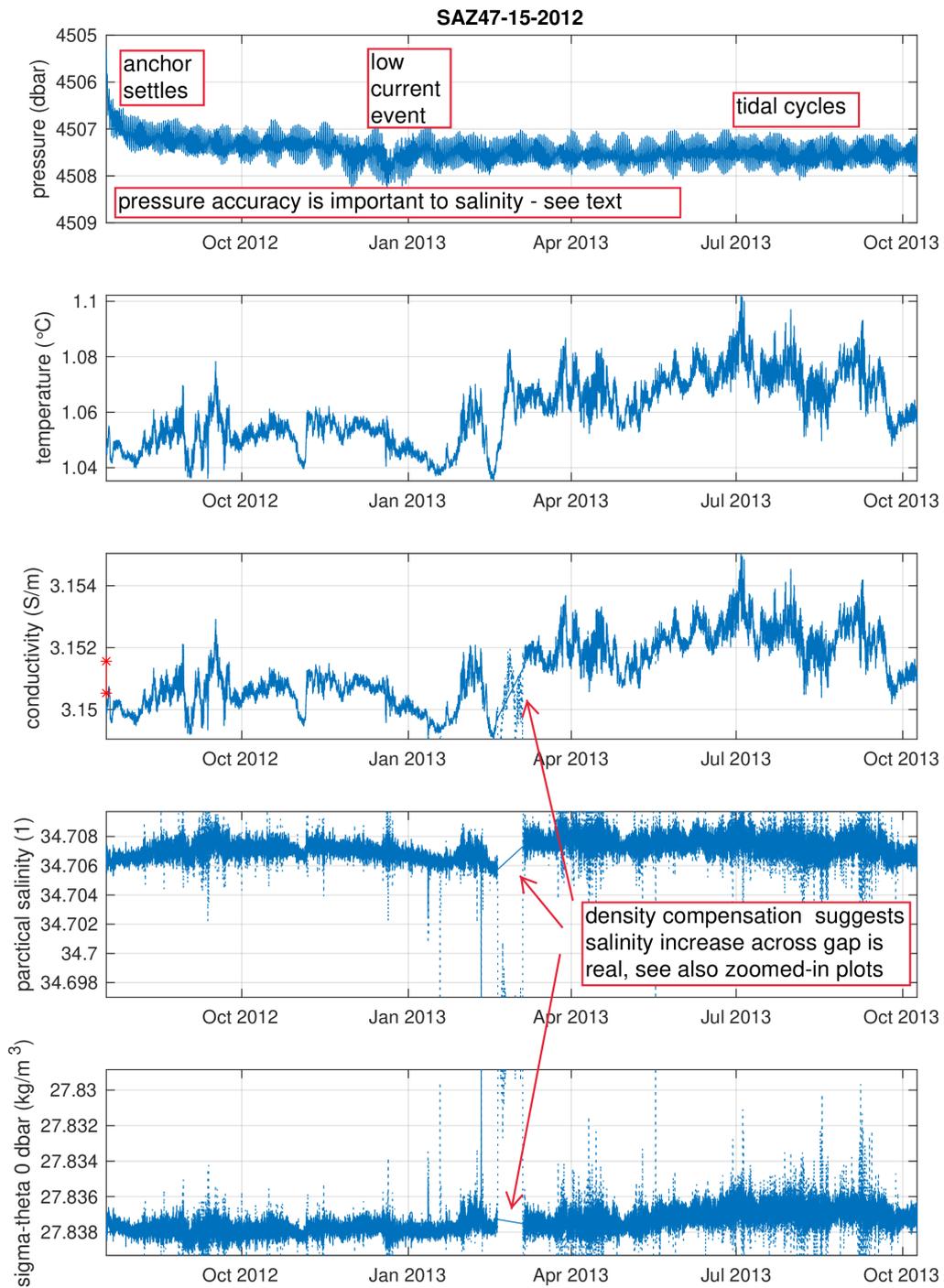


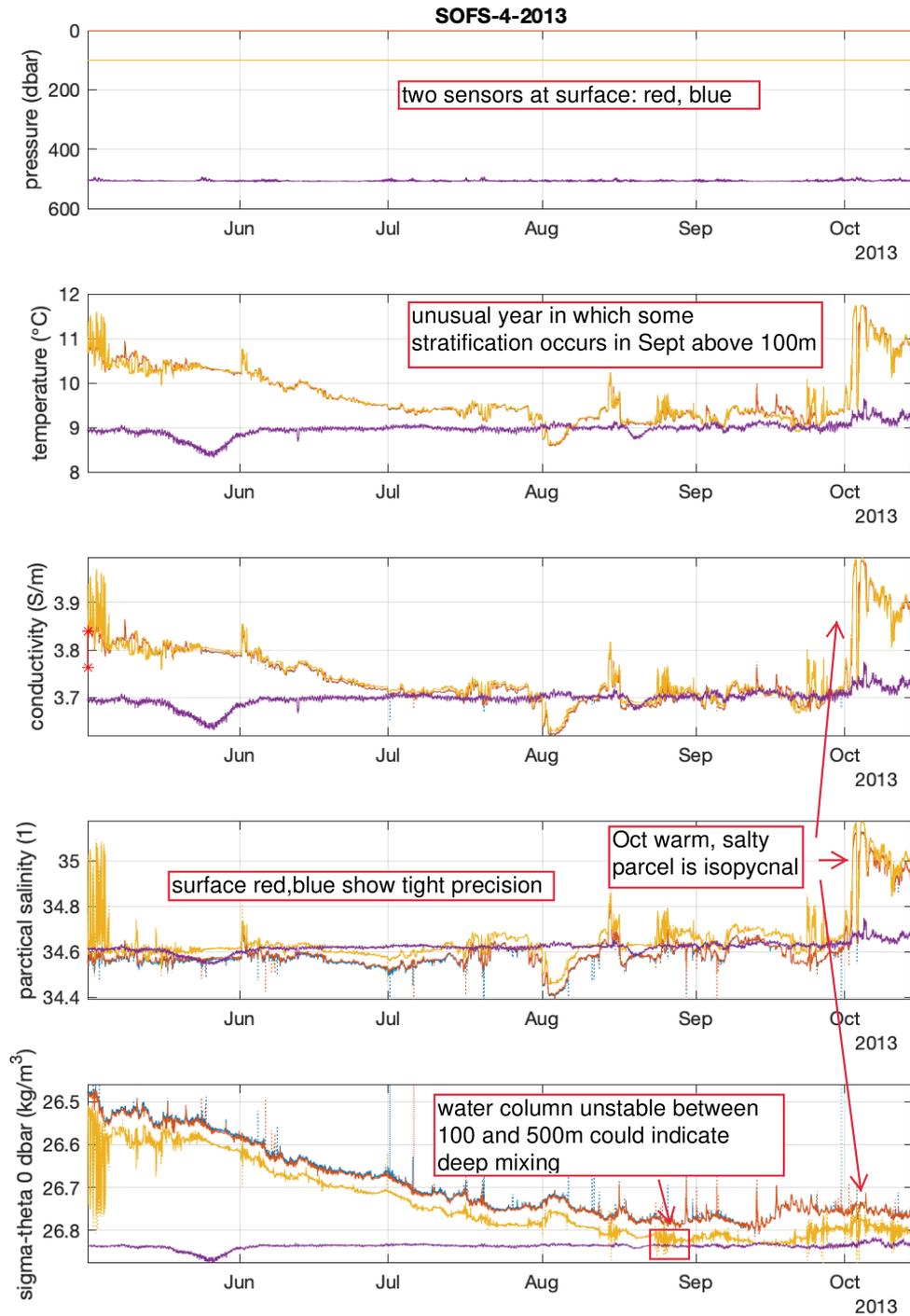




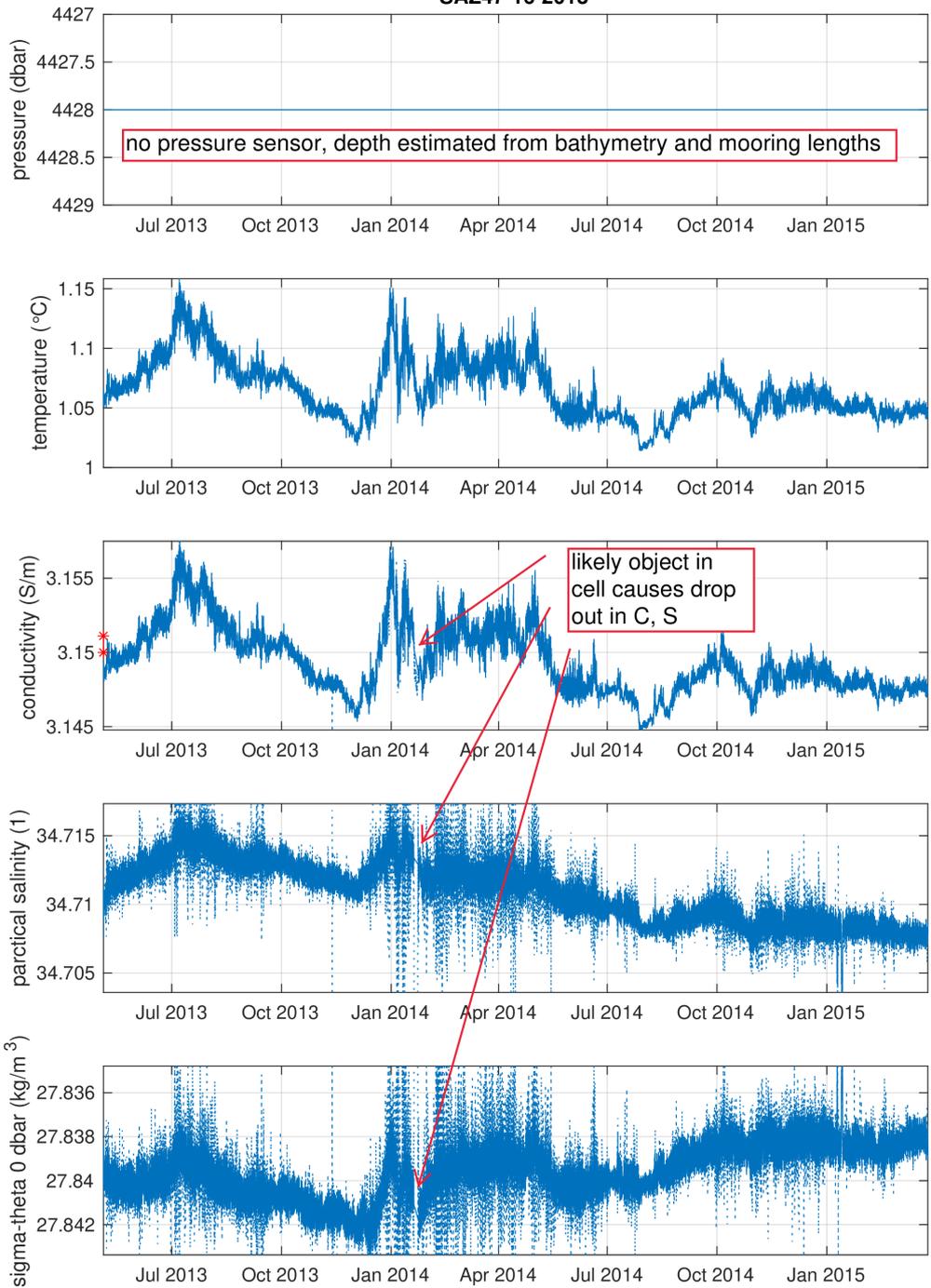


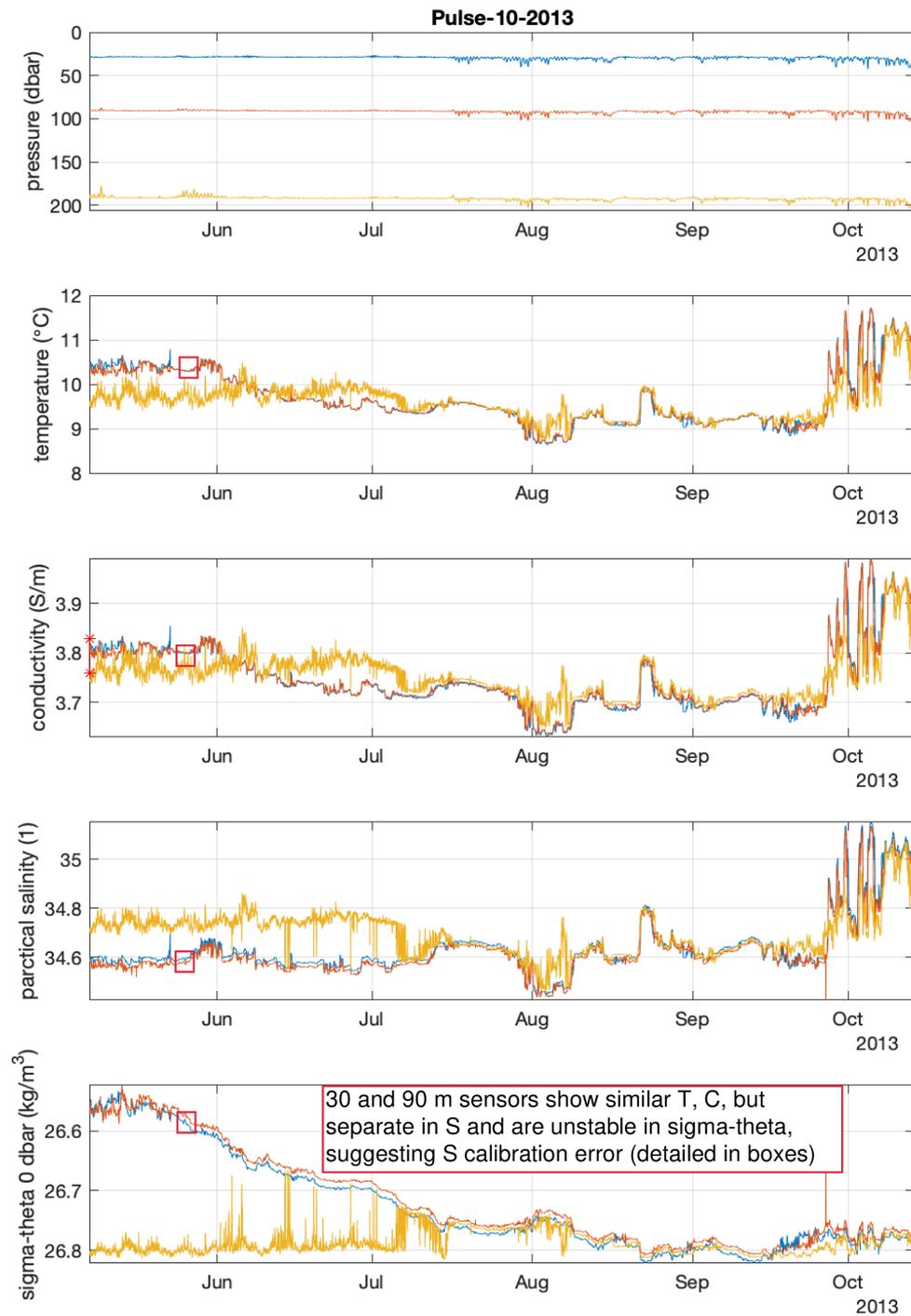


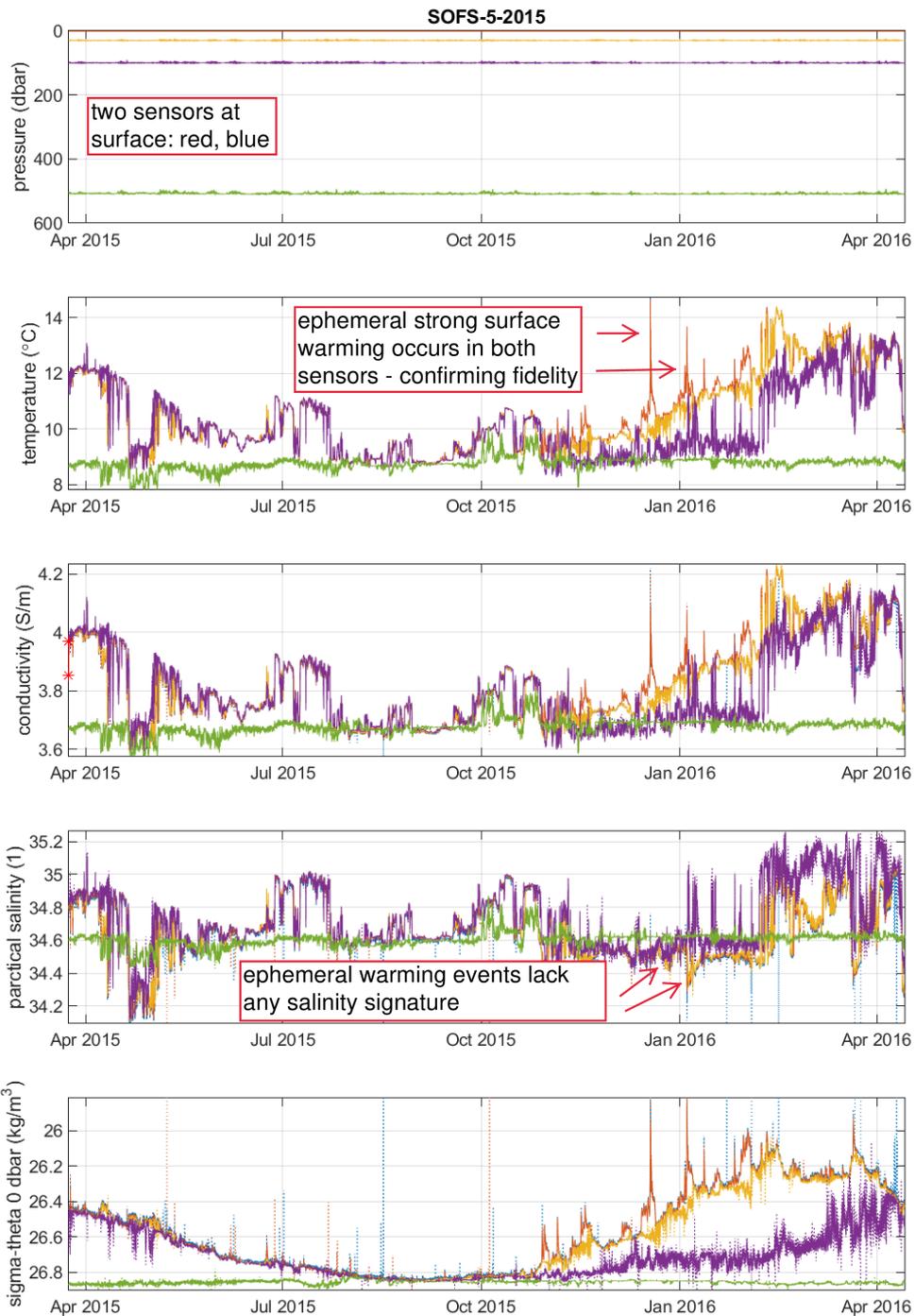


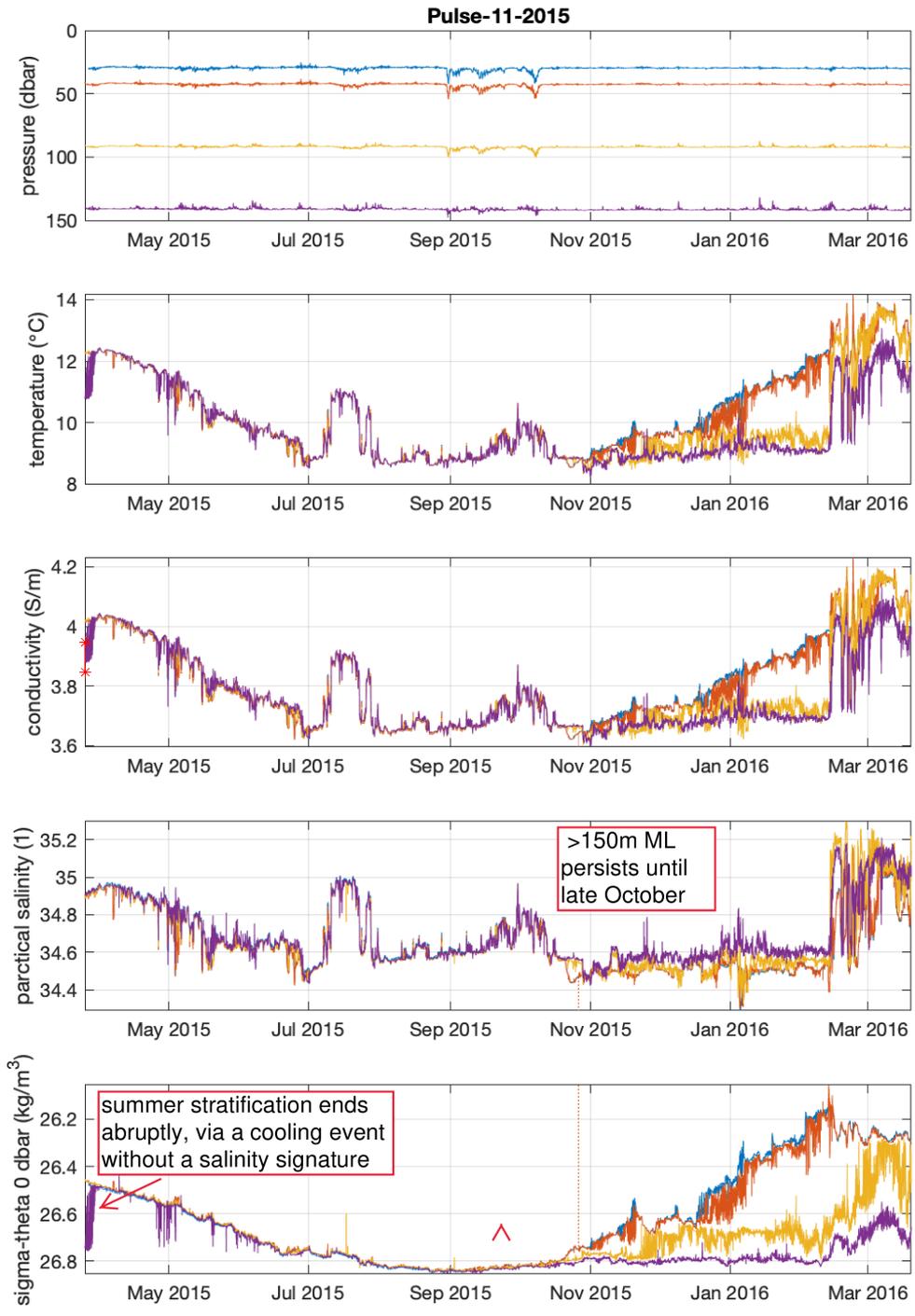


