Recommended updates to BGC <PARAMETER>_ACCURACY and <PARAMETER>_ADJUSTED_ERROR specifications

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Purpose of this discussion:

1. Review current specifications for <PARAMETER>_ACCURACY AND <PARAMETER>_ADJUSTED_ERROR FOR DOXY, NITRATE, AND PH
2. Identify areas where these specifications require modification, and provide recommendations. **Recommendations are highlighted in purple throughout.**

Motivation:

AOML and MBARI need to better utilize these fields

- AOML – **<PARAMETER>_ACCURACY** and <PARAMETER>_RESOLUTION remain empty
- MBARI – **<PARAMETER>_ADJUSTED_ERROR** is filled, but not at required granularity and not always in accordance with definitions listed in Argo parameter documentation

- Current accuracy specs do not represent what is observed in the field, especially for pH
- And, from Bittig et al, 2019: "Sea-Bird Scientific claims an initial stated accuracy of ±0.05 pH"
- Recommended change to documentation:
  - NITRATE_ACCURACY = **3 µmol/kg**
  - PH_IN_SITU_ACCURACY = **0.05**

NITRATE (NITRATE_ACCURACY[1] = 2 µmol/kg)
First offset* adjustment from SAGE QC matrix, by sensor type:

Sensor	N	Mean (µmol/kg)	Median (µmol/kg)	Std (µmol/kg)
Navis – SBE SUNA	24	2.582	2.279	2.462
APEX – MBARI ISUS	159	0.649	0.374	3.210

pH (PH_IN_SITU_TOTAL_ACCURACY[2] = 0.005)
First offset* adjustment from SAGE QC matrix, by sensor type:

Sensor	N	Mean	Median	Std
Navis – SBE DURA	16	-0.0382	-0.0329	0.0800
APEX – MBARI DURA	140	-0.030	-0.0194	0.0512

[1]Processing Bio-Argo nitrate data at the DAC level https://archimer.ifremer.fr/doc/00350/46121/55922.pdf
[2]Processing BGC-Argo pH data at the DAC level https://archimer.ifremer.fr/doc/00460/57195/61336.pdf
* Offset = float-reference at 1500m

NITRATE_ADJUSTED_ERROR

- Recommendation for in-situ data calibrated to reference algorithm (in DM):

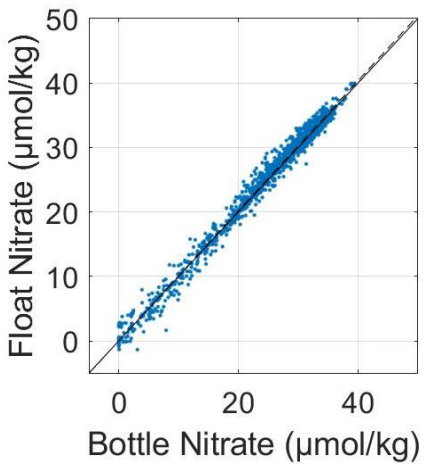
NITRATE_ADJUSTED_ERROR = **1 µmol /kg** + DOXY_ADJUSTED_ERROR /10

- No change to RT error specification

NITRATE_ADJUSTED_ERROR = elast + 1 umol/kg year-1 · (T – Tlast)

	Nitrate 1st-year drift (µmol kg^{-1} yr^{-1})	Nitrate 2nd-year drift (µmol kg^{-1} yr^{-1})
Median	-0.173	0.058
Mean	-0.507	-0.092
Std dev	1.581	0.978

	Bottle-Float nitrate
mean	-0.245
median	-0.153
stdv	0.928



PH_IN_SITU_TOTAL_ADJUSTED_ERROR

- Recommendation for in-situ data calibrated in DM (using reference algorithm):

PH_IN_SITU_TOTAL_ADJUSTED_ERROR = 0.01 + **DOXY_ADJUSTED_ERROR*0.0016**

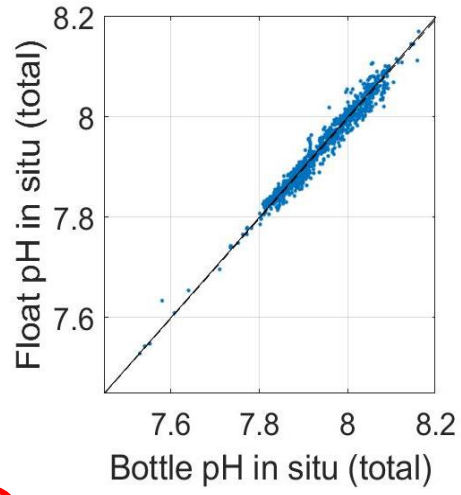
(0.0016 ref Williams et al, 2016 supplemental)

