# Data processing - observational pathway from collection to quality assured/control data sets

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# GO-SHIP: High Quality Ocean Reference Data

The Need

- GO-SHIP collects a comprehensive set of ocean observations: temperature, salinity, oxygen, nutrients, carbon, transient tracers, velocity and more
- GO-SHIP is the reference dataset for the Argo array and other autonomous platforms.

# IAPSO Working Group on Ship-Based CTD-$O_2$ Processing and Calibration Procedures

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# THE IAPSO CTDO2 WORKGROUP


## About the Working Group

- International group of scientists and technicians
  - Led by Bernadette Sloyan at CSIRO
- 2-year goal of assembling a forum capable of assessing global CTDO2 data processing status and routines
- Intercomparing CTDO2 data processing between labs/institutions/countries

*Acronyms*

- IAPSO - International Association for the Physical Sciences of the Oceans
- CTDO2 – Instrument package that continuously measures conductivity, temperature, depth, and oxygen

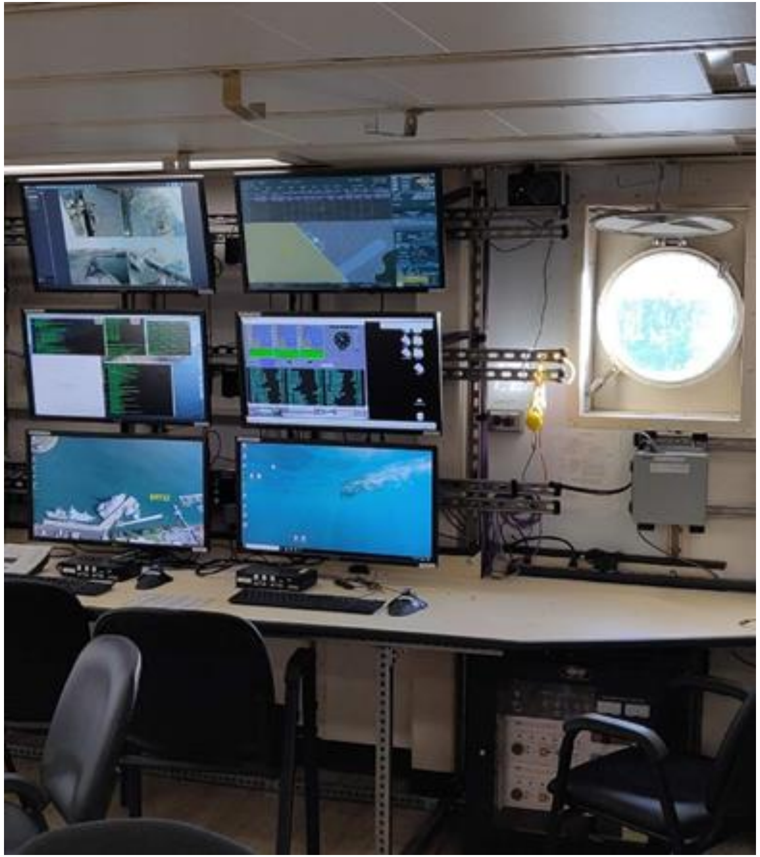
# MOTIVATION

1. $CTDO_2$ data is important
   - Monitoring and assessing ocean change
   - Calibration and validation of autonomous and unattended observations
   - Interpreting ecosystem observations and monitoring

1. Unknown differences in how data is processed around the world
   - Leading to uncertainties in data quality and missed opportunities
   - GO-SHIP cruises are completed by highly-qualified and experienced science and technical teams to produce climate-quality data, but the GO-SHIP manual is 15 years old; technology has changed; and differences in procedures are emerging between groups
   - Quality $CTDO_2$ data is also needed beyond GO-SHIP, e.g. in marginal seas and the coastal ocean

1. Numerous international programs are associated with aspects of $CTDO_2$ processing
   - ICES WGOH; US UNOLS R2R and GO-SHIP working groups (including CCHDO); EuroGO-SHIP European Infrastructure project; German DAM Underway research data project

1. Coordination to address:
   - Is there a "best" or "better" procedure for data processing for high-quality products?
   - Is it well-enough described and useable by groups with different resources and requirements?
   - How is a group to know if they are getting the most out of their data?



# Approach

Survey of 33 participants

- Antarctica only continent w/o representation

CTD intercomparison project

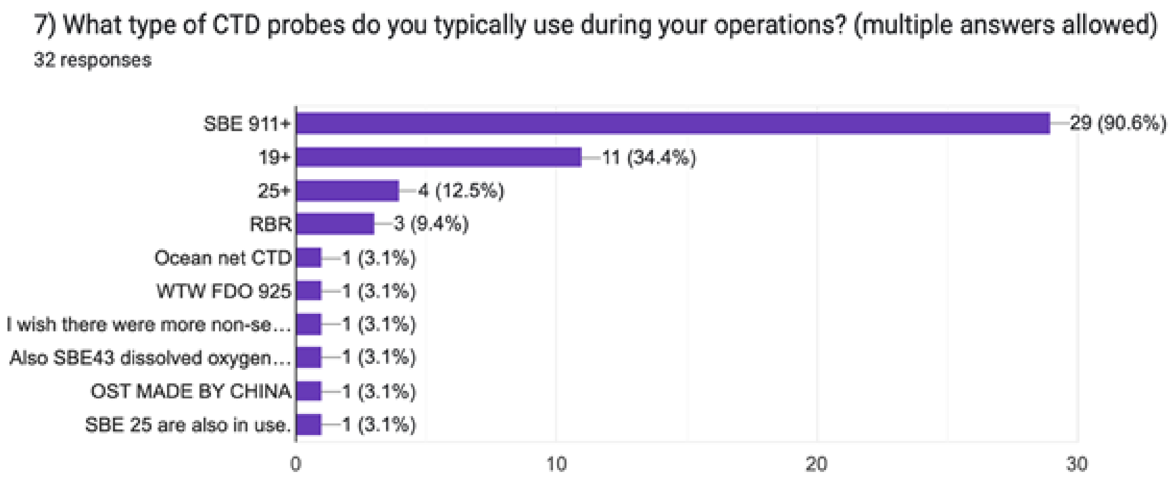
- 18 international participants
- Process GO-SHIP line A02
- Statistical analyses
- Reported methods

Other experiments

- CTD salinity and $O_2$ relative to bottle oxygen
- Changing processing step order

2017 GO-SHIP line A02 sample track, undertaken on the *Celtic Explorer* (45CE20170427)

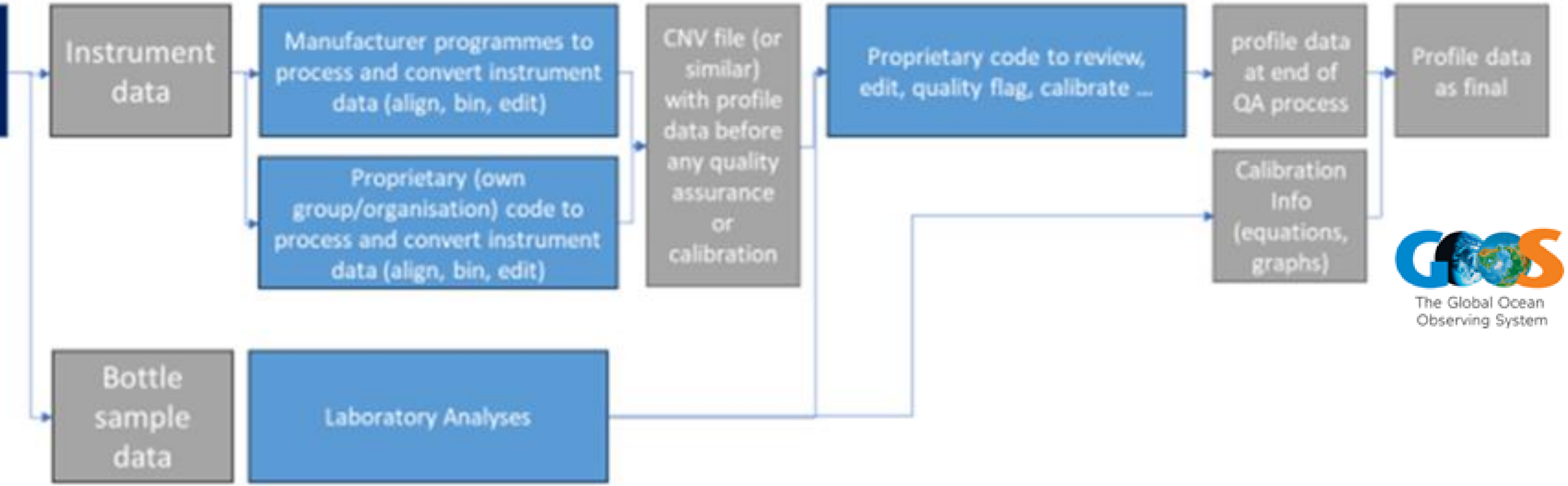
# Conductivity, Temperature, Depth (CTD) with Oxygen




→ The ocean community mainly relies on one manufacture of the CTD instrument.

Diversity is required, while maintaining accuracy and manufacture quality.

# Background: CTDO2 data steps




The Global Ocean Observing System

# Background: Discrete sample analysis



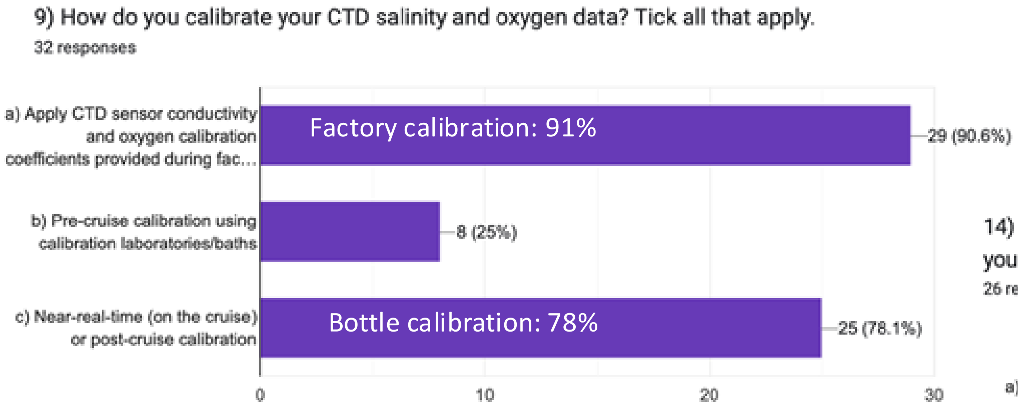
Salinity measurements

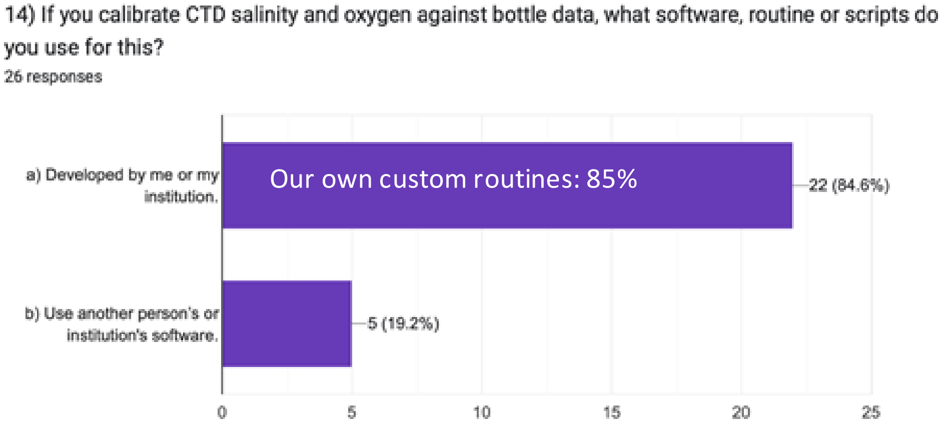
Guildline *Portasal* Salinometer with OSIL standard seawater for salinity measurements from bottles