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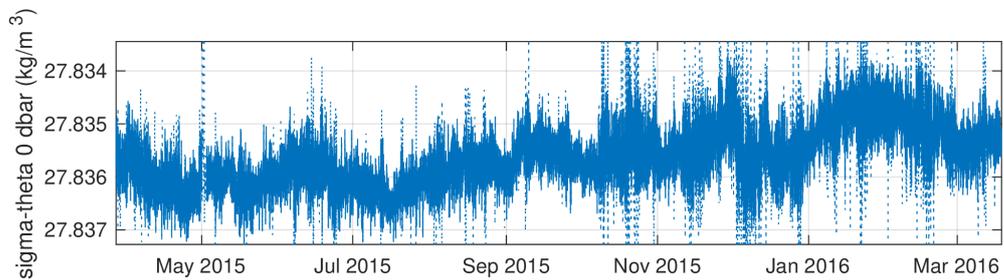
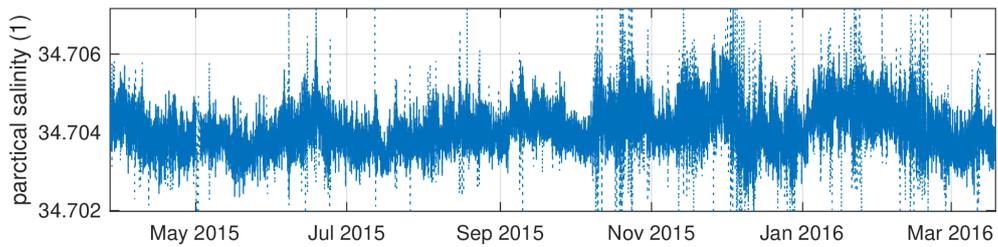
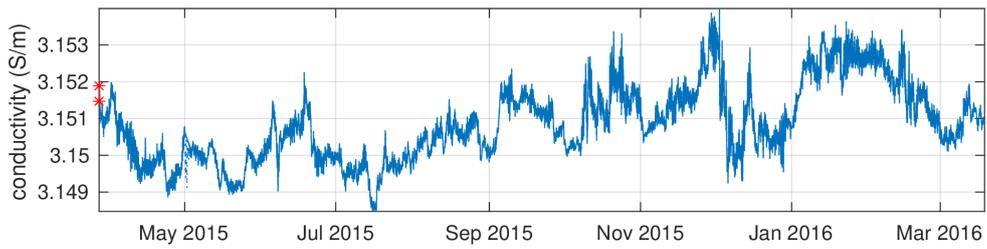
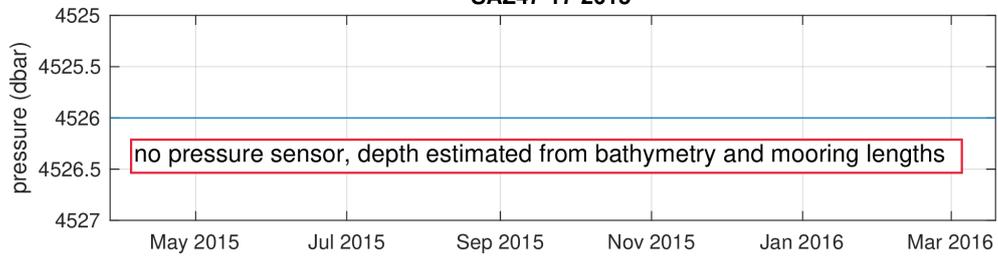