- Recommendation for in-situ data calibrated in RT:

PH_IN_SITU_ADJUSTED_ERROR = elast + **0.03year-1** · (T – Tlast)

	pH 1st-year drift (yr^{-1})	pH 2nd-year drift (yr^{-1})
Median	-0.001	-0.003
Mean	-0.021	-0.004
Std dev	0.062	0.036

	Bottle-Float pH
mean	0.003
median	0.003
stdv	0.015



DOXY_ADJUSTED_ERROR

- In Argo Quality Control manual for dissolved oxygen concentration https://archimer.ifremer.fr/doc/00354/46542/59751.pdf , DOXY_ADJUSTED_ERROR specifications are in units mbar, to be converted to µmol/kg-equivalent by the data manager.
- *Units of mbar are not as meaningful to users*, and also issues with specification around 0-oxygen
- Recommendation:

In O2 QC manual:

- Keep one value/small range for error in units of mbar as recommendation; Data managers convert to umol/kg equivalent for population of DOXY_ADJUSTED_ERROR
- Add explanatory sentence on magnitude of approximate conversion, ie "2 mbar (equivalent to 2-5 umol/kg depending on in-situ TEMP and PSAL"
- Add additional text describing that a constant 2mbar error may not be appropriate in all cases (ie near O2 minimum zones, Johnson et al, 2019; Wojtasiewicz et al, 2018)

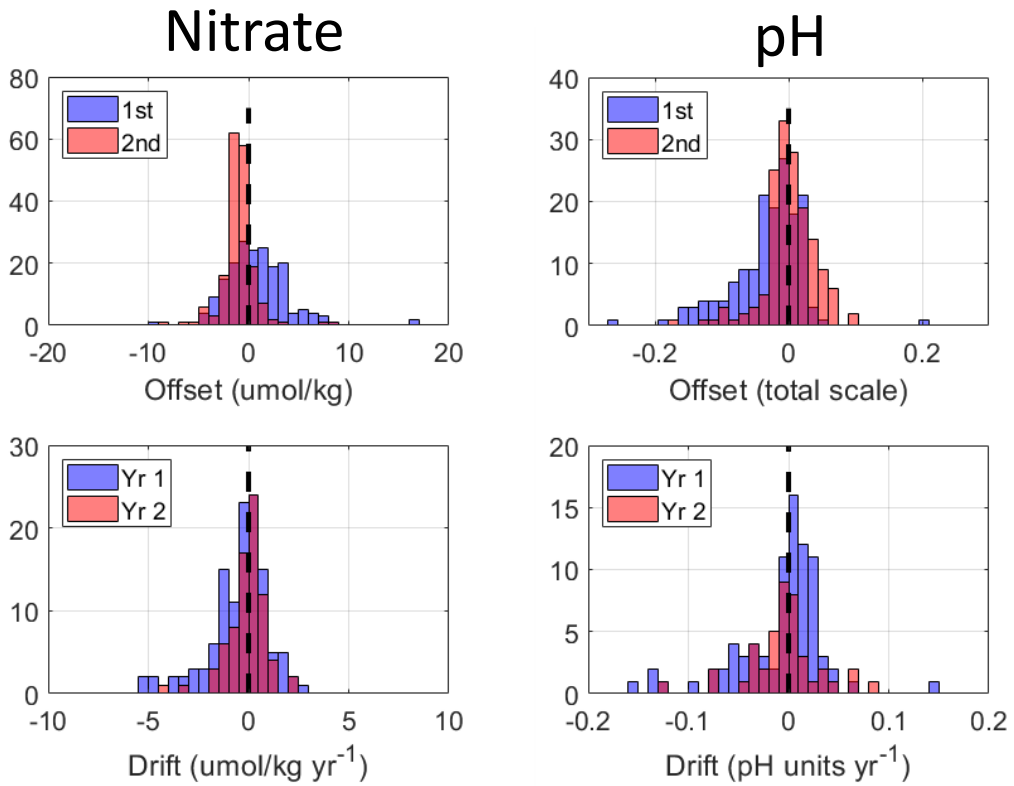
In profile files:

- Add SCIENTIFIC_CALIB_COMMENT field, ie:

"DOXY_ADJUSTED_ERROR recomputed from a PPOX_DOXY_ERROR = [xx] mbar"

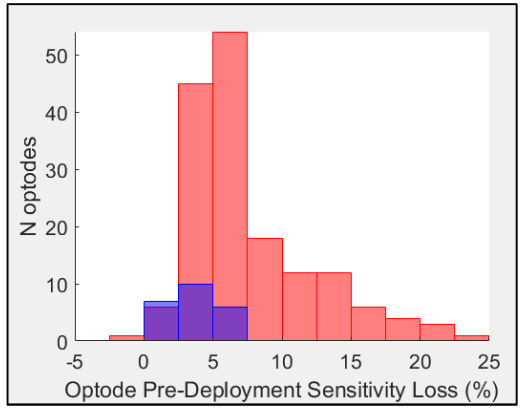
Delayed-mode adjustments improve accuracy. How much should we be adjusting data??

