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Nitrate and pH (underway)

Data quality flag designation: 2 = acceptable; 3 = questionable

A prototype instrument (BGC-SUMO; Y. Takeshita - yui@mbari.org) for measuring seawater nitrate and pH was integrated into the *R/V Sally Ride's* underway seawater line (intake located at ~5 meters depth). Nitrate was measured using an In Situ Ultraviolet Sensor (ISUS) [*Johnson and Coletti*, 2002]. pH was measured using a Deep-Sea-Durafet (DSD) sensor [*Johnson et al.*, 2016]. An SBE45 MicroTSG thermosalinograph was located directly downstream (< 10 cm) of the instrument flow cell for underway temperature and salinity measurements near the sensors. The instruments were powered through an isolation transformer to prevent ground loop issues. The system was polled using a LabView interface and pH measurements were made every 30 seconds while nitrate measurements were made every 4 minutes. pH and nitrate sensor data were calibrated using discrete pH (n = 21) and nitrate (n = 11) samples, respectively, collected from the underway line throughout the cruise. BGC-SUMO pH data were converted from pH values measured at the BGC-SUMO TSG temperature to in situ pH at the ship intake temperature (MET), which was ~0.5 °C cooler than the BGC-SUMO TSG (Figure1). This pH temperature conversion calculation was performed using the program CO2SYS applying total alkalinity values estimated from the CANYON-B algorithm [*Bittig et al.*, 2018]. Nutrient concentrations were set to zero in these calculations. Large spikes in salinity, nitrate, and pH were identified using salinity deviations exceeding 0.8 units from the mean salinity over the cruise period. Small spikes in salinity, nitrate, and pH were defined as neighboring salinity values differing by > 0.03. A quality flag of 3 was given to "spike" data (Figure 2). Nitrate values that were negative or collected during the sensor warm-up phase or near-shore (during the transit back) were flagged as questionable (QF = 3). An offset of -0.93 µmol L^{-1} was applied to the underway nitrate data based on a comparison with the discrete nitrate samples (Figure 3). The nitrate sensor was cleaned regularly to minimize effects due to biofouling. Based on the QC method, flags for pH should be considered conservative, further evaluation by the data user may be needed.

Underway ship (MET) and BGC-SUMO data were interpolated to the BGC-SUMO pH timestamps of 30 seconds