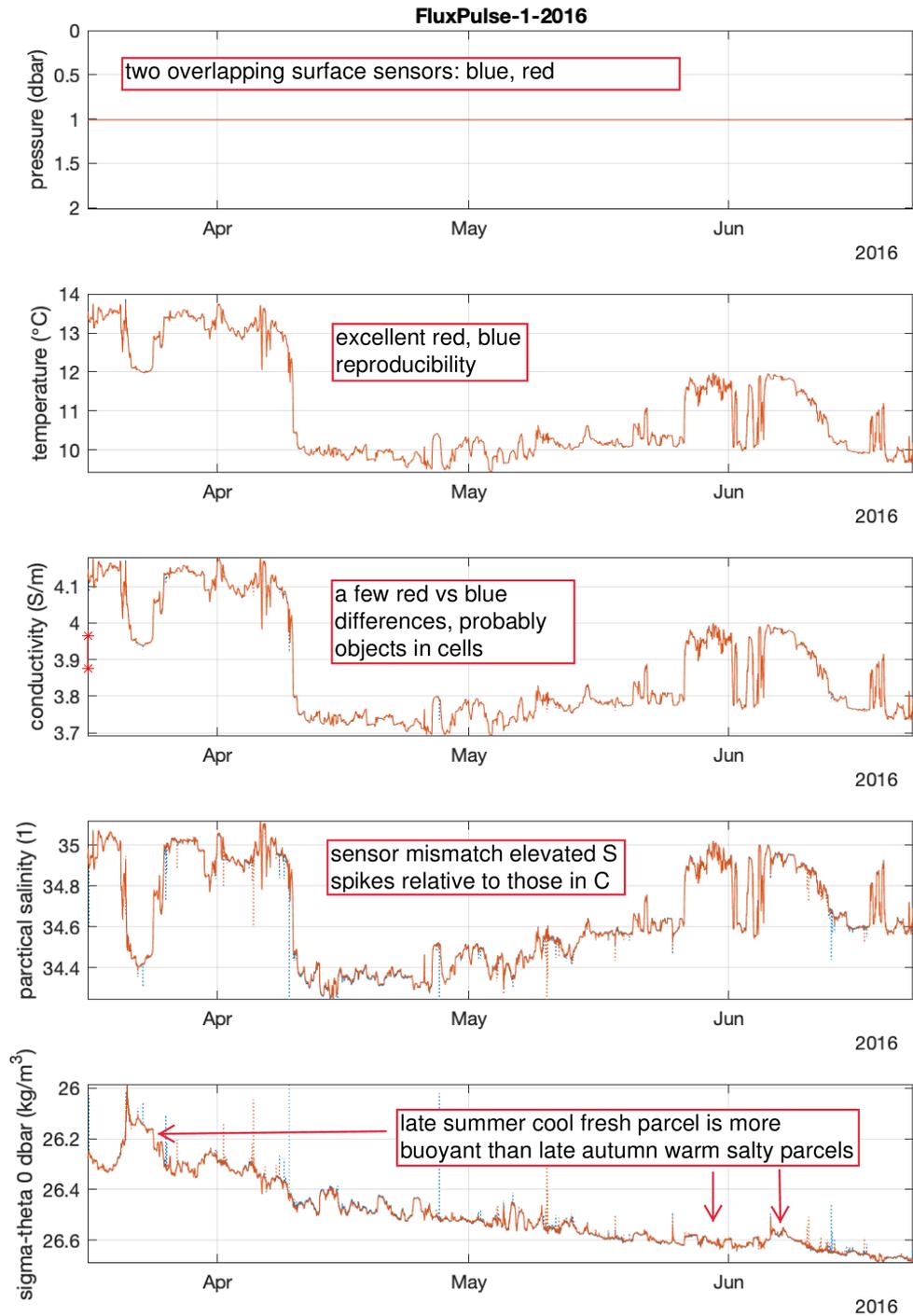


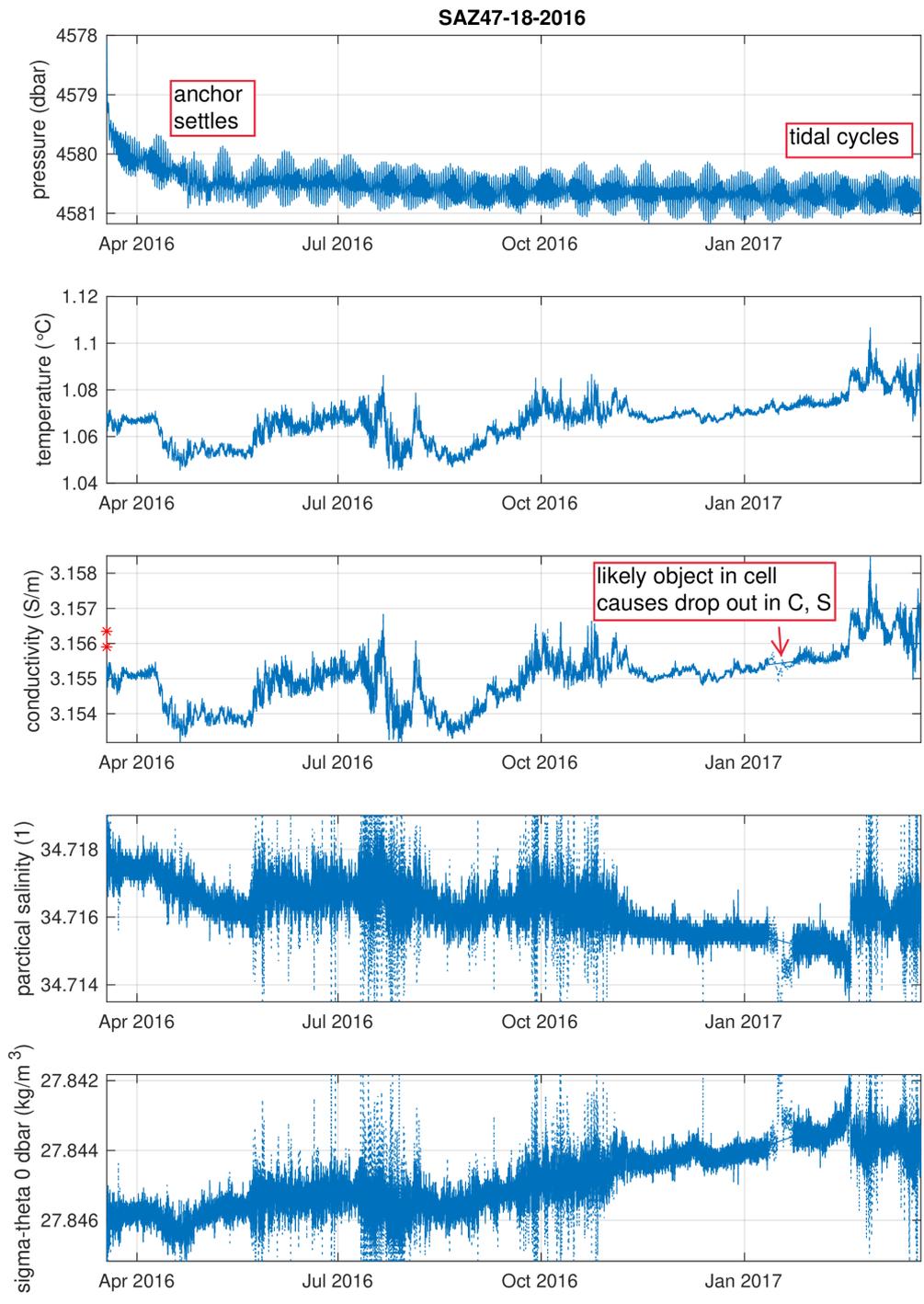


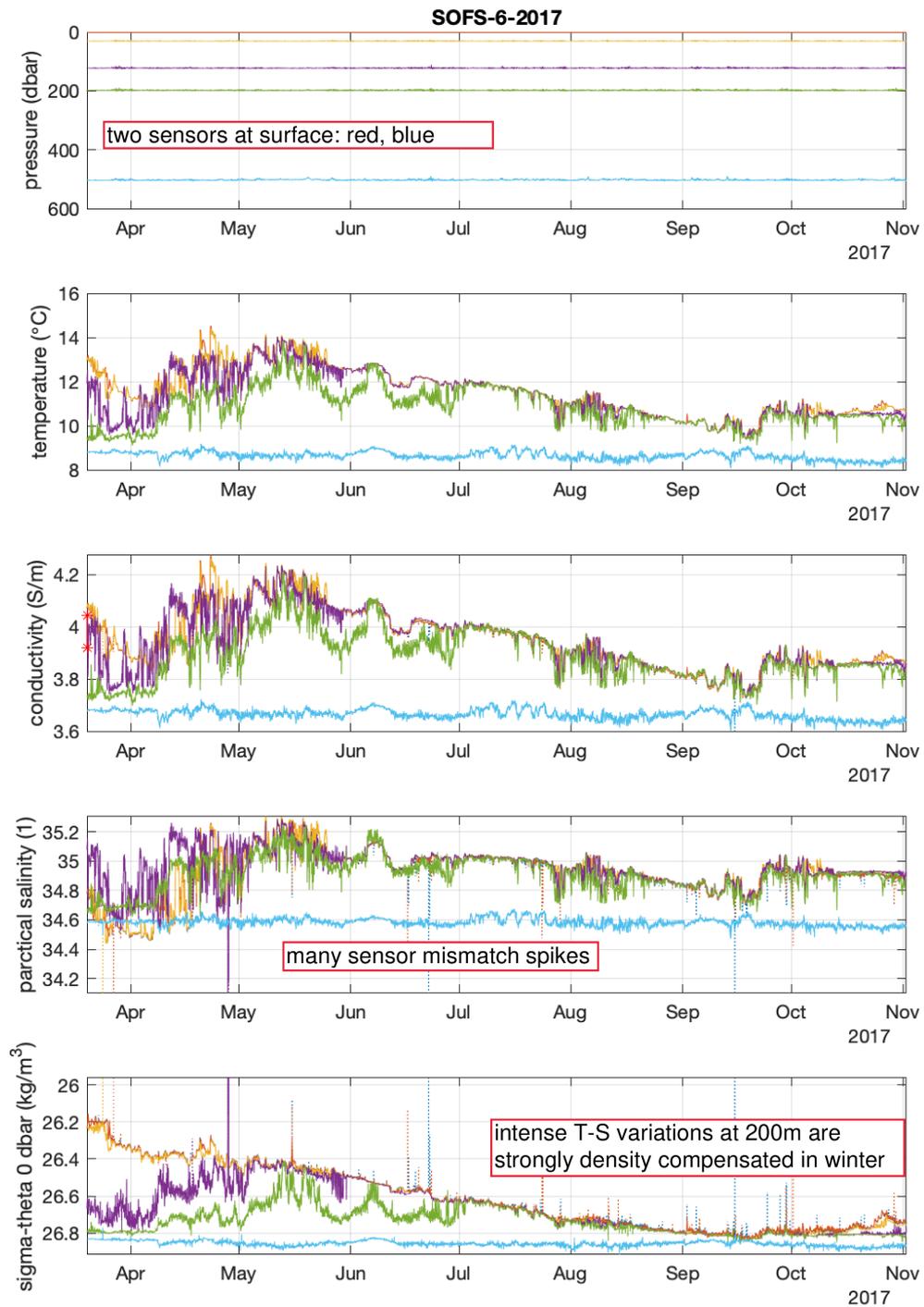


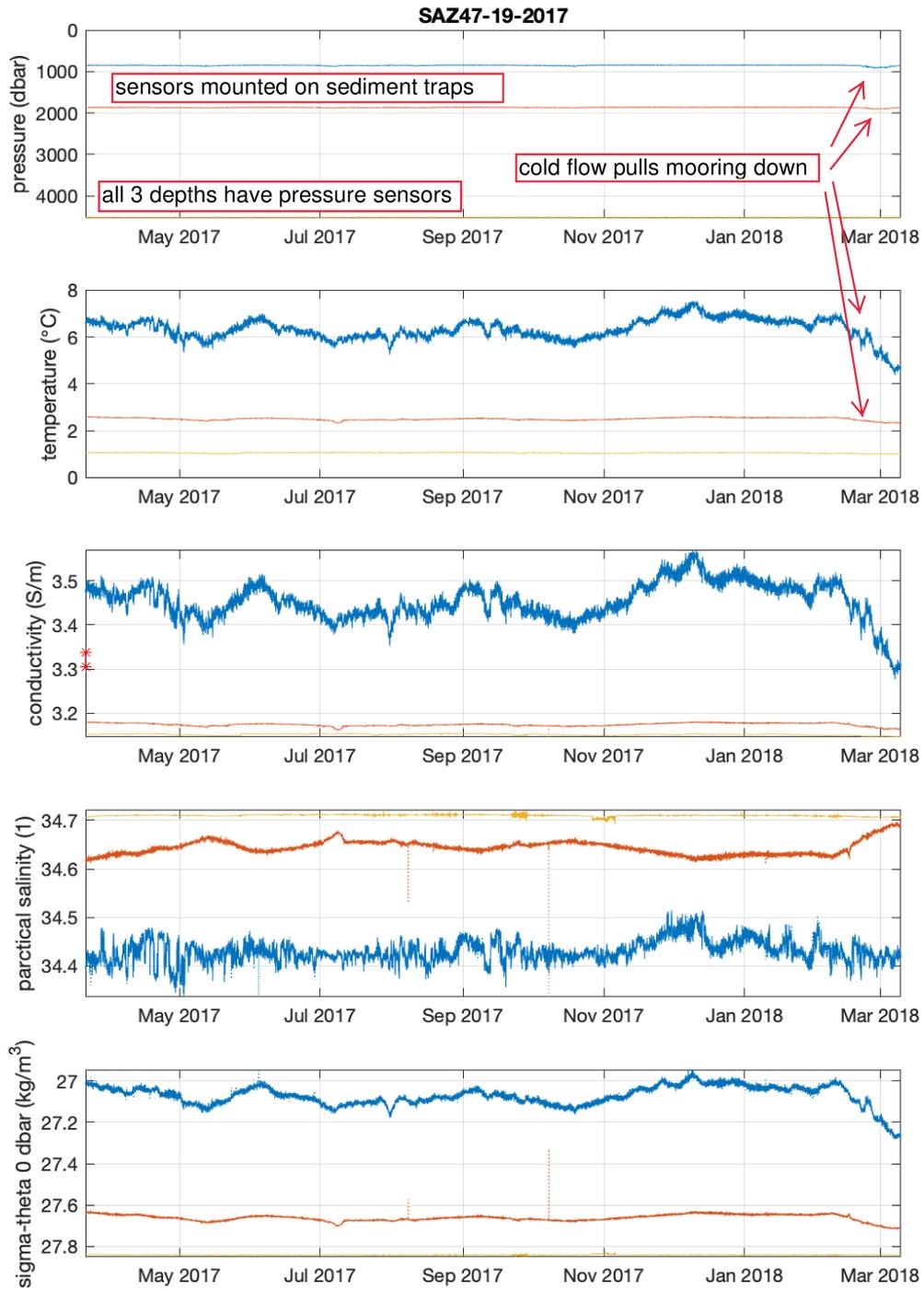
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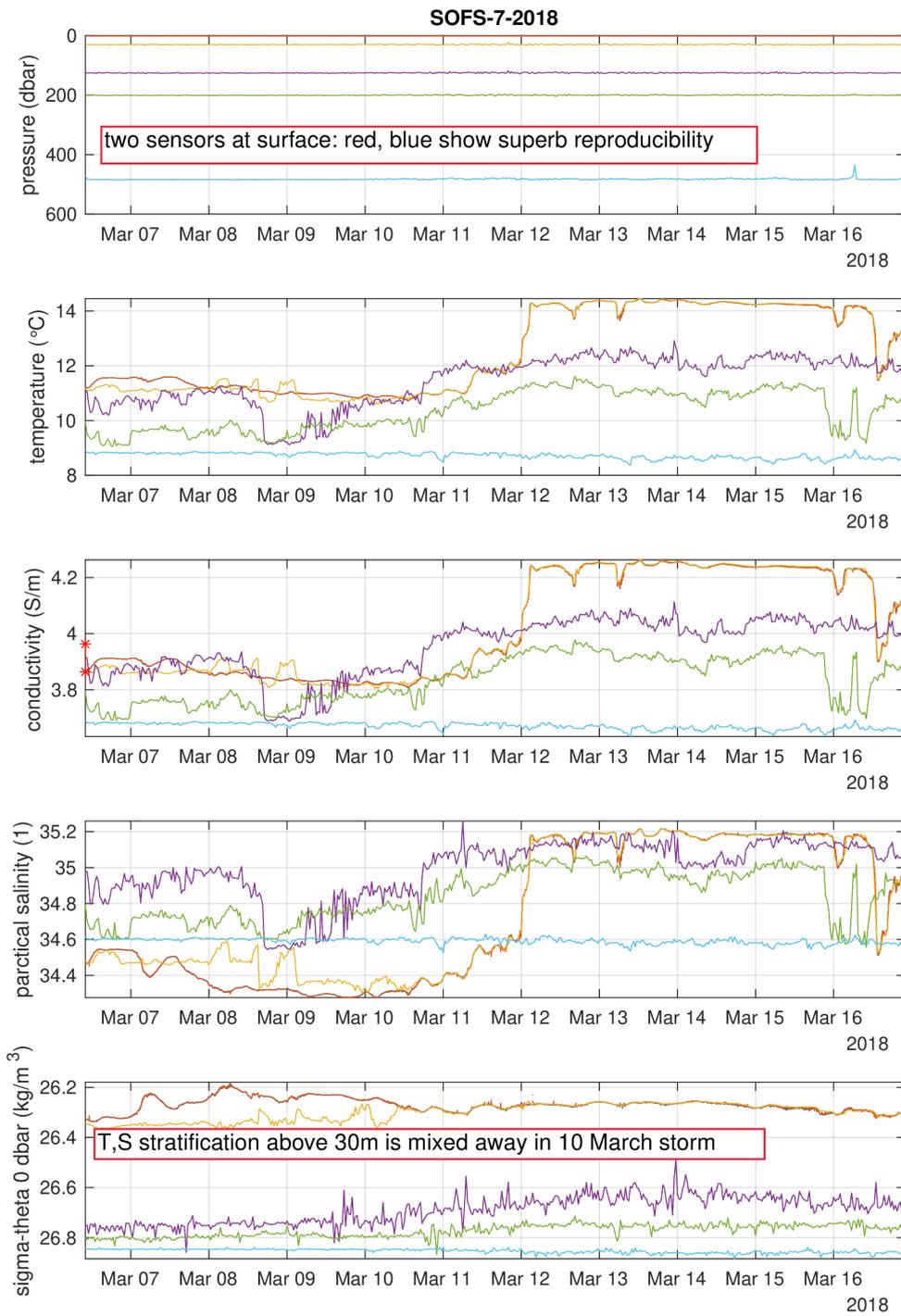