1st and 2nd offsets for nitrate and pH across SOCCOM array derived using SAGE software (float minus reference)



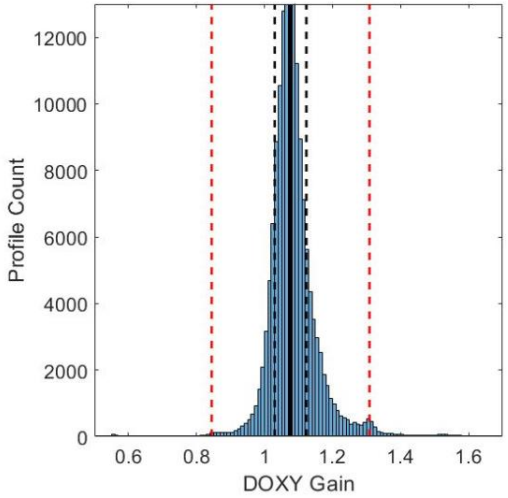
SOCCOM optode gains
(by float, computed using in-air, WOA or shipboard data)

Median = 5.6% sensitivity loss
MAD = 3.4%



BGC Argo DOXY gains
(by profile, computed using WOA)

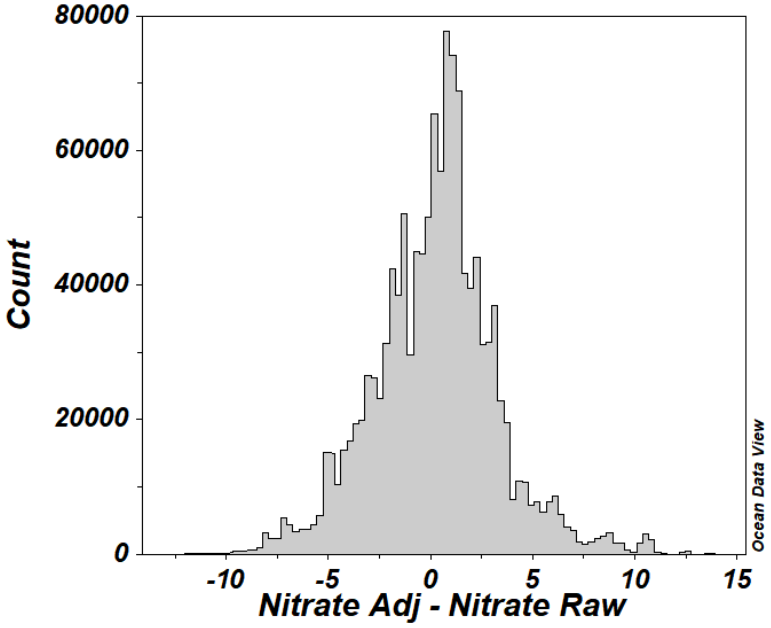
Median = 7.7% sensitivity loss
MAD = 4.6%



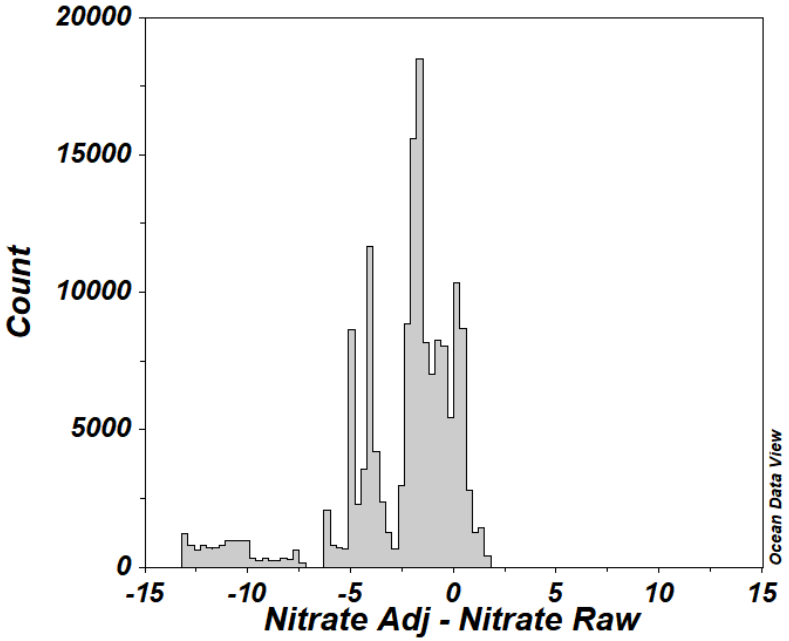
- Bulk statistics of initial adjustments can also guide DMQC operators in identifying sensor anomalies
- Larger-than-normal adjustments can occasionally indicate problems with sensor cals -- *should we be adjusting this data*?