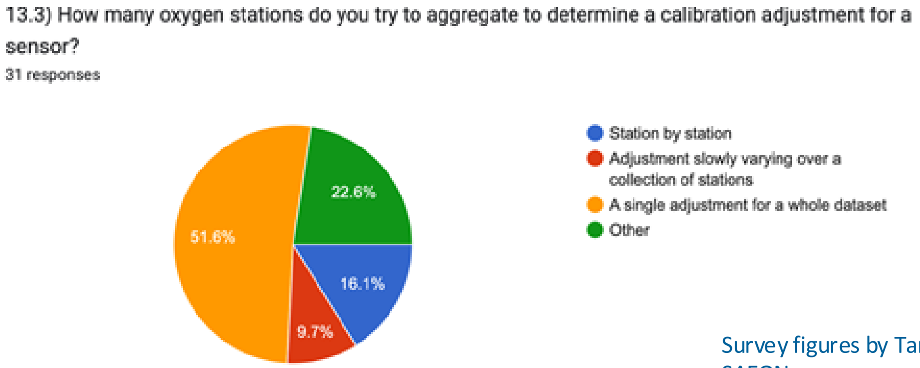
Winkler Oxygen Titration system
Colorimetry
Automated and portable

Winkler titration workbench using iodate standards for bottle oxygen measurements

# Survey results: Different methods




Survey figures by Tamaryn Morris, SAEON

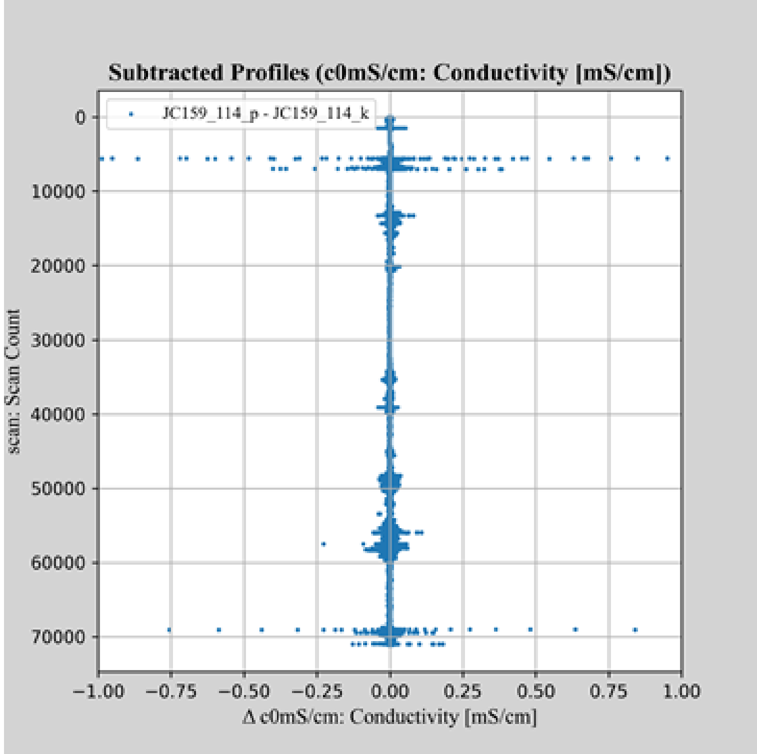
# Intercomparison results: Different methods

CTD intercomparison project

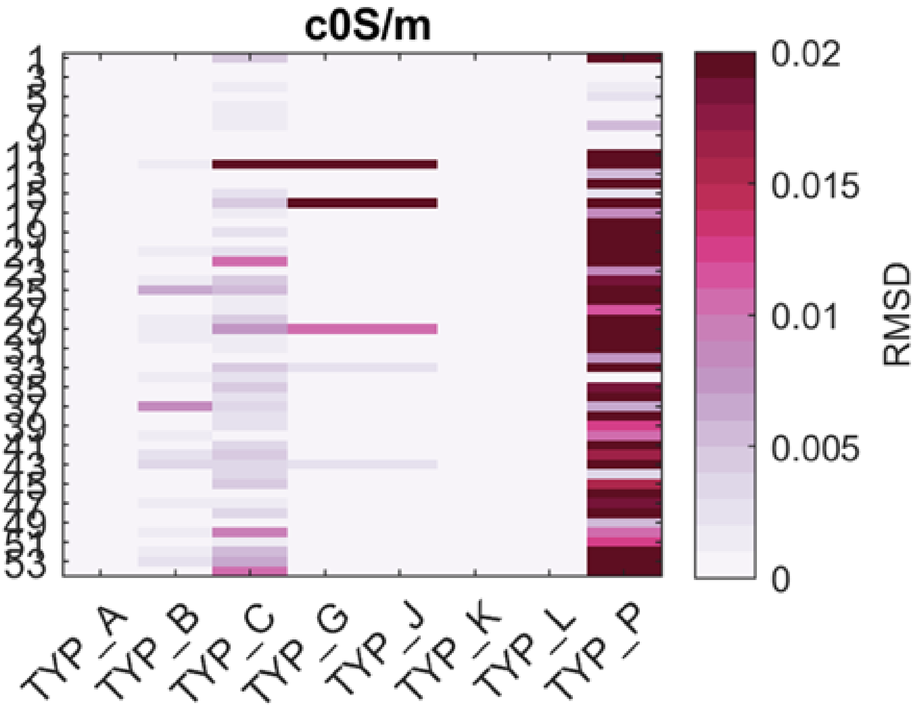
- Each group processes differently
  - Steps, settings, post-corrections
- Most participants inherited their routine and have not derived it themselves
- No one follows SeaBird or GO-SHIP recommended series of steps ("typologies")
- Statistically, the most "average" groups run two processing typologies
  - A, B, C
  - H, J
  - Unprocessed typology is "P"

| Typology | A | B | C | H | J |
|---|---|---|---|---|---|
| # Part. | 2 | 1 | 2 | 1 | 1 |
| Steps order | # datcnv | # datcnv | # datcnv | # datcnv | # datcnv |
| | # wildedit | # wildedit | # wildedit | # filter | # alignctd |
| | # filter | # filter | # filter | # alignctd | # filter |
| | # alignctd | # celltm | # alignctd | # celltm | # loopedit |
| | # celltm | # loopedit | # celltm | # loopedit | # celltm |
| | # loopedit | # wfilter | # loopedit | # wfilter | # binavg |
| | # binavg | # binavg | # binavg | # binavg | # file |
| | # file | # file | # wfilter | # file | |
| | | | # file | | |

# Intercomparison results: different methods and effect on T, S




Conductivity changes for unprocessed data vs typology "K" (GO-SHIP)

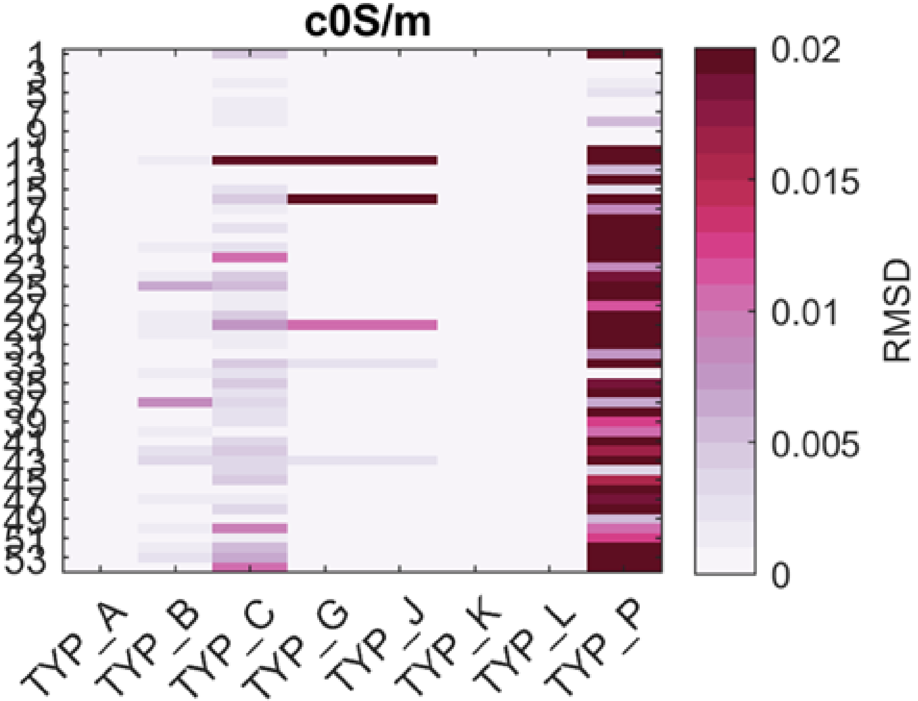



Visualizing root mean square deviation for different typologies against type A. Type P is unprocessed (Figure credit Dr. Berx, Scottish Marine Directorate)

# Intercomparison results: different methods and effect on T, S

Finding "significant" steps

- Few groups did pressure adjustments external to SBEDataProcessing
- *# celltm* is a very minor improvement
- *# wfilter* placement matters
- Groups use *# alignctd* with different settings




Visualizing root mean square deviation for different typologies against type A. Type P is unprocessed (Figure credit Dr. Berx, Scottish Marine Directorate)

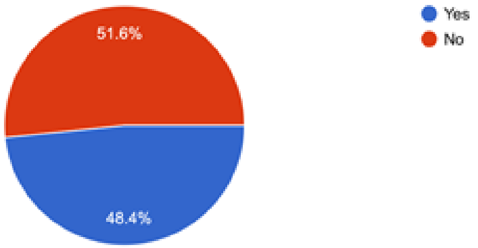
# Other survey results: Temperature

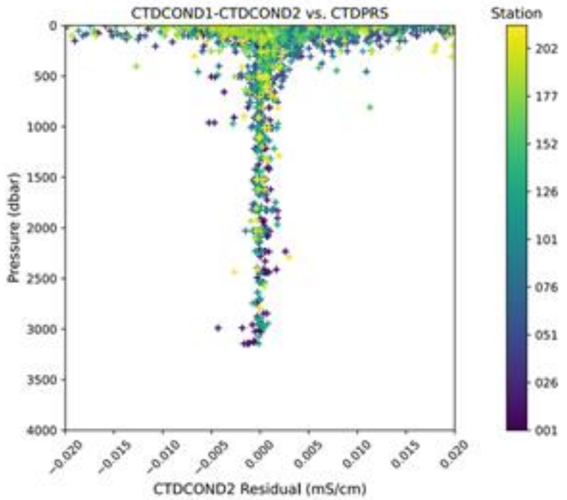
SBE35 sensor discontinued somewhere in the 2010s

- Existed to emulate traditional glass reversing thermometers

11) Do you calibrate for temperature?