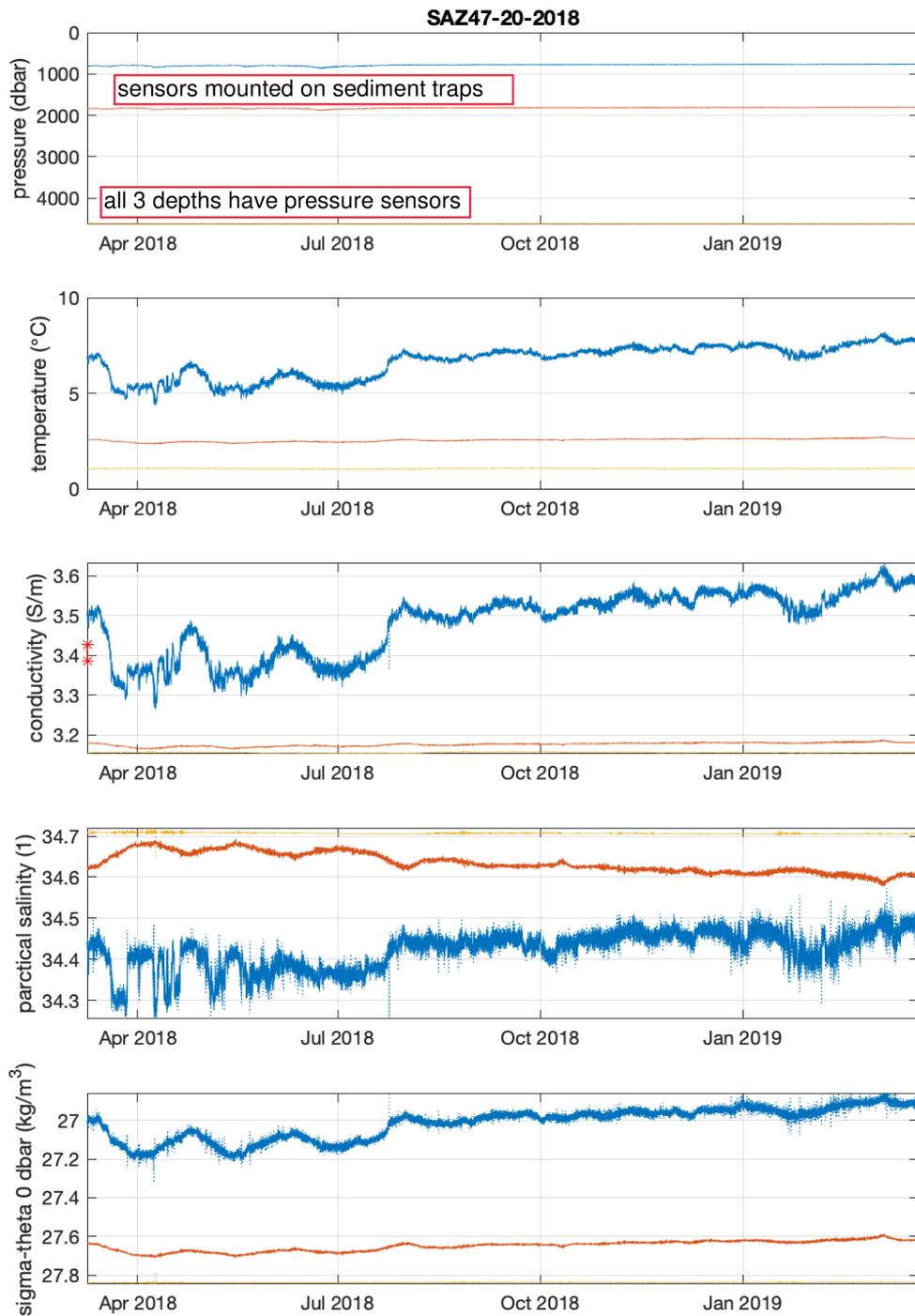


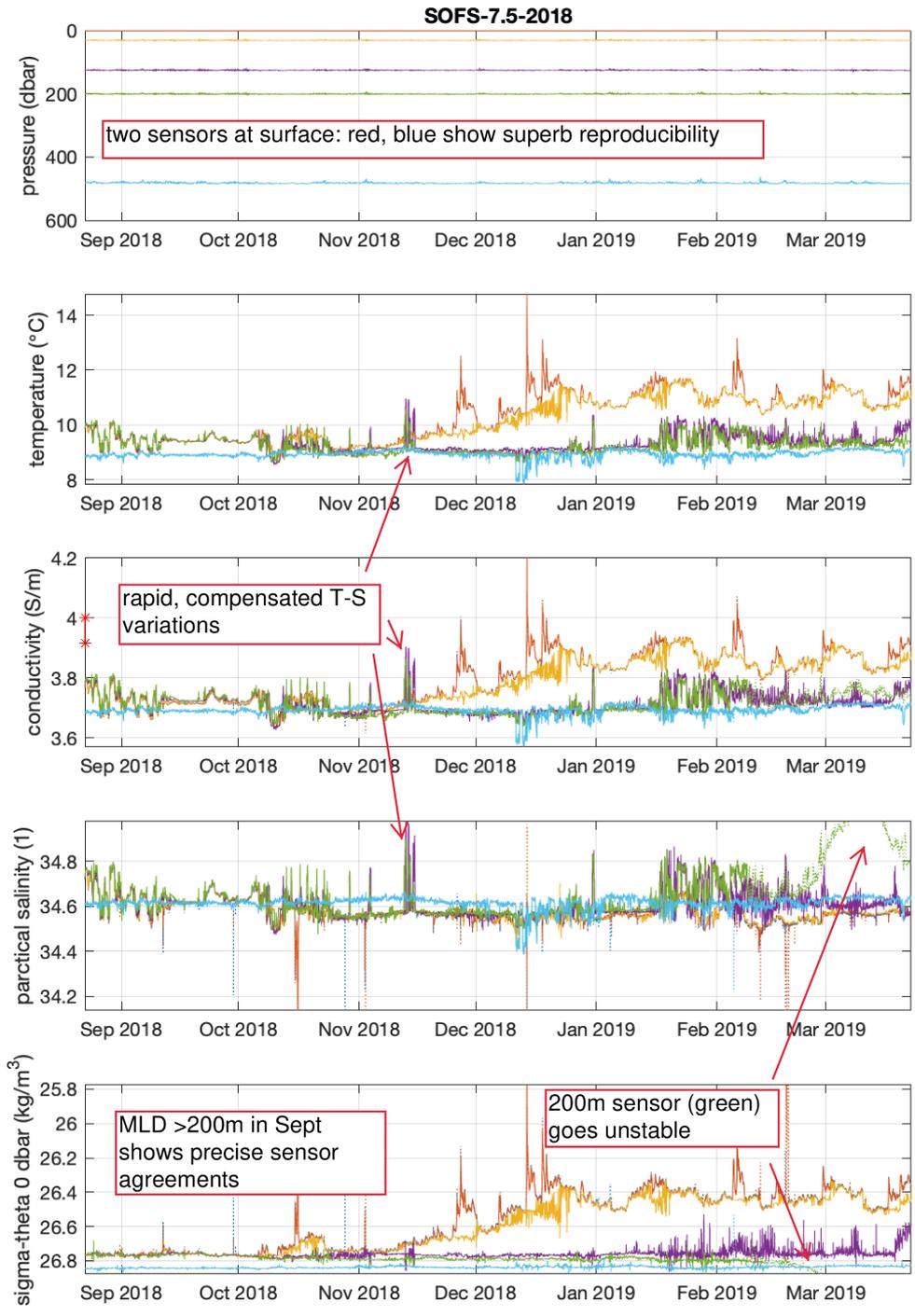


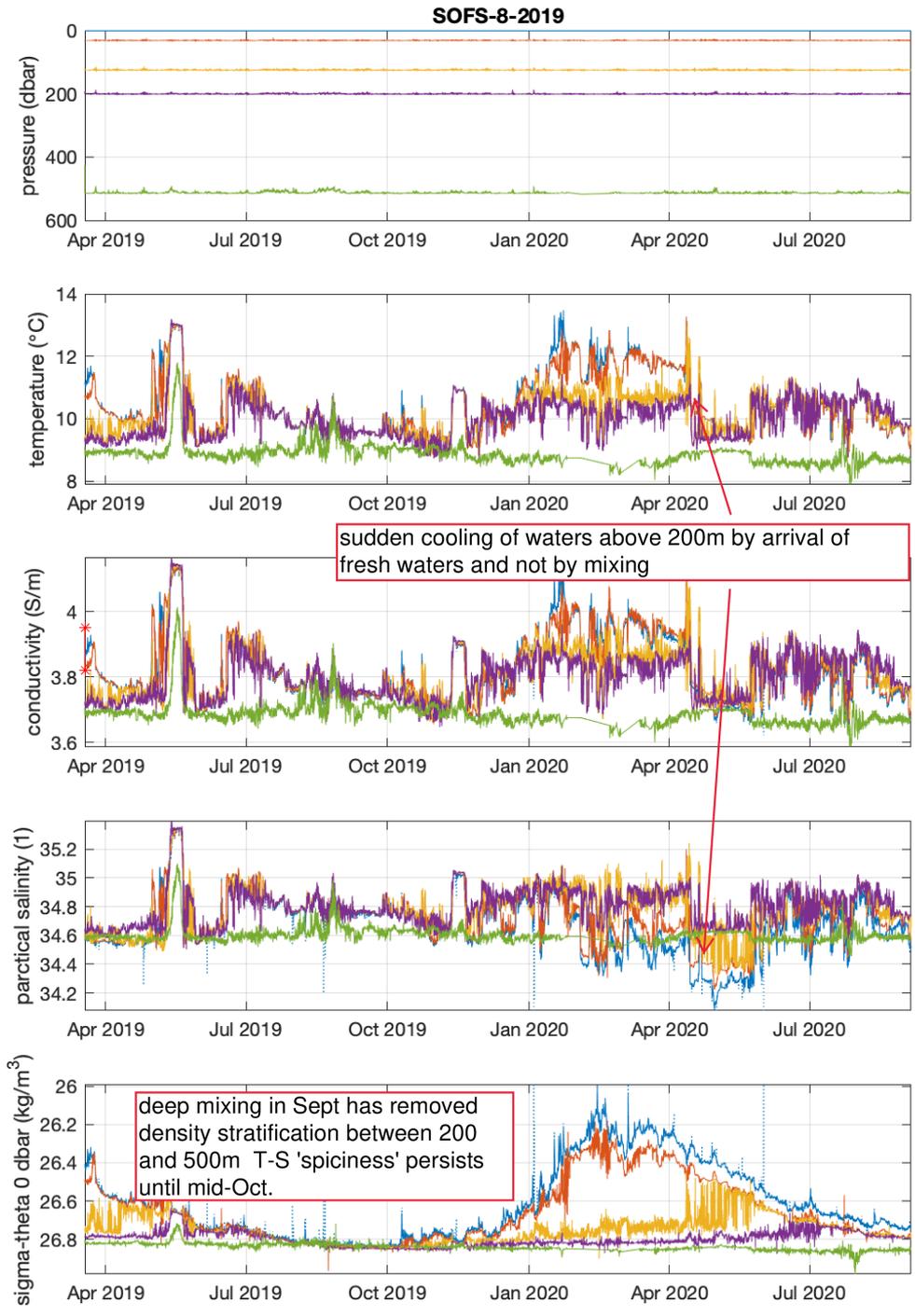


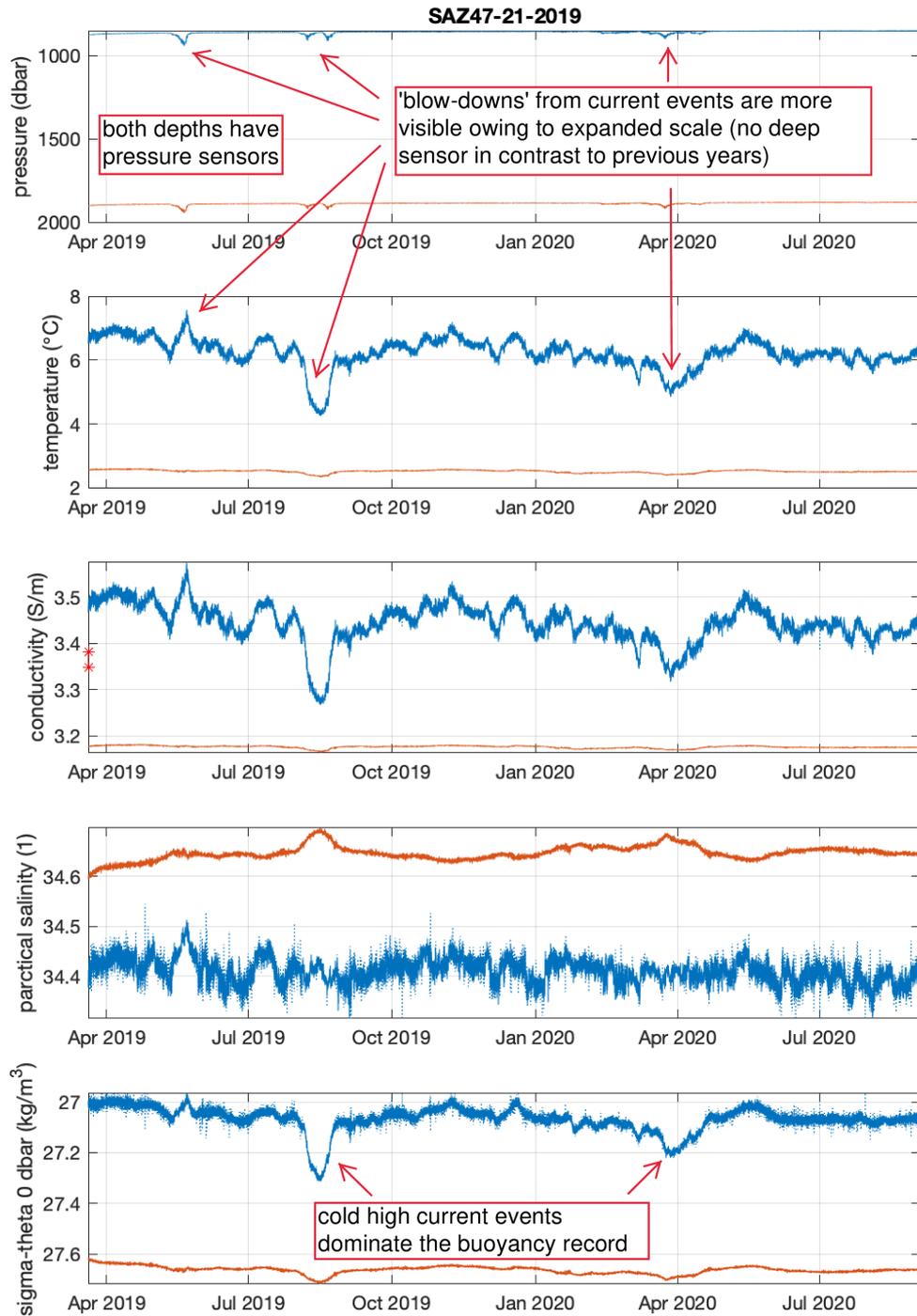


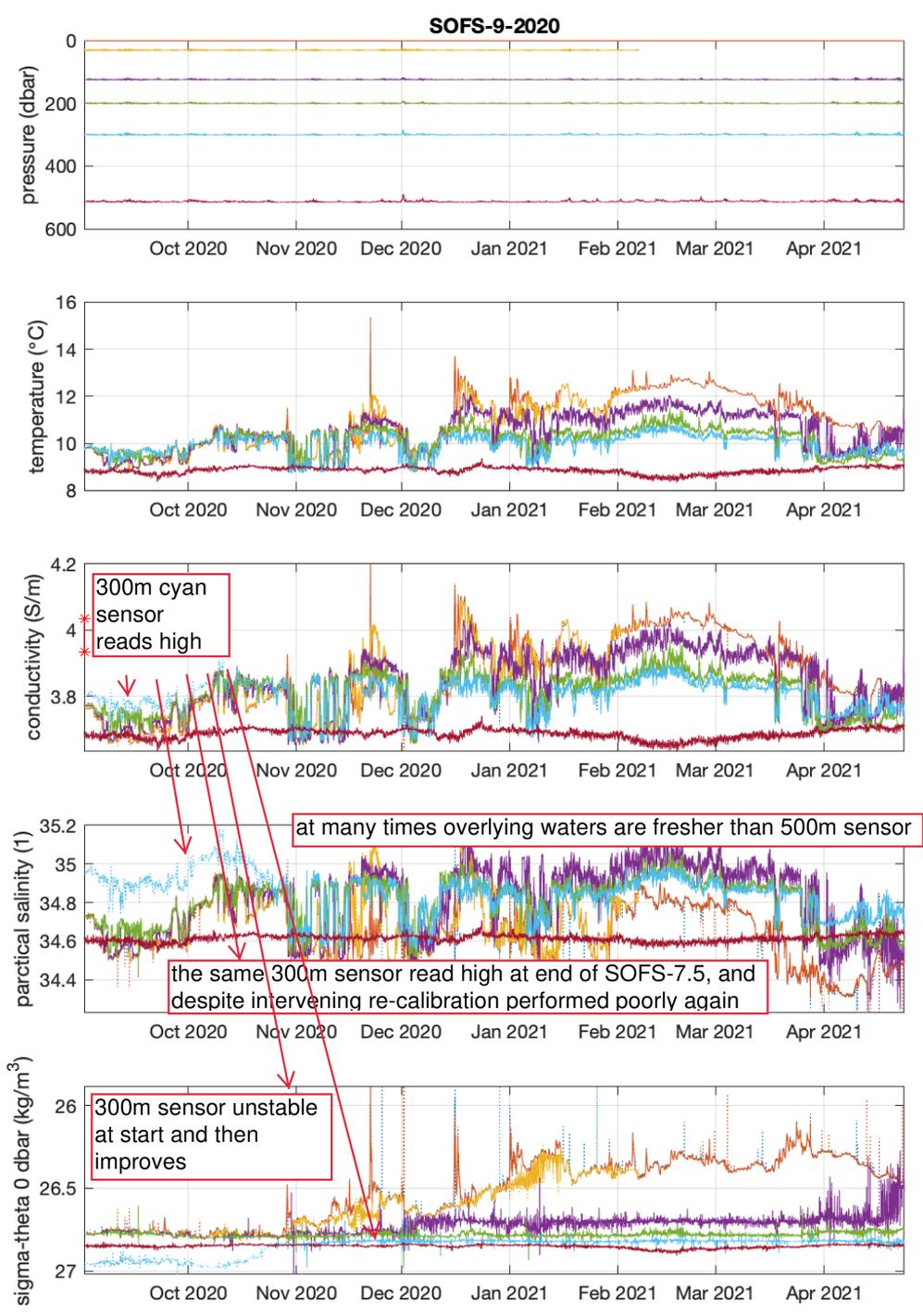




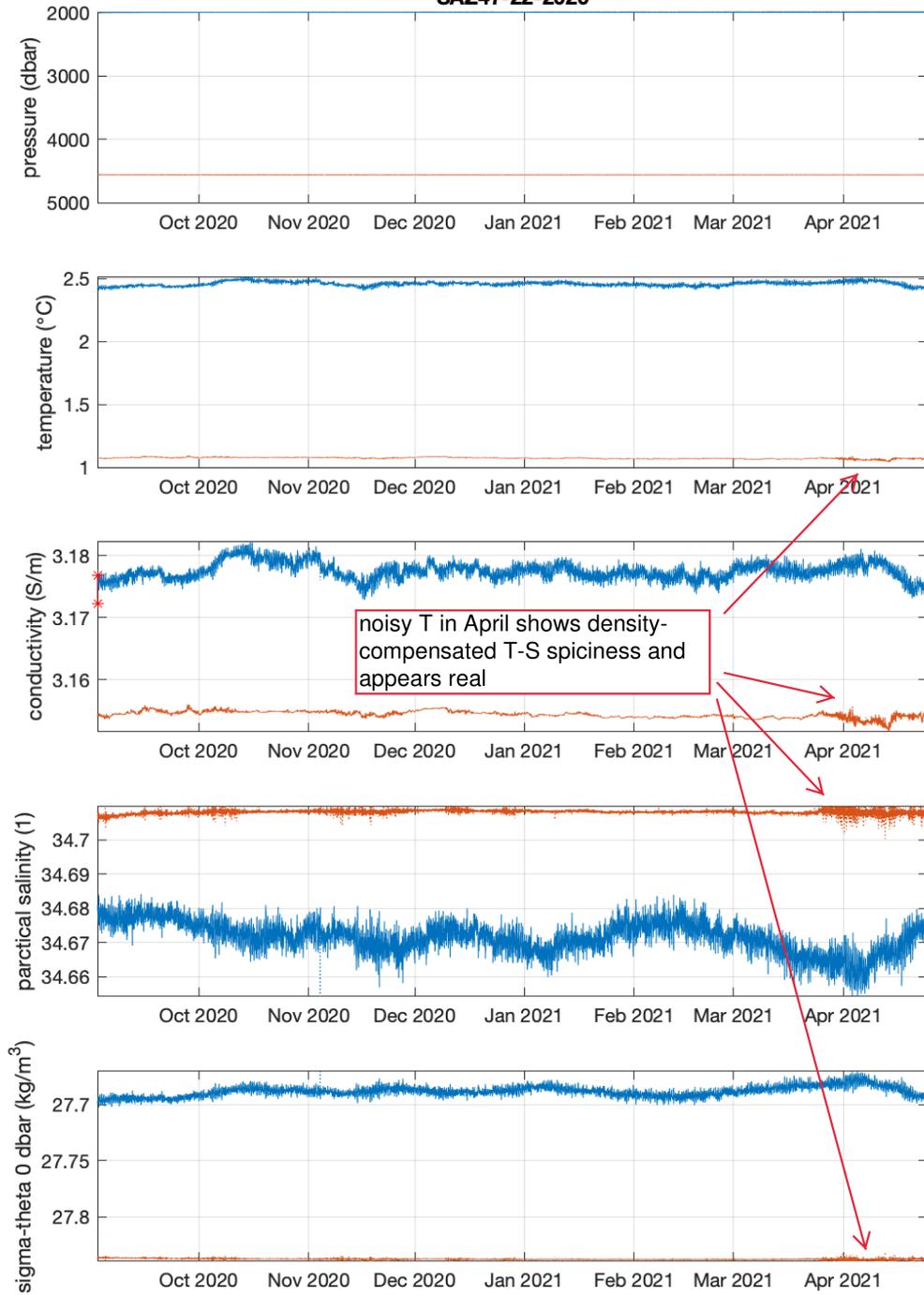


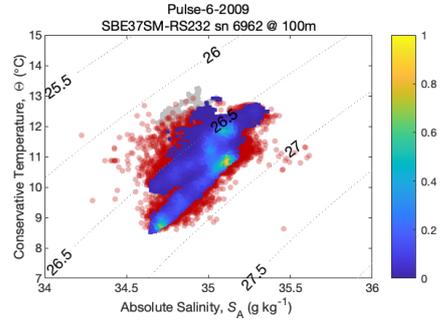
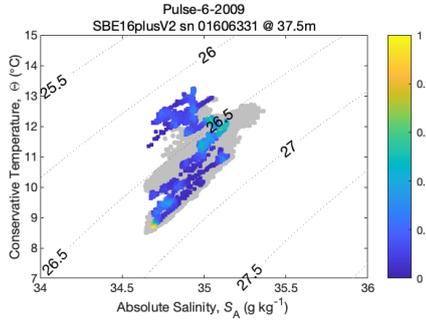


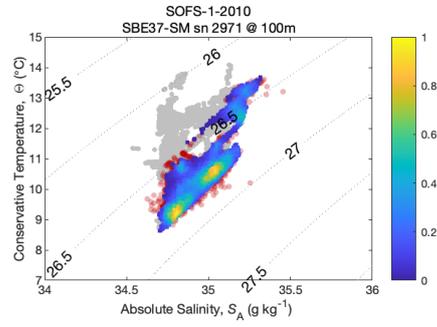