Nitrate Adjustments on the GDAC, separated by platform/sensor

All UWMBARI Apex floats. ISUS nitrate sensor calibrated at MBARI. Mean = 0.2 umol/kg



All UW/MBARI Navis floats. SUNA nitrate sensor calibrated at Sea-Bird. Mean = -2.6 umol/kg



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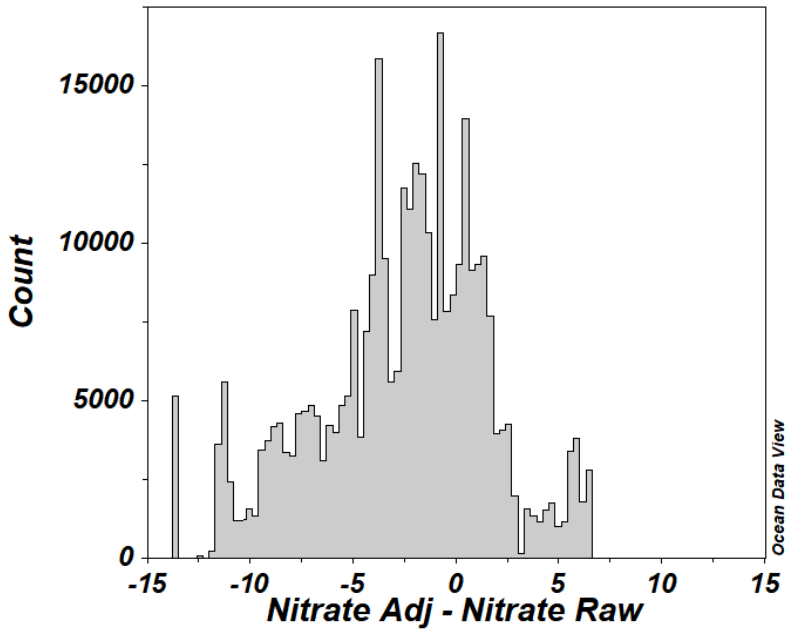

- Larger adjustments typically required for SUNA sensors vs ISUS
- Adjustments >> 10 umol/kg are acceptable but error estimates likely should be increased by 10% of the correction (Johnson et al 2013)

Final thought: Similar to core Argo, BGC should develop adjustment thresholds for chemical data beyond which data should be deemed "adjustable only under careful scrutiny", or "adjustable only with an increased error estimate"? (Not to be enforced)

- **Possible adjustment thresholds to assist in guiding DACs in delayed mode QC of DOXY, NITRATE, PH_IN_SITU_TOTAL**
- **Adjustments beyond these thresholds, while acceptable, should be considered with care as they may suggest sensor calibration (or other) issues**
- **A starting point, open to discussion, modification, inflation?**

	DOXY	NITRATE	PH
Initial Offset	--	7 µmol/kg [a]	0.1[a]
Drift	0.6% yr^{-1} [b]	2 µmol/kg yr^{-1} [c]	0.07 yr^{-1} [d]
Gain	20% [e]	?	--

[a] 2σ of first offset for APEX sensors in SOCCOM as a guide (see slide 7, extended ppt)
[b] drift range +/- 0.6%yr^{-1} for individual optodes, from Bittig et al, 2018; range for SOCCOM floats is larger at +/-1%yr^{-1}
[c] 2σ of 2nd yr drift across SOCCOM array as a guide (see slide 16, extended ppt)
[d] 2σ of 2nd yr drift across SOCCOM array (see slide 18, extended ppt)
[e] median+2xMAD of global BGCArgo profile gains (using WOA) ~=15% (see slide 9, extended ppt; note: MAD used in DOXY audit but is similar to stdv as a metric)

End