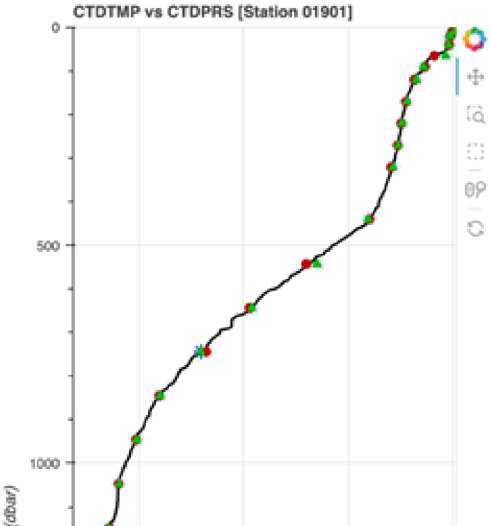
31 responses

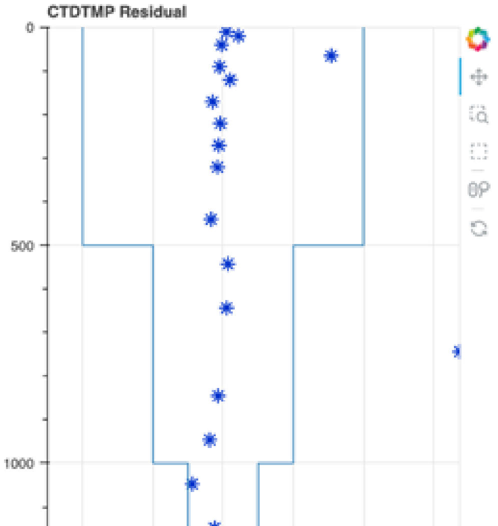



All Station Data:

| # | SSSCC | Bottle | CTDPRS | CTD Param | Reference | t_res | s_res | o_res | Flag | Comments |
|---|---|---|---|---|---|---|---|---|---|---|
| 0 | 01901 | 25 | 10 | 20.108 | 20.1085 | 0.0005 | -0.0071 | -0.8645 | 2 | |
| 1 | 01901 | 24 | 19.5 | 19.8525 | 19.8548 | 0.0022 | -0.0073 | -0.4055 | 2 | |
| 2 | 01901 | 23 | 39.7 | 19.8111 | 19.8109 | -0.0002 | -0.0071 | -0.5047 | 2 | |
| 3 | 01901 | 22 | 64.6 | 19.6637 | 19.6791 | 0.0154 | -0.0073 | -0.284 | 2 | |
| 4 | 01901 | 21 | 89.8 | 18.6055 | 18.6049 | -0.0005 | -0.007 | 0.2468 | 2 | |
| 5 | 01901 | 20 | 119.9 | 18.2632 | 18.2642 | 0.001 | -0.0076 | 0.1254 | 2 | |
| 6 | 01901 | 19 | 170 | 17.8119 | 17.8104 | -0.0015 | -0.0059 | -0.1233 | 2 | |
| 7 | 01901 | 18 | 219.8 | 17.5673 | 17.5669 | -0.0004 | -0.007 | 0.4819 | 2 | |
| 8 | 01901 | 17 | 270.3 | 17.3925 | 17.392 | -0.0006 | -0.0068 | 0.6886 | 2 | |
| 9 | 01901 | 16 | 320.4 | 17.151 | 17.1502 | -0.0008 | -0.0074 | 0.2735 | 2 | |
| 10 | 01901 | 15 | 439.9 | 15.9637 | 15.962 | -0.0017 | -0.0068 | -0.1063 | 2 | |
| 11 | 01901 | 14 | 542.5 | 13.512 | 13.5127 | 0.0007 | -0.0046 | 0.104 | 2 | |
| 12 | 01901 | 13 | 643.2 | 10.3943 | 10.3948 | 0.0005 | -0.0025 | 0.6452 | 2 | |
| 13 | 01901 | 12 | 743.6 | 7.939 | 7.9727 | 0.0337 | -0.0011 | -0.3594 | 3 | T_resid harms derived params |
| 14 | 01901 | 11 | 844.9 | 5.995 | 5.9943 | -0.0007 | -0.001 | -1.4211 | 2 | |

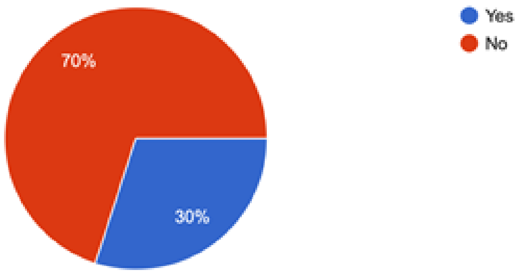


# Other survey results

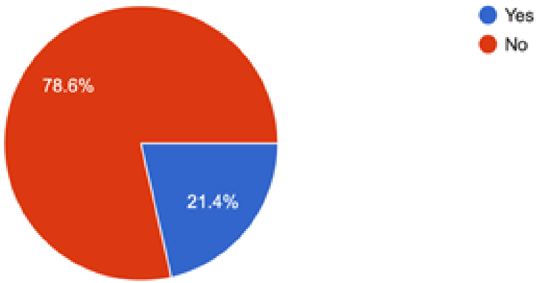
20) Do you correct the pressure dependency of your temperature sensor?

30 responses



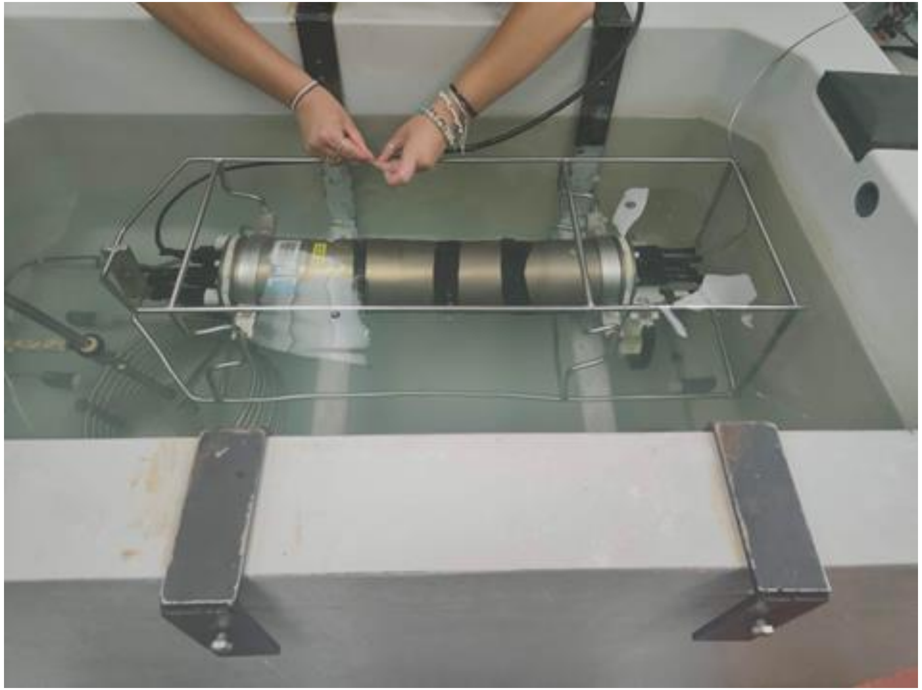

21) Do you routinely identify and adjust the pressure dependence of your conductivity sensor , eg change CpCor if a SeaBird CTD?

28 responses



# Pressure adjustments

- SeaBird recommends recalculating the pressure offset with routine adjustments to the XMLCON file (deck testing).
- In the SIO calibration laboratory, it can take 3-4 minutes for a CTD to equilibrate
  - +0.41 dbar when turned on
  - -0.11 dbar after 195 seconds
  - 0.52 dbar of difference before going in the water. Helpful to zero in on “0”.
- In the field, pressure should be done cast by cast
  - Pressure before cast: -0.15 dbar
  - Pressure after cast: -2.09 dbar
  - 1.96 dbar difference during the cast changes where samples came from
- SBE9 calibrations drift over time, even if unused

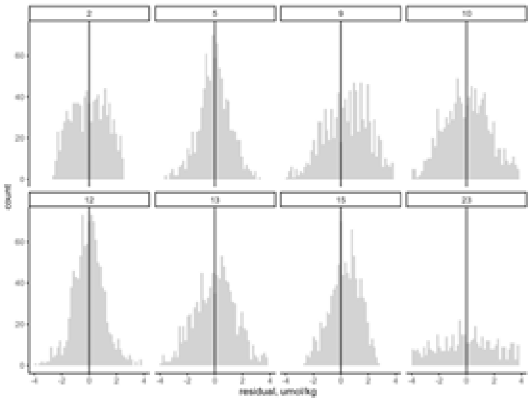


# Intercomparison results: different methods and effect on O2

Oxygen comparisons

- 3 different methods for calculating oxygen from voltage
- Some groups did not QC Niskin bottles
- Hysteresis correction is important

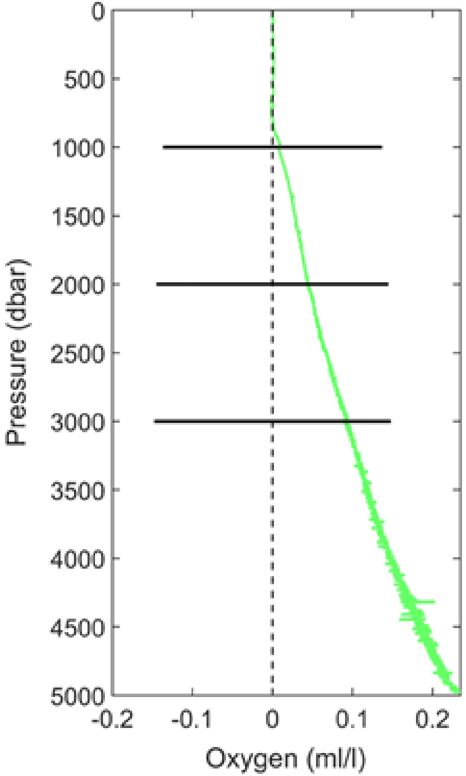
Histograms of residuals (all participants)



umol/kg

| Participant | mean residual | RMSE |
|---|---|---|
| 2 | -0.005 | 1.3 |
| 5 | -0.043 | 1.1 |
| 9 | 0.708 | 2.9 |
| 10 | 0.304 | 3.5 |
| 12 | -0.009 | 1.2 |
| 13 | 0.016 | 1.6 |
| 15 | 0.306 | 1.1 |
| 23 | 3.9 | 6.0 |