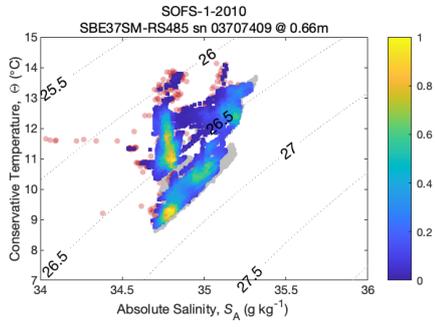


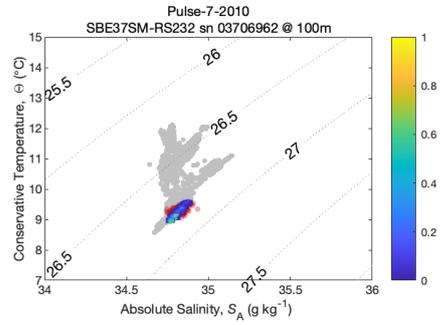
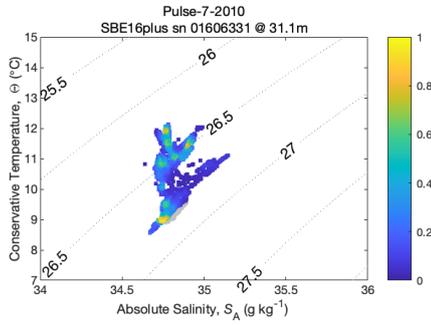


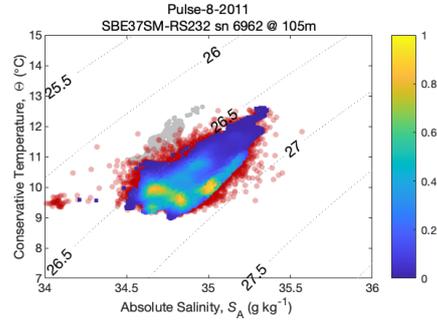
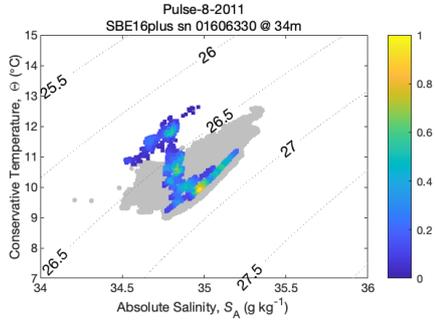
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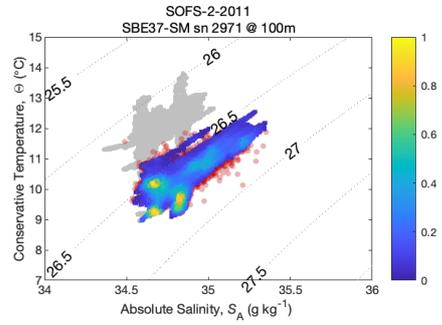
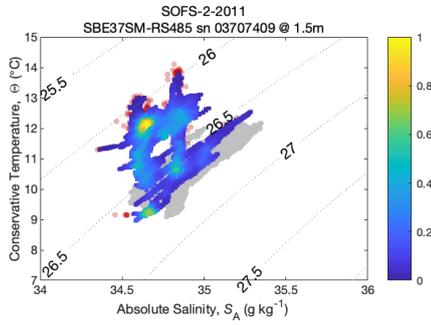


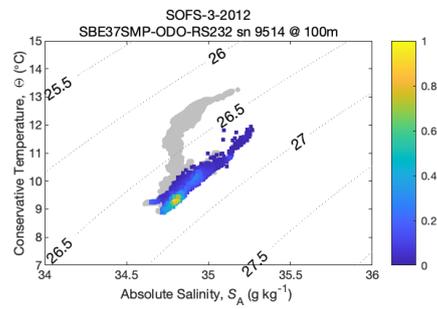
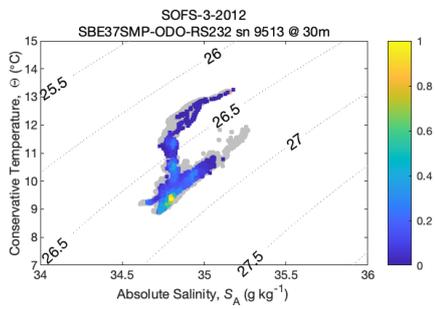
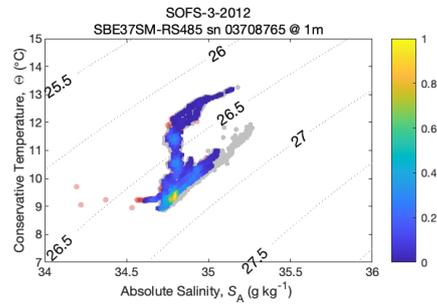
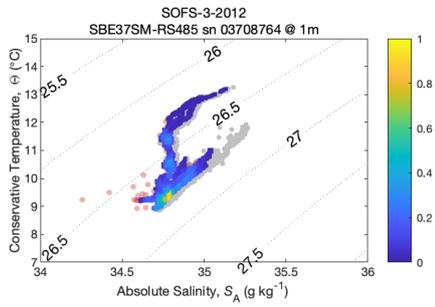


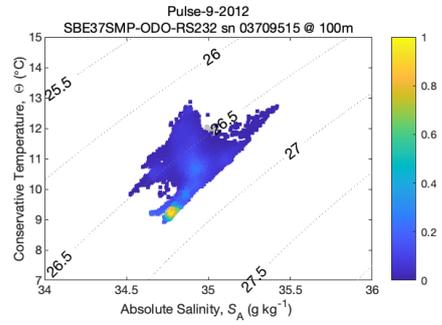
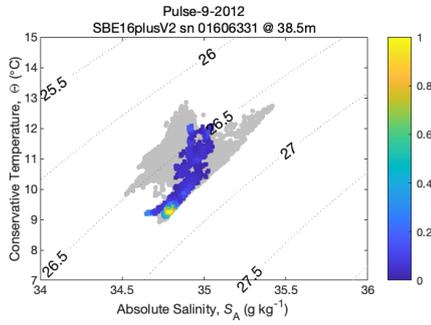


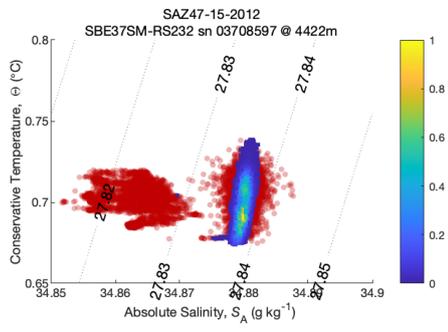


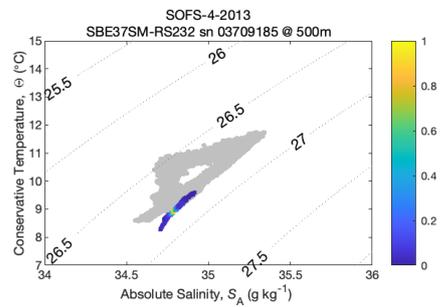
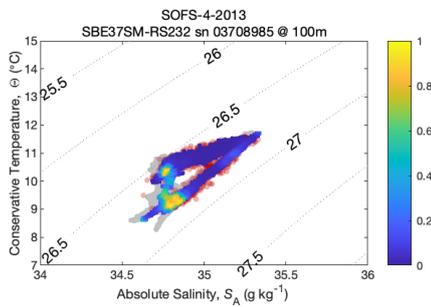
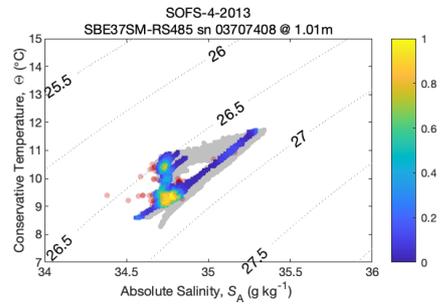
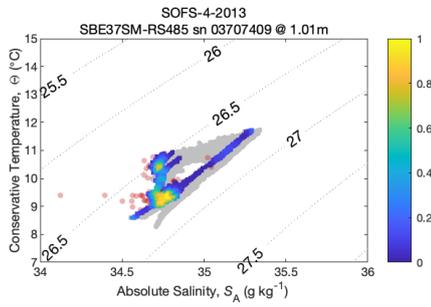