Oxygen comparison histogram (Figure credit Dr. Langdon, RSMAS)



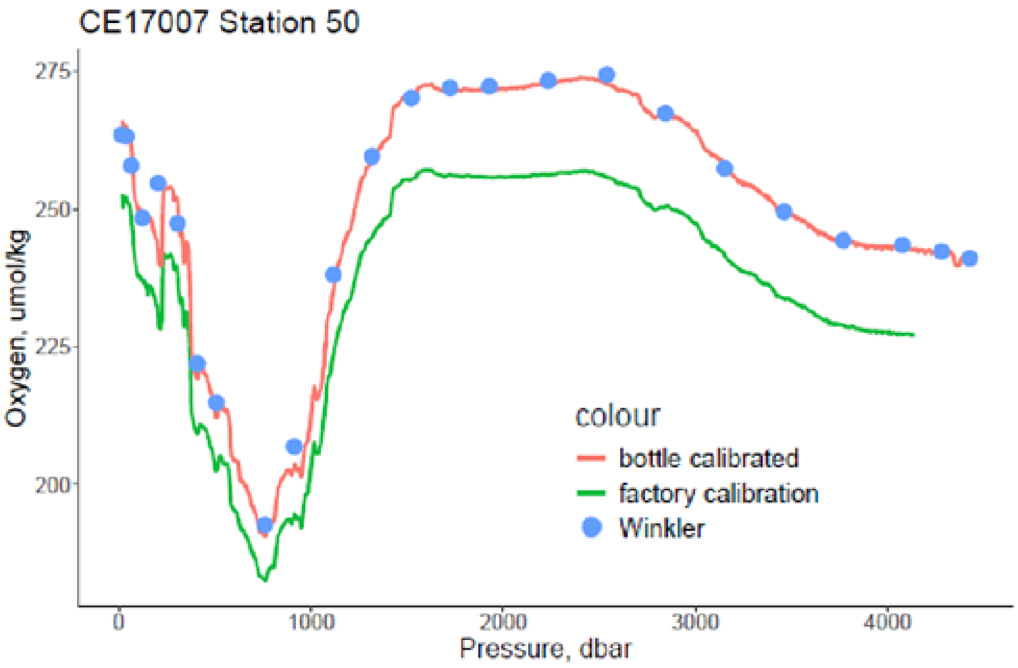

Hysteresis Vs No Hysteresis

# Experiment results: effect of bottle calibration on O2

<u>Oxygen comparisons</u>

- 3 different methods for calculating oxygen from voltage
- Some groups did not QC Niskin bottles
- Hysteresis correction is important
- 8 participants used Niskin bottles for oxygen analysis

- Bottle calibration is very important
  - Example from CE17007: the factory calibration of the SBE43 (green line) results in under estimation of bottle oxygen (blue circles) by 15 umol/kg



# Experiment results: effect of bottle calibration on O2

Oxygen comparisons

- 3 different methods for calculating oxygen from voltage
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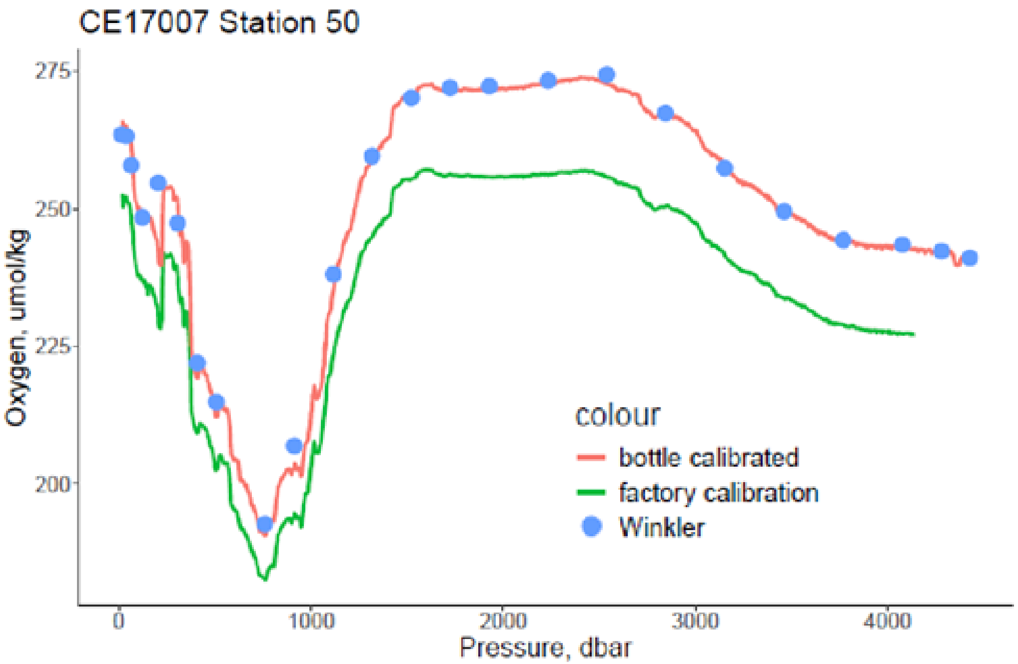
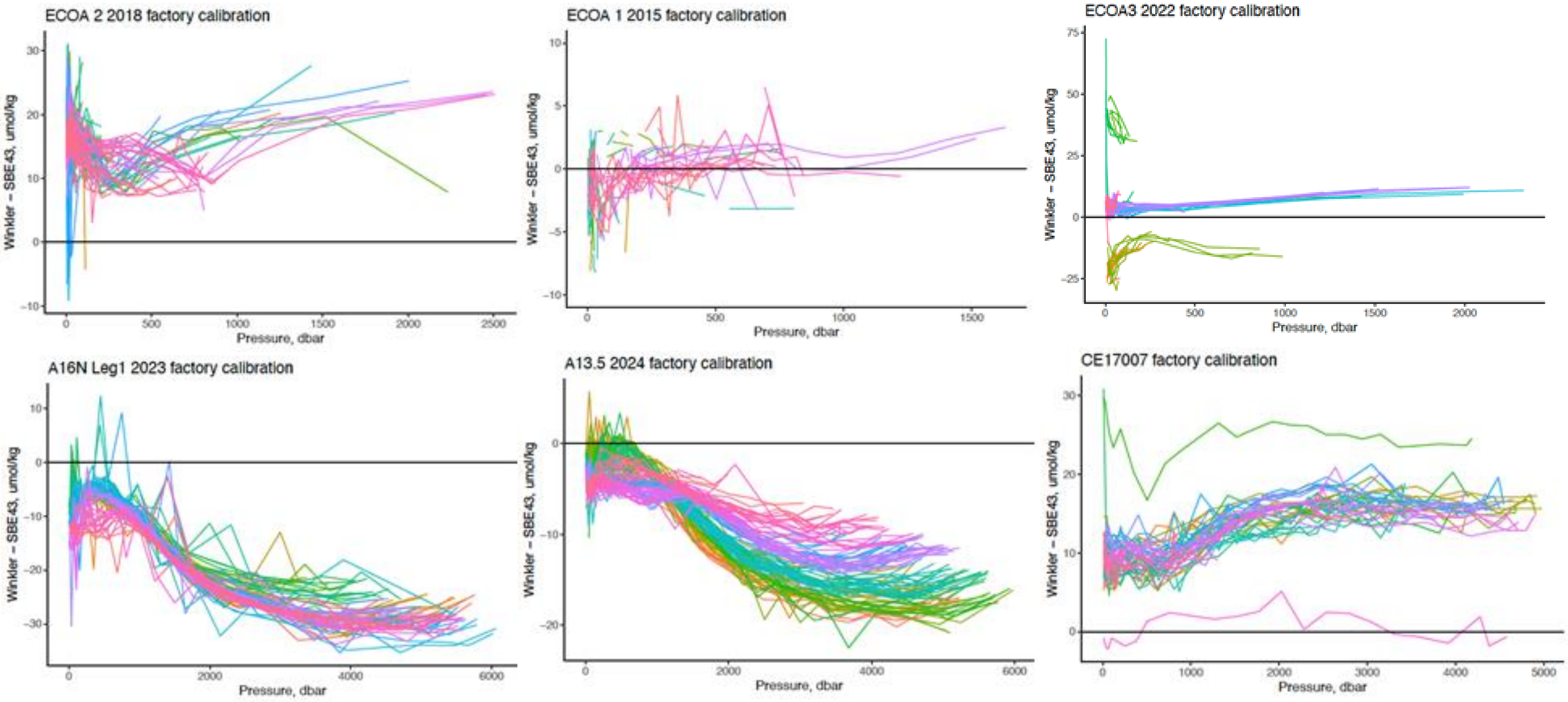
  Example from CE17007: the factory calibration of the SBE43 (green line) results in under estimation of bottle oxygen (blue circles) by 15 umol/kg