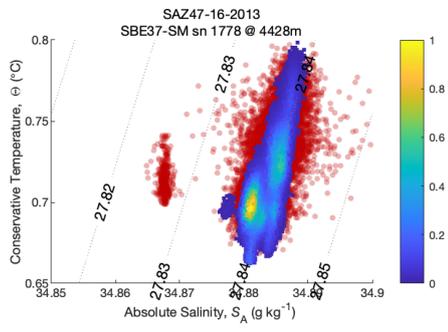


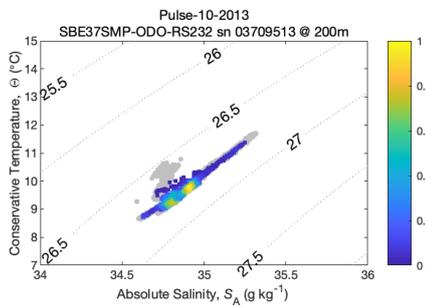
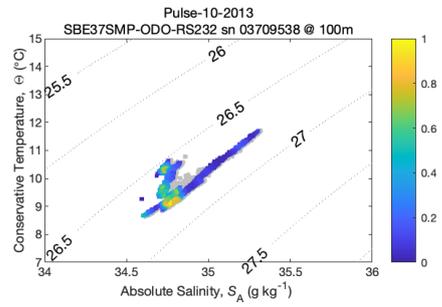
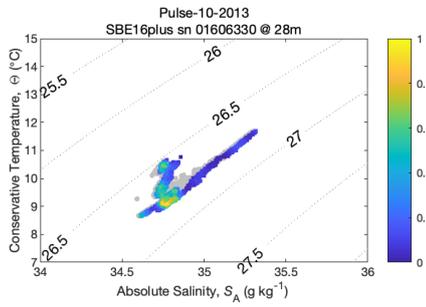


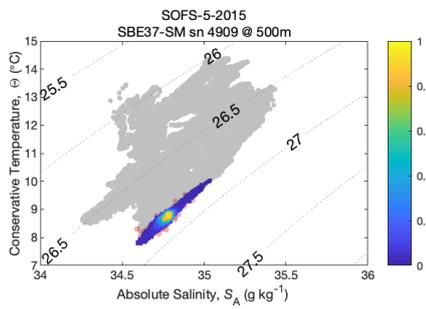
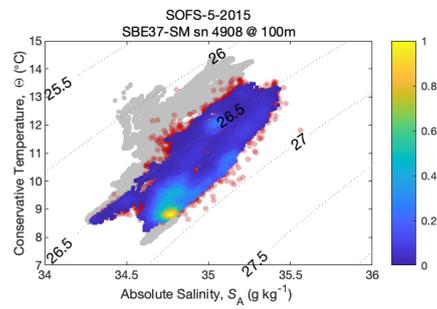
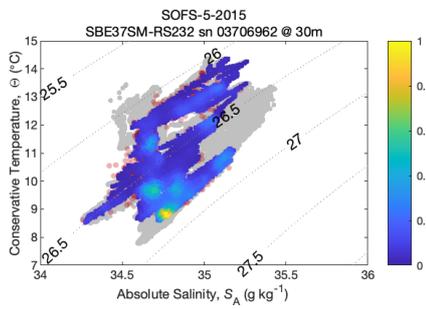
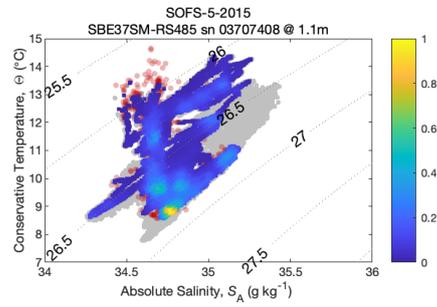
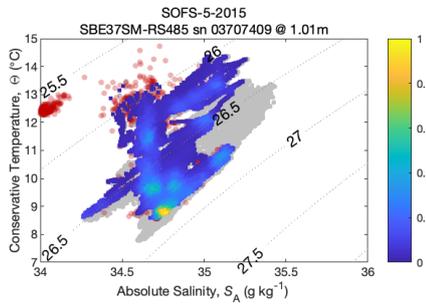


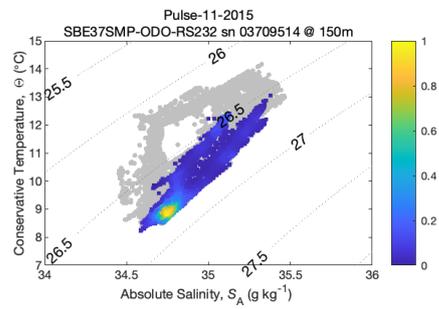
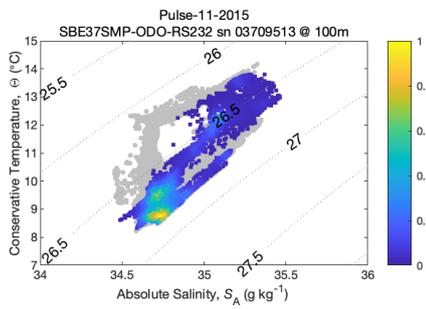
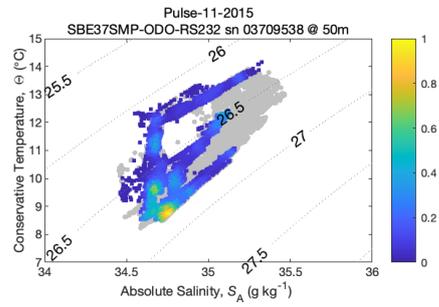
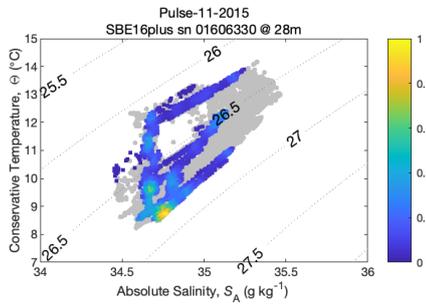


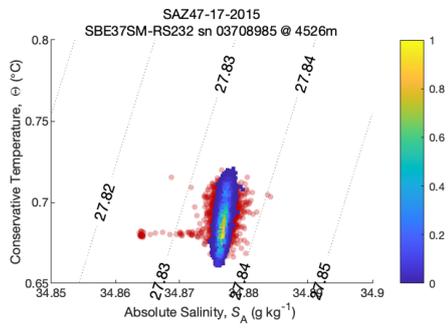


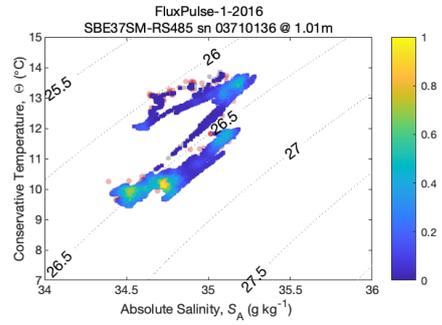
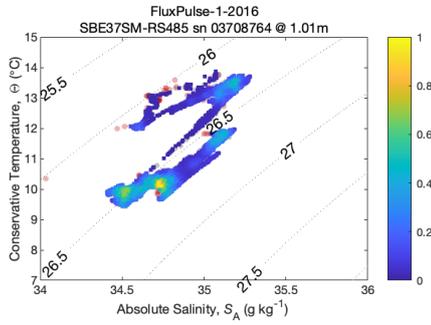


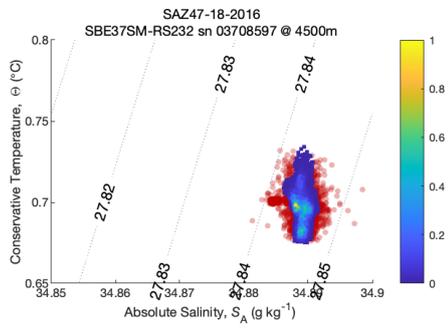


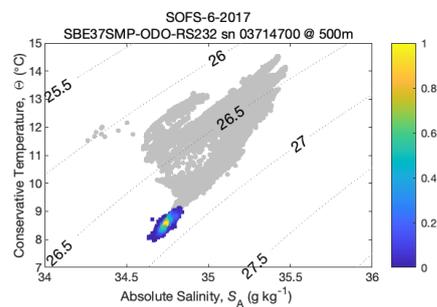
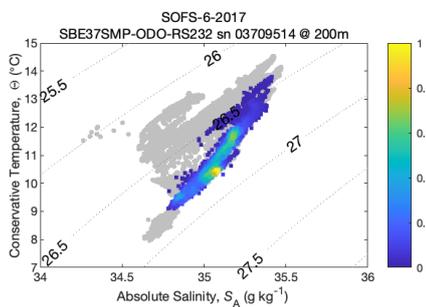
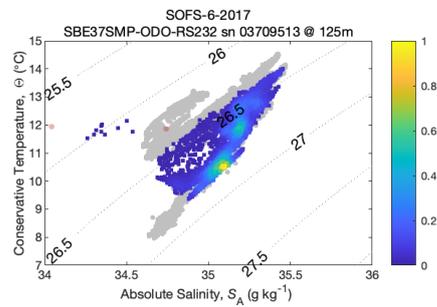
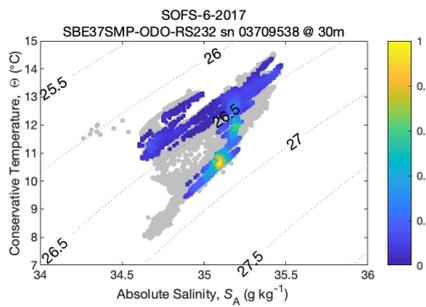
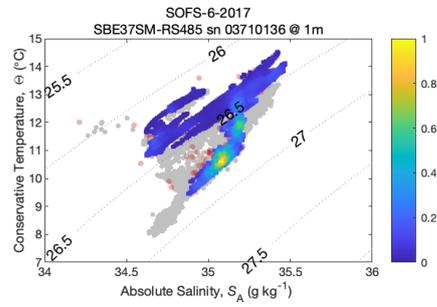
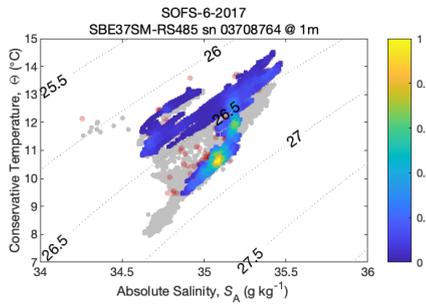


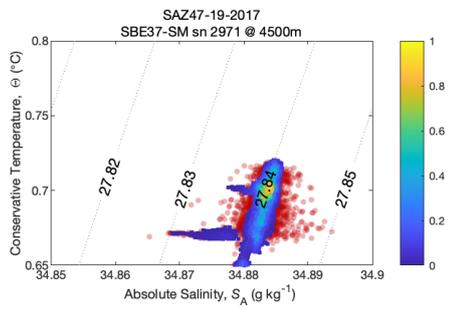
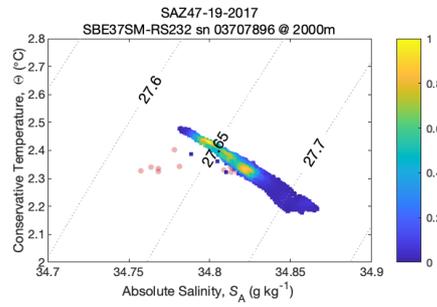
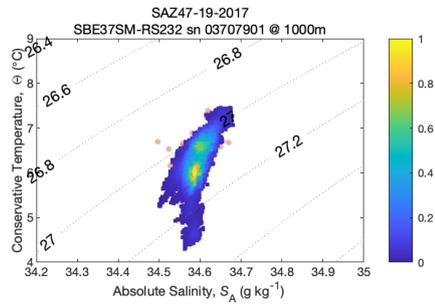