  Adjustment of Voff, Soc and E coefficients results in good fit to bottle data

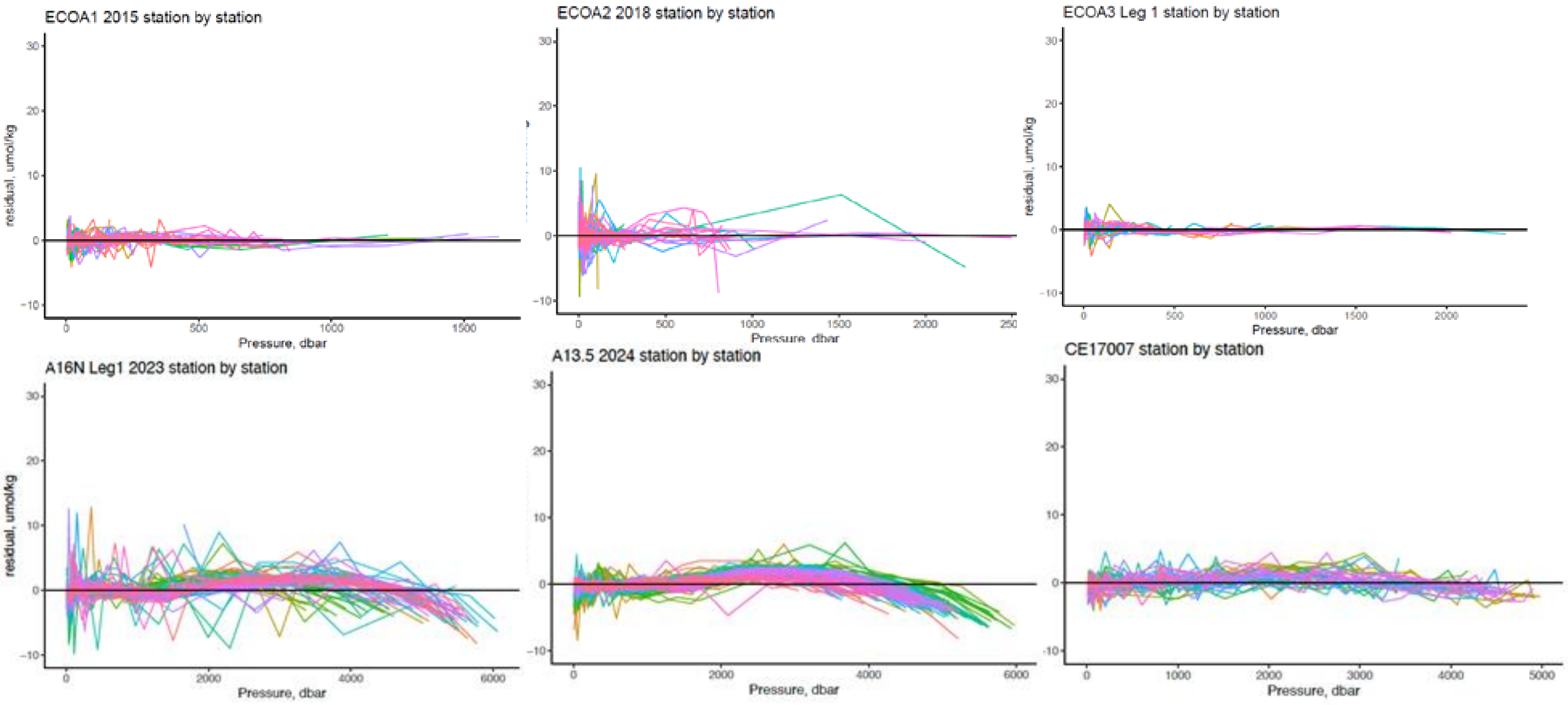



| Coefficient | factory | Fit to bottle data |
|---|---|---|
| Voff | -0.5093 | -0.551 ± 0.01 |
| Soc | 0.5902 | 0.594 ± 0.004 |
| E | 0.036 | 0.0395 ± 0.0006 |

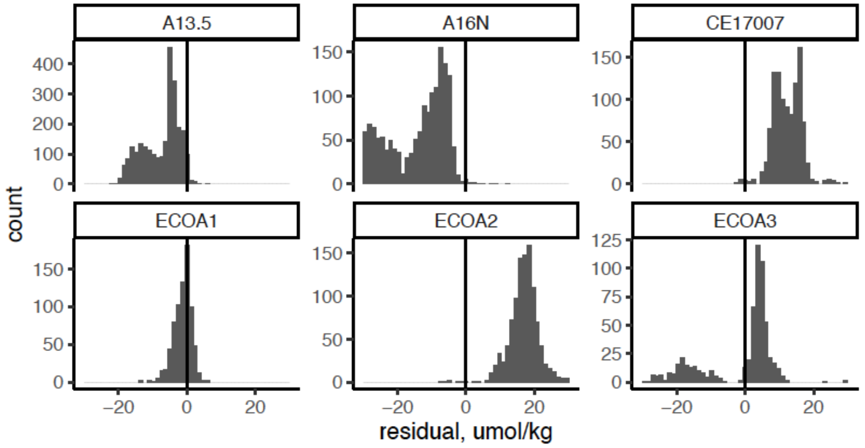
# Experiment results: effect of bottle calibration on O2



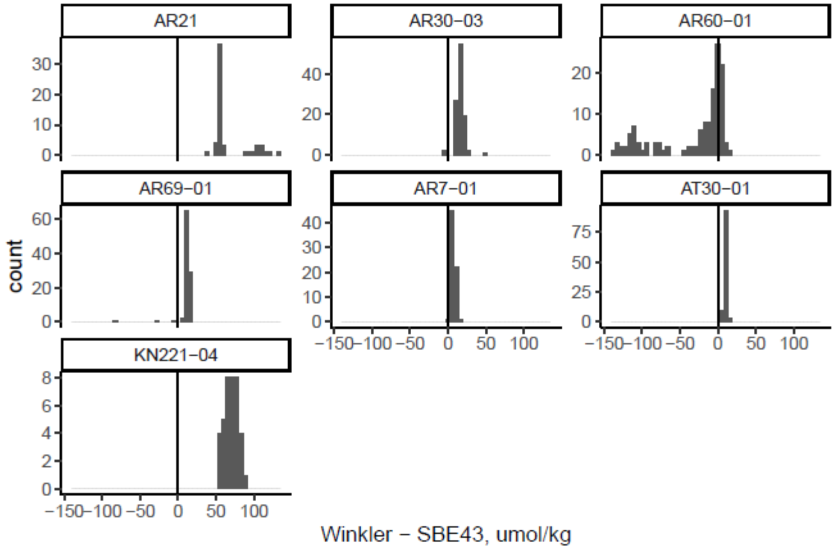
# Experiment results: effect of bottle calibration on O2



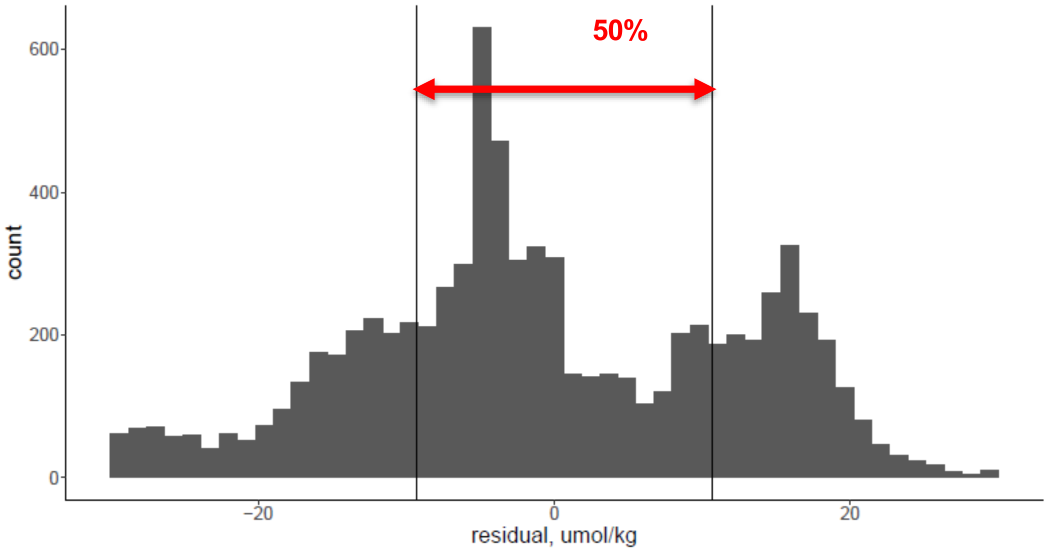
# Bottle calibration of O2




residuals based on factory calibration. Analysis: Langdon

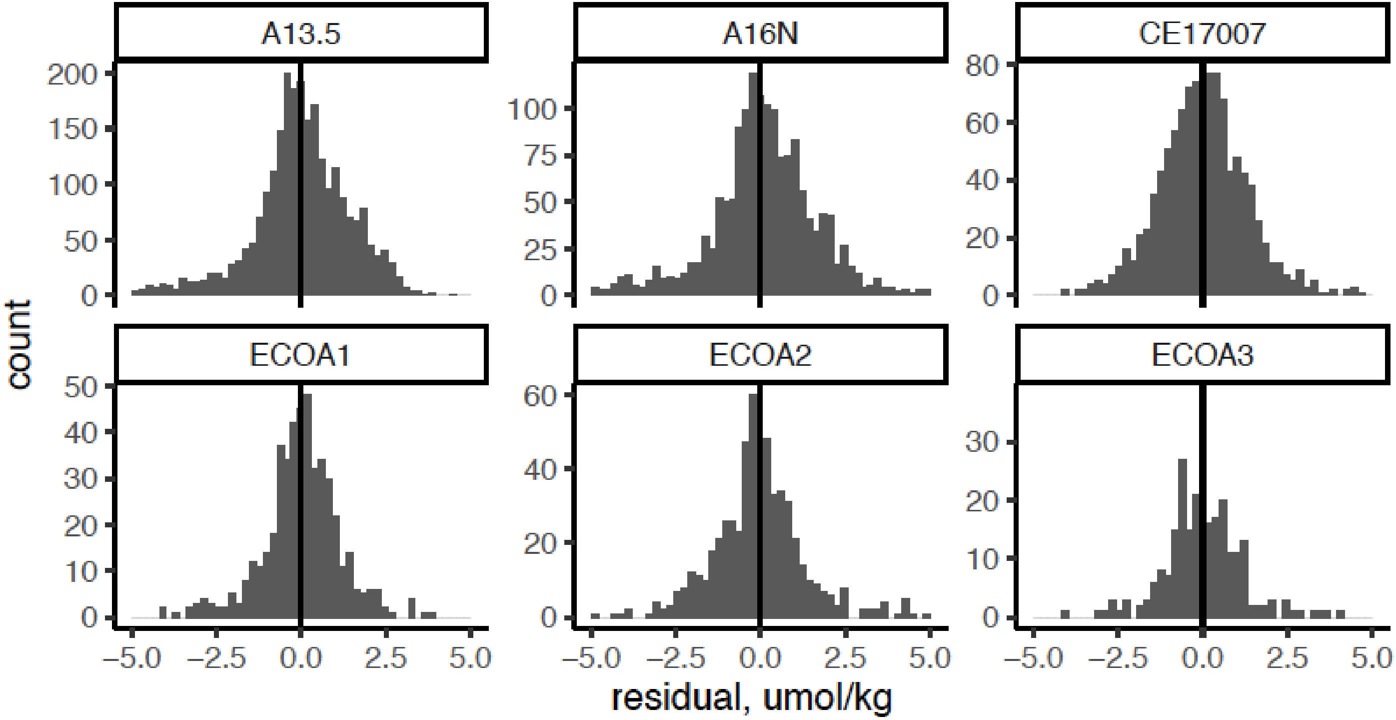


# How are accurate are uncalibrated CTD $O_2$ data?




Based on the analysis of data from 13 cruises, 50% of the uncalibrated data can be expected to be high or low by more than 10 umol/kg. Analysis: Chris Langdon

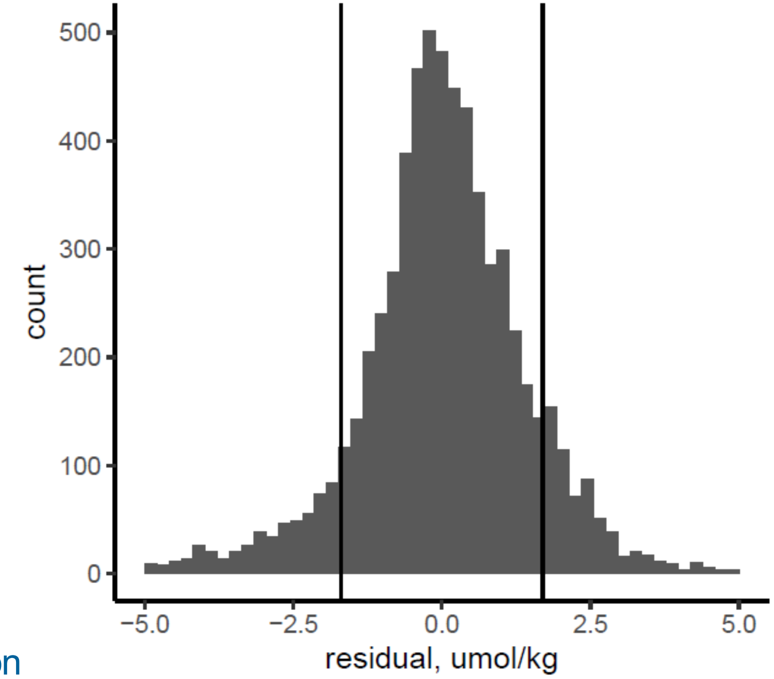
# Oxygen residuals when post calibrated by station




Analysis: Chris Langdon

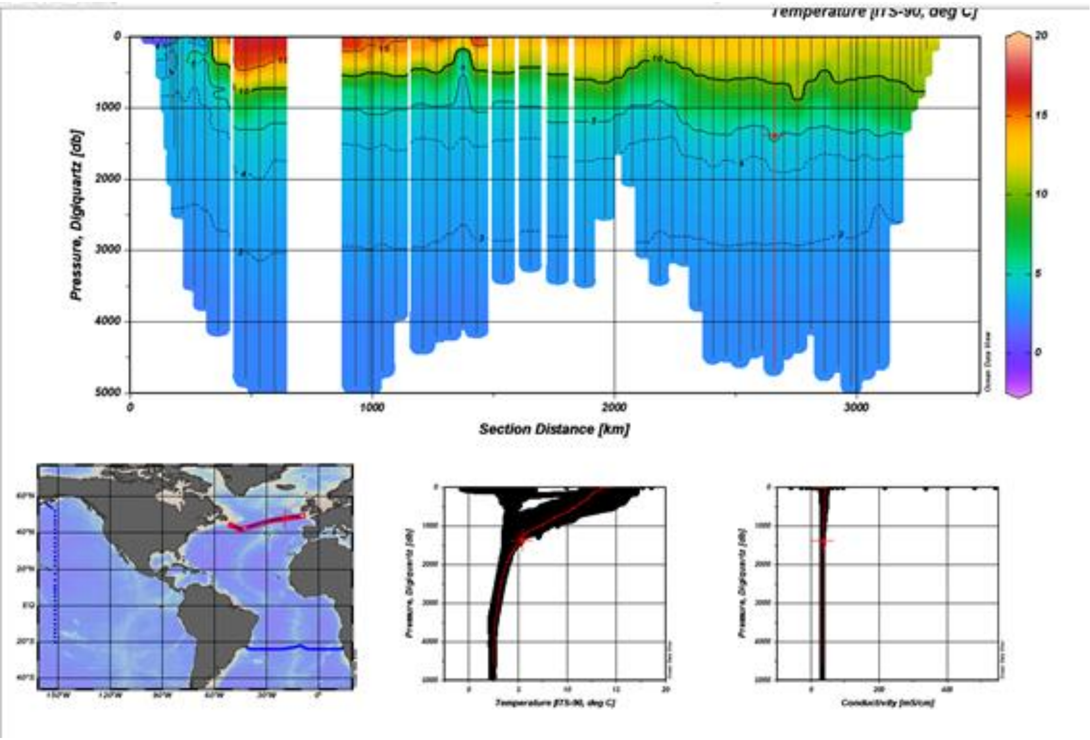
# Oxygen accuracy when post calibrated by station

If the CTD O2 data is calibrated, 90% of the data fall within the range -1.7 to + 1.7 umol $O_2$/kg



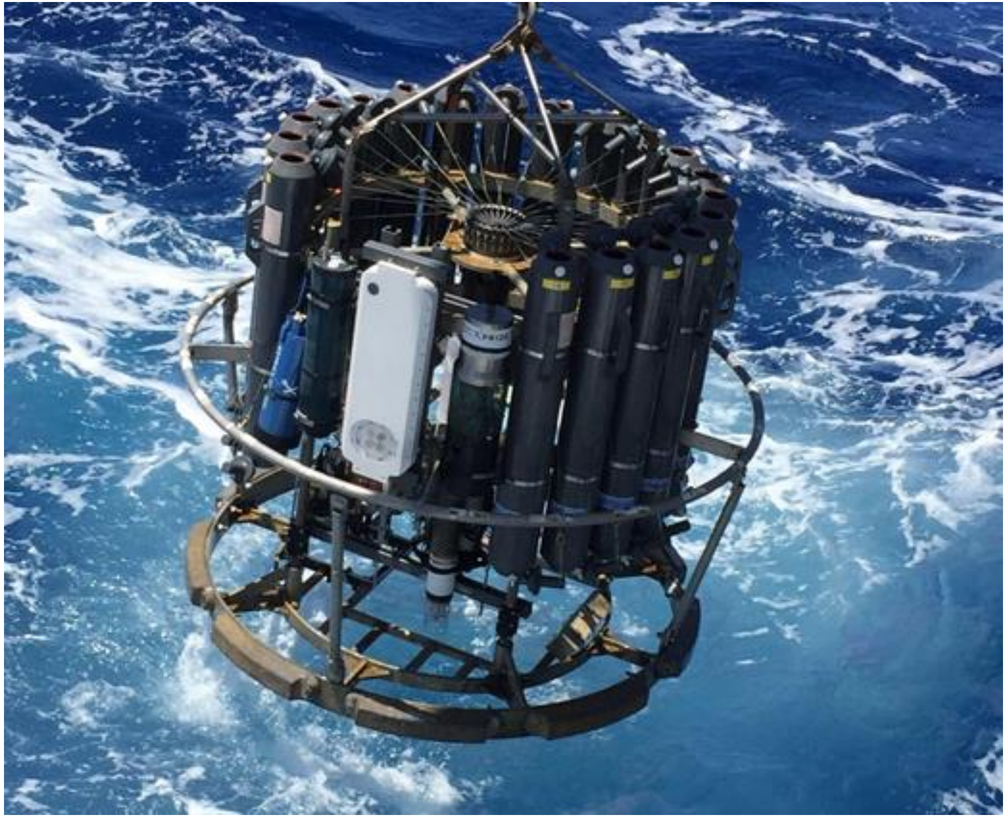

Analysis: Chris Langdon

# What's next for our analyses

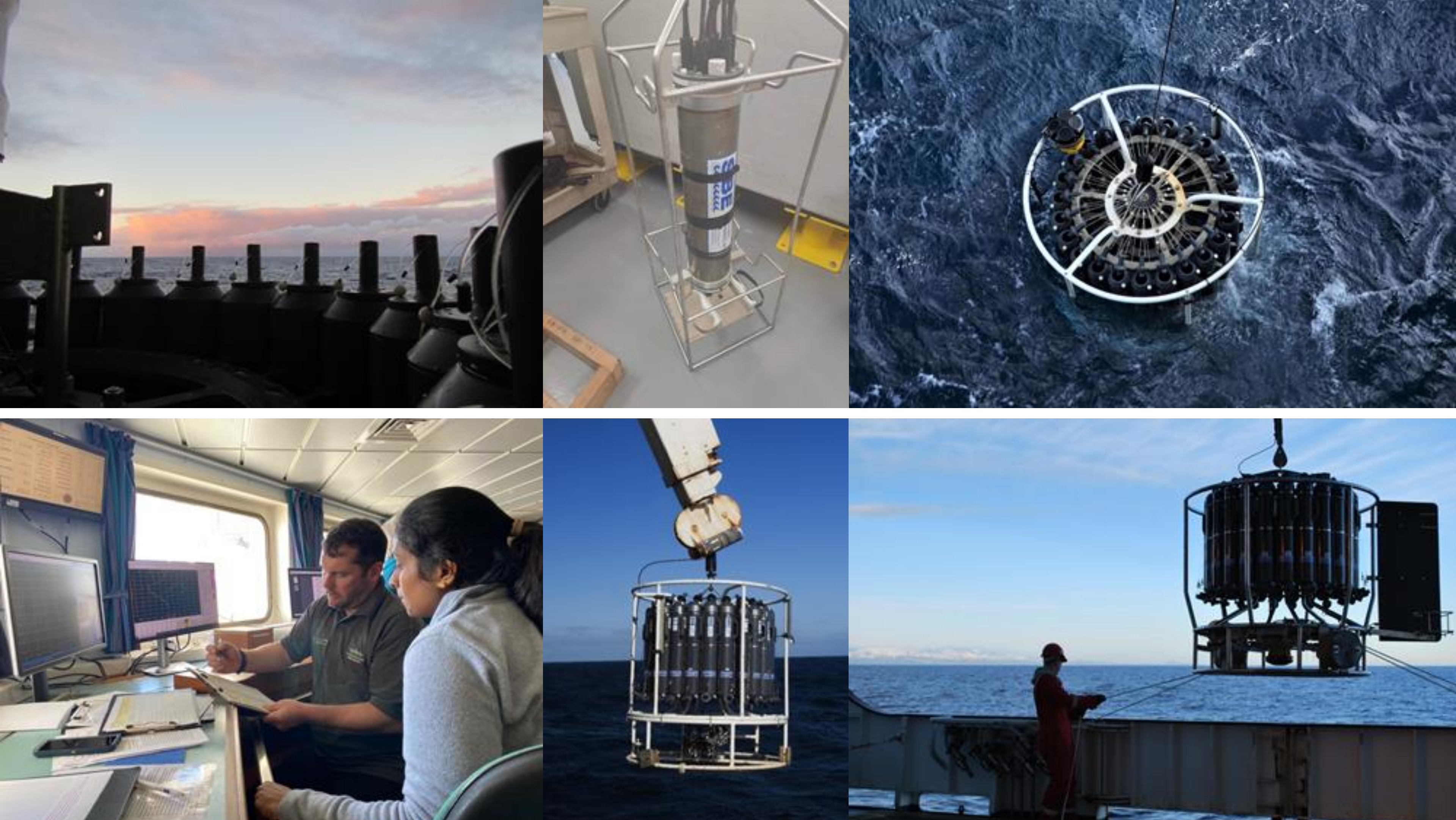



- Future analyses
  - Looking into *step settings*, rather than just typologies
    - Disentangle statistical bias
  - Expanding to a meridional section
  - Oxygen optimizations