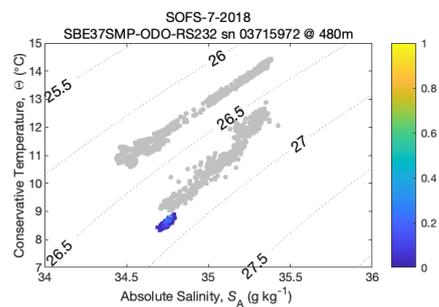
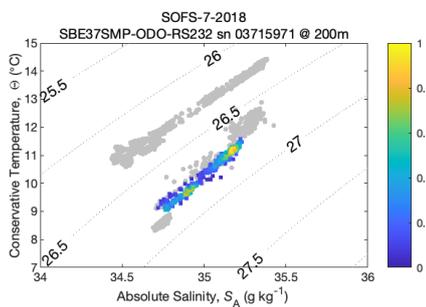
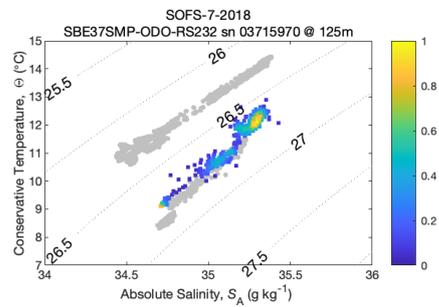
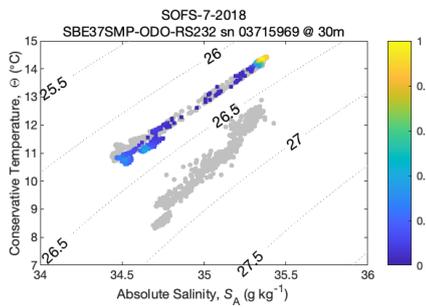
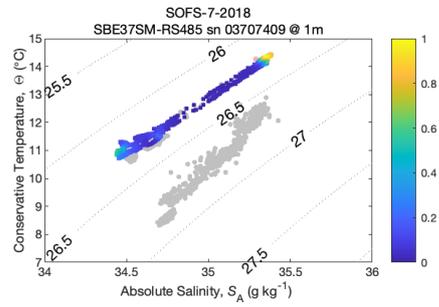
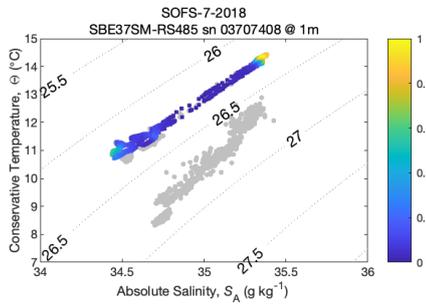


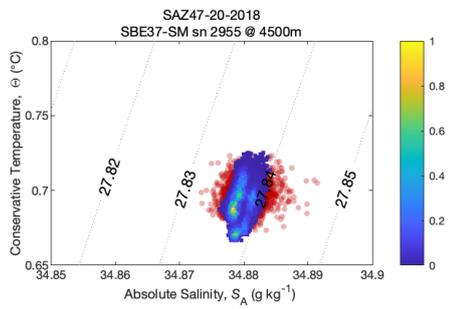
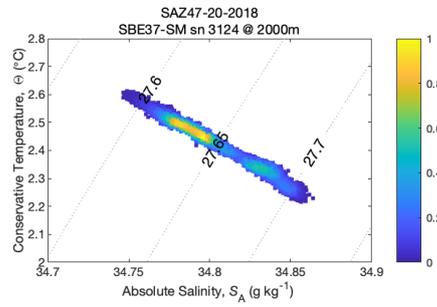
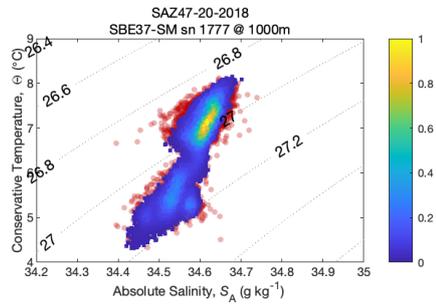


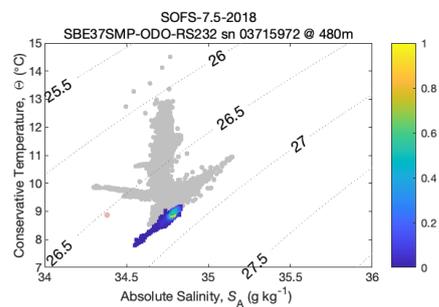
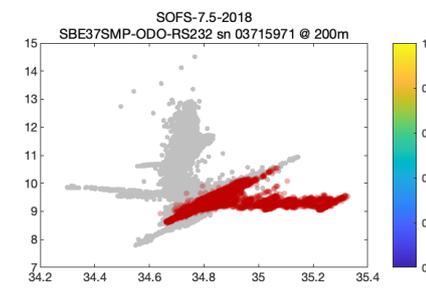
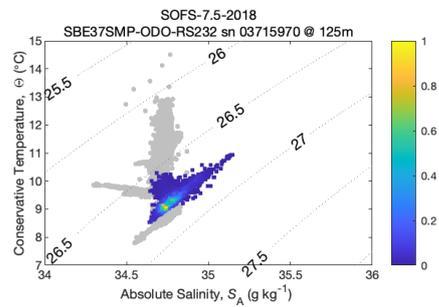
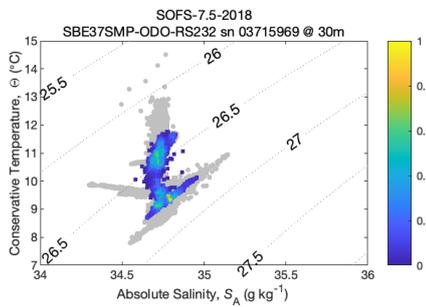
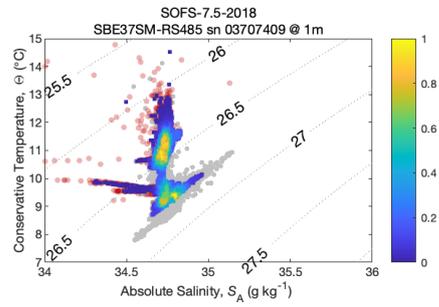
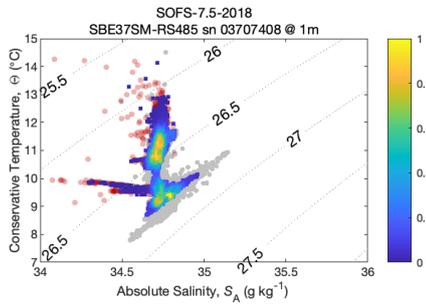


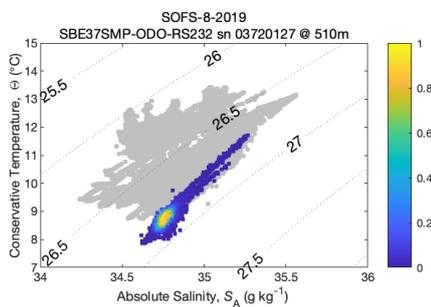
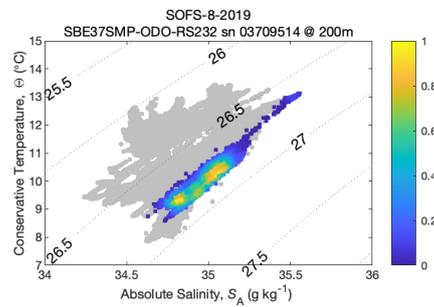
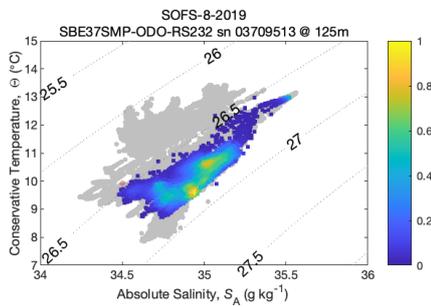
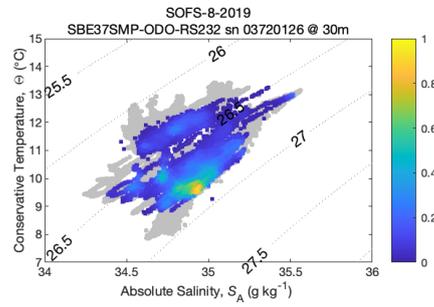
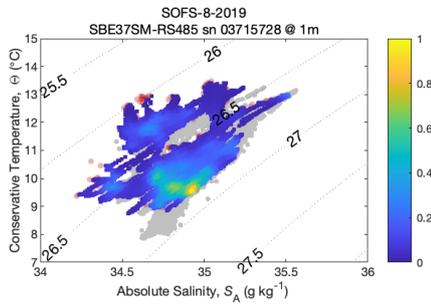


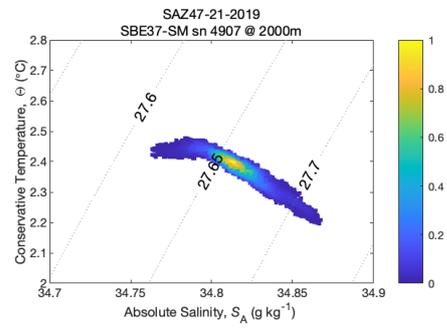
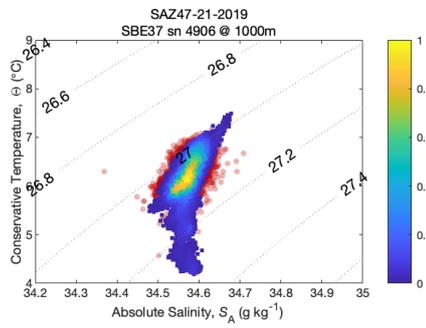


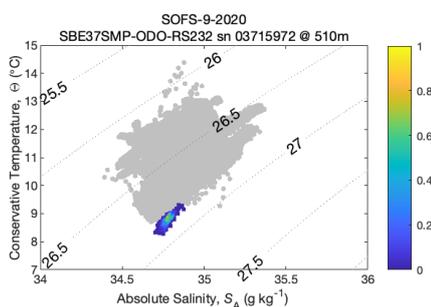
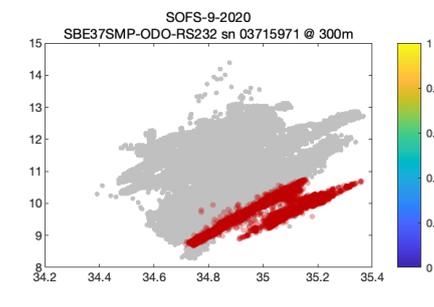
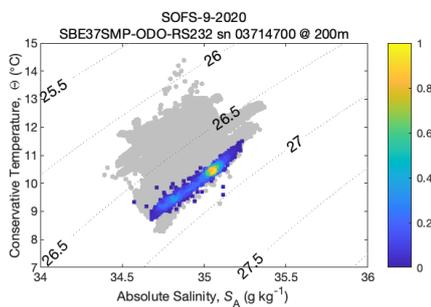
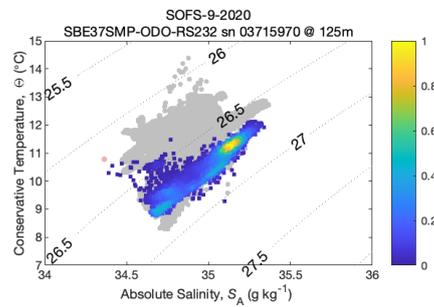
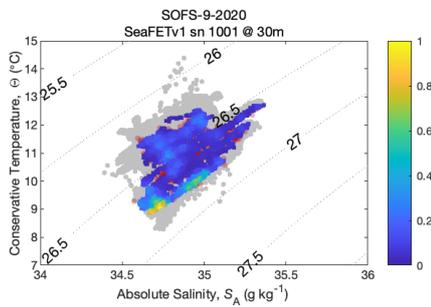
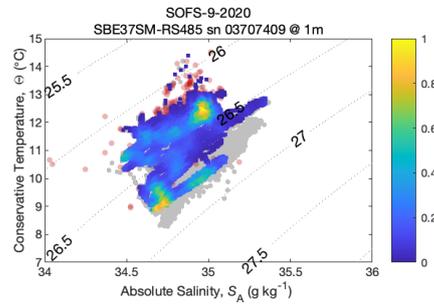
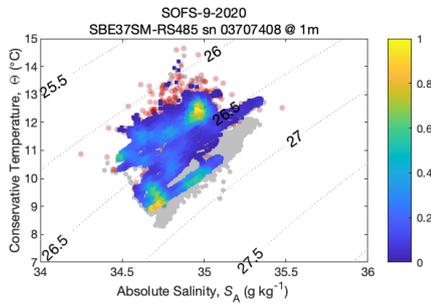


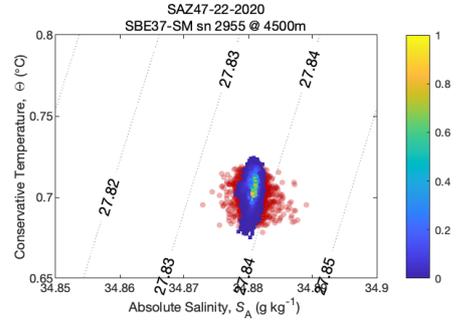
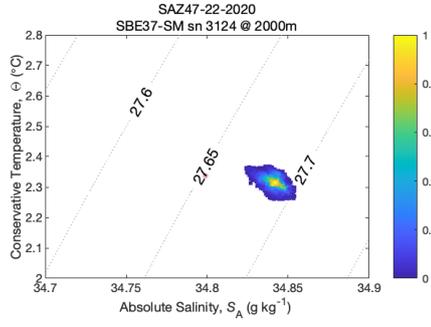












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Version	Date	Change Description	Revision Author
1.0	8 Oct 2021	Original Issue	Jansen, Shadwick and Trull