# Next steps for the working group and community

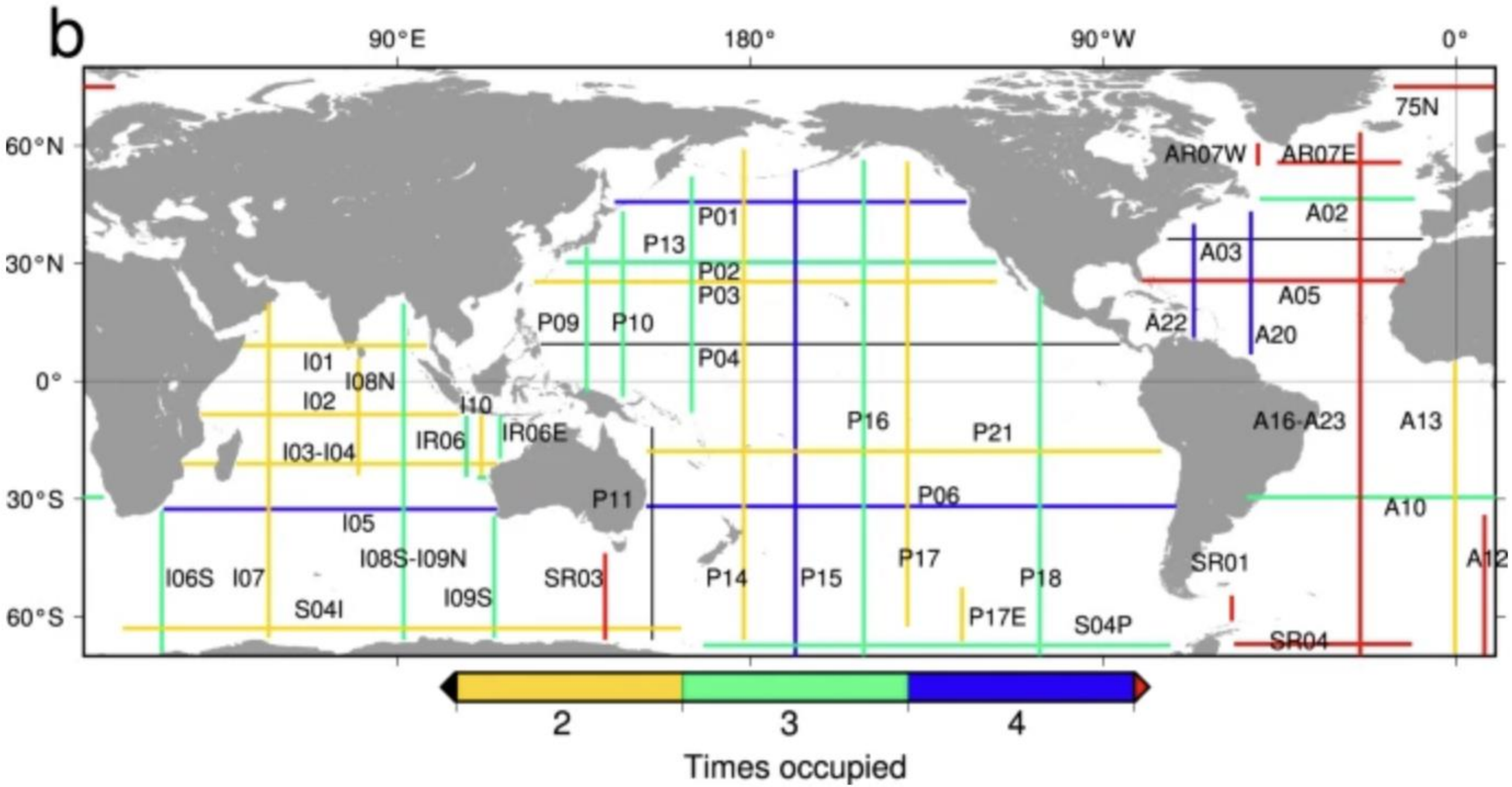


- Publish results from survey and $CTDO_2$ intercomparison.
- Revised GO-SHIP Standard Operating Procedures (SOP)
- Develop Library of Tools and Practices - software, training resources.
- Benchmark datasets for testing your procedures.
- Establish CTDO2 practitioners and users community.

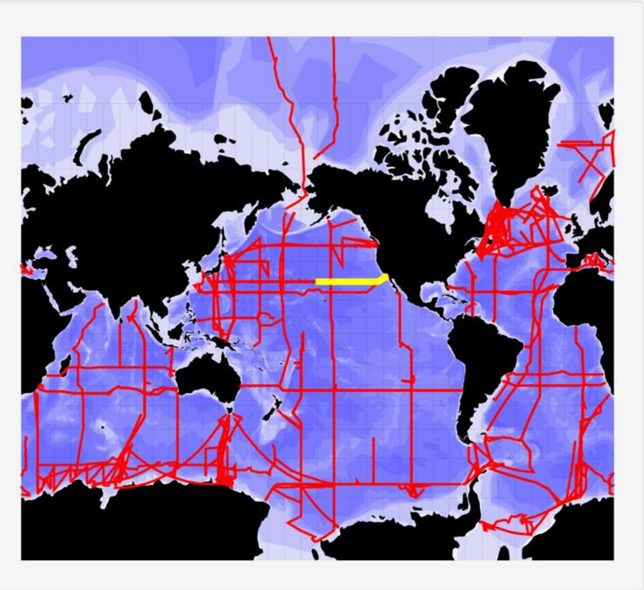


# Data Products: GO-SHIP Easy Ocean and GLODAP

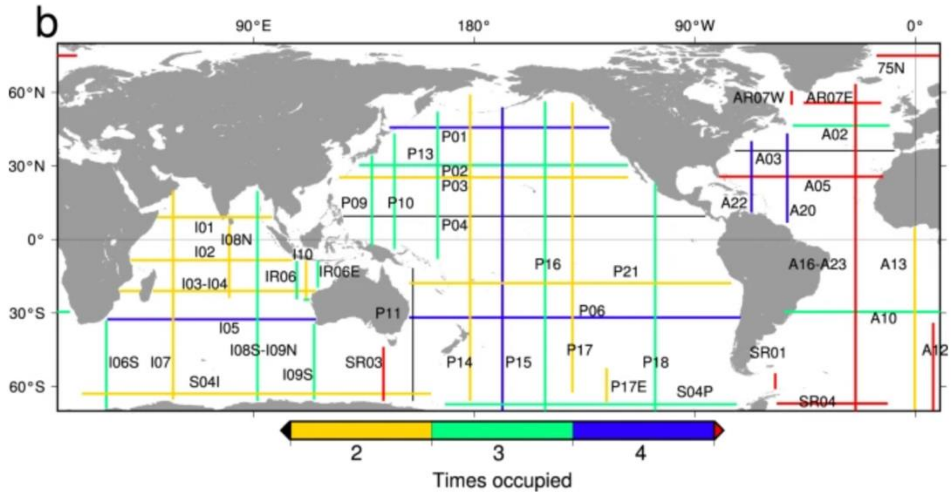
# GO-SHIP Easy Ocean



# Gridding to standard x, y, z

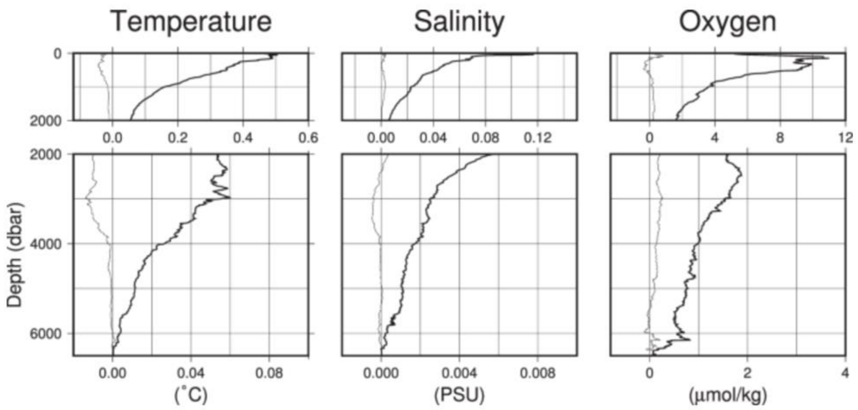


GO-SHIP basin sections are long, and not always completed by on one voyage or one research ship. They are broken into multiple sections. For many science application you need a complete section that is on the same grid.




CCHDO – is the global data center for all GO-SHIP data.

# Gridded Data product



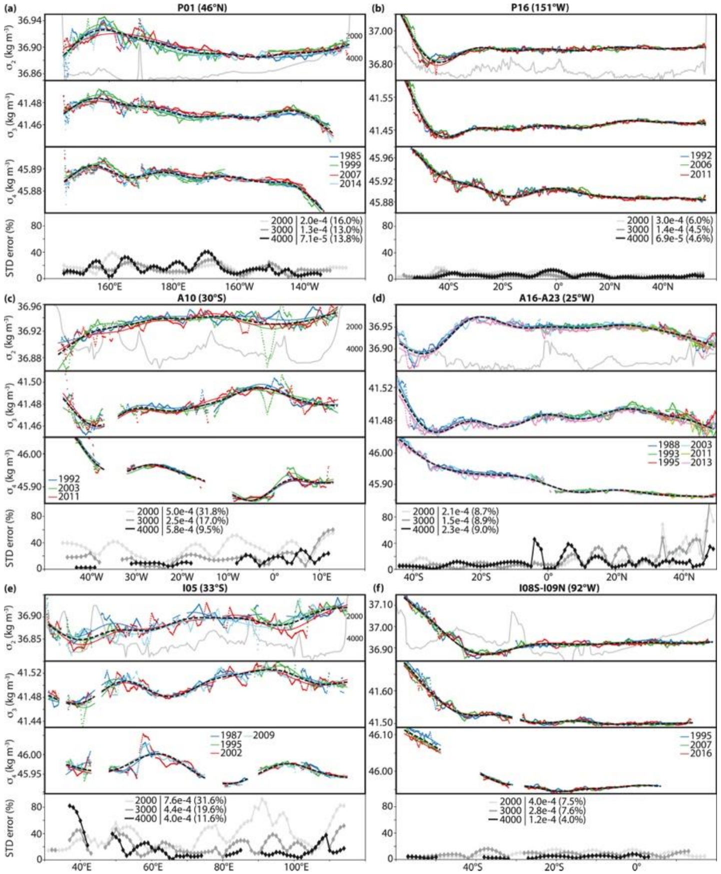

Errors introduced in the gridding procedure. The thin lines show the average of the errors (biases) and the thick lines show the standard deviation of the errors estimated at each depth.

The meridional or zonal station data are interpolated to a standard 0.1° horizontal grid. Vertically, the data were interpolated to a 10 dbar grid with a Gaussian filter. We used an objective mapping method by Roemmich.

The mapping is performed in two steps; the first for the large-scale field with a horizontal scale of 40 station spacing (approximately 2200 km, signal-to-noise ratio 0.1) and the second for the eddy field with a scale of two station spacing (approximately 110 km, signal-to-noise ratio 0.3).

The distance of 40 stations varies less than 40% among occupations and the gridding is not sensitive to the choice of the correlation length

# Testing the assumption of a steady state ocean

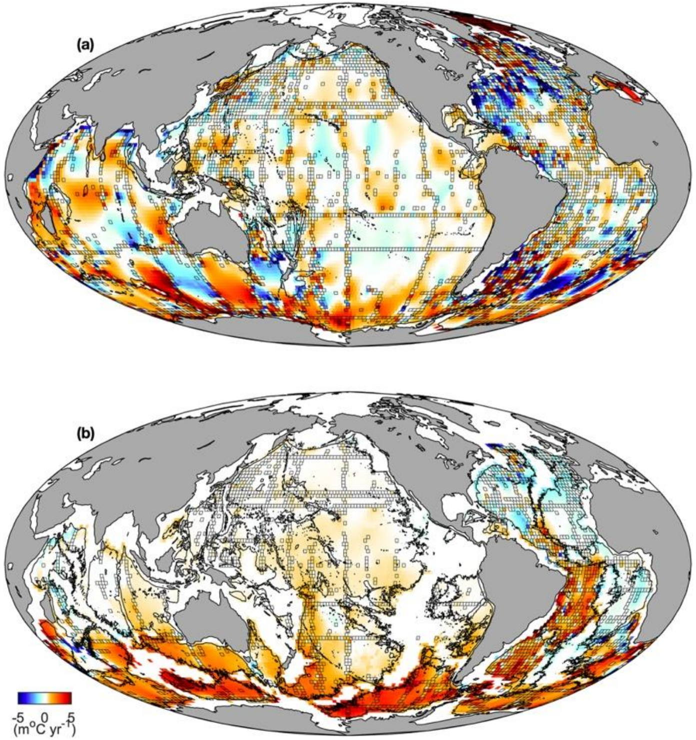



Hautala and Finucane 2022, find that away from boundary currents, planetary-scale potential density gradients in most parts of the deep ocean are stable from occupation to occupation, with higher variability in a few expected regions and for shorter sections.

Median standard errors from all sections are 12%–17% in the Pacific, 10%–23% in the Atlantic, and 11%–36% in the Indian Ocean, with the highest values at 2,000 dbar and lowest at 4,000 dbar.

Representative sections from the Pacific (a and b), Atlantic (c and d), and Indian Ocean (e and f) with the *Easy Ocean* nominal latitude or longitude in parentheses.

# Decadal Ocean Change




Combining GO-SHIP and deep Argo for deep ocean change.

Map of (a) deep (2,000–4,000 dbar) and (b) abyssal (4,000–6,000 dbar) pressure-averaged decadal temperature trends in 167 × 167 km bins with the 2,000 and 4,000 dbar isobars of bottom bathymetry contoured, respectively (black lines). Bins with directly measured trends are bordered by light black lines, with the remaining bins values interpolated by natural neighbor ( Johnson and Purkey, 2024).

# GLODAP – using QC GO-SHIP data

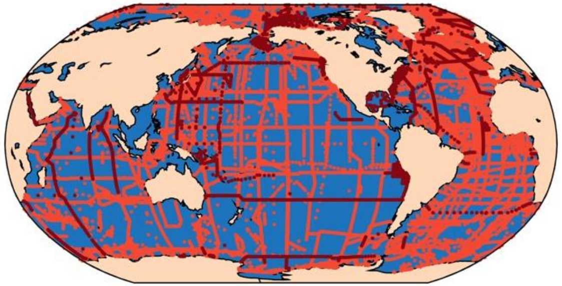
GLODAP does a secondary quality control of salinity, oxygen, nutrients, TCO2, and TAlk was carried out through crossover and in- version analyses.

This uses least-squares models (Menke, 1984; Wunch, 1996) to calculate the set of corrections required to simultaneously minimize all cruise- by-cruise offsets.

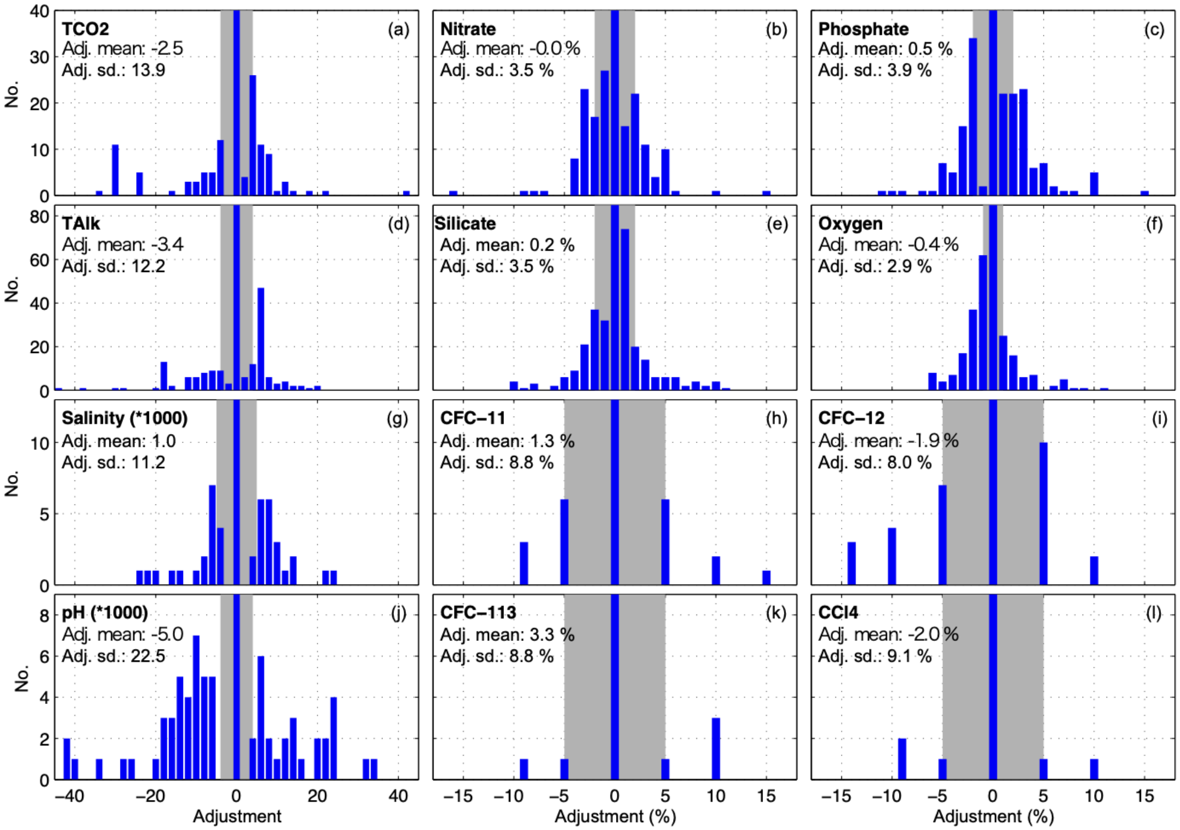
Let **G** be the model matrix of size *o* x *n*,
where *o* is number of crossovers and **n** number of cruises, *d* is the *o* crossover offsets, and *m* is the *n* corrections such that

$\mathbf{G} \times m = d$,
then
$m = \mathbf{G}^T \times (\mathbf{G} \times \mathbf{G}^T)^{-1} \times d$.

This model is known as simple least squares (SLSQ). Johnson et al. (2001) also introduced the weighted least squares (WLSQ) and weighted damped least squares (WDLSQ) models.

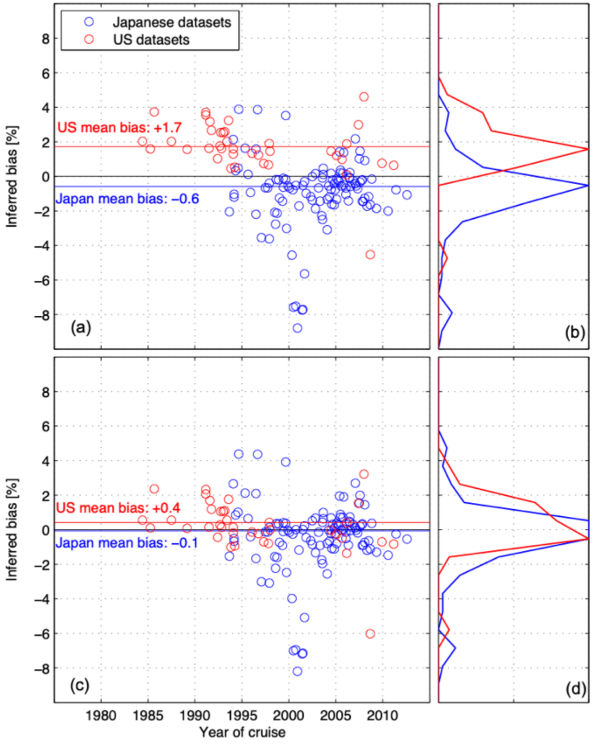


# GLODAP Error analysis




Size distribution of applied adjustments for each core variable that received secondary QC. Gray areas depict the initial minimum adjustment limit. (A. Olsen et al., 2016)

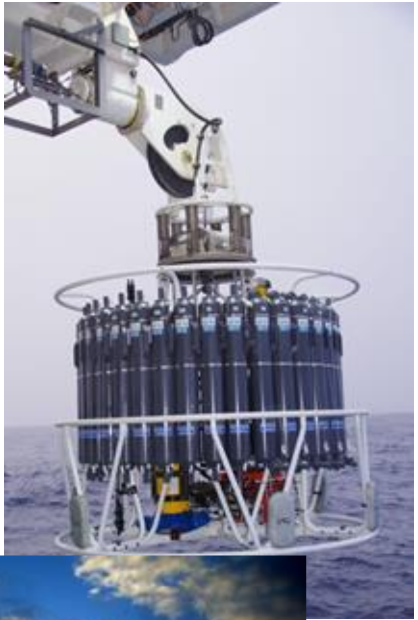
# Comparison by Country




Silicate biases between US and Japanese efforts before (a, b) and after (c, d) pre-adjustments (US:−1 %; Japan: +1 %) were applied to the data (see main text for details).

Data from “Line P” and many small-scale cruises in the variable Kuroshio region were excluded from this analysis. Red and blue horizontal lines indicate countries’ approximate mean offsets.


RP 32
RP 31
RP 30
RP 29
RP 28



# Summary

Data quality assurance and control is a continuous process;

- Pre-deployment – are the instruments calibrated are these calibrations  up-to-date.

- On voyage – constant checking of data collected.

- Post-voyage – detailed comparison of data, check consistency of data

- Submit data with error estimates

- Make data product – add gridding errors.

Repeat these steps.

# Q&A and open discussion

# Experiment results: Adjusting Individual Seabird Steps

Adjust only one processing step, re-process and calculate changes

**Wild edit**: 5-7 decimal places (T & C)
*massive on DO

**Filter**: 5-7 decimal places

**Loop Edit**: 5+ decimal places (0.25 vs 0.05 $ms^{-1}$)

**Align CTD**: 4 decimal places on C (+0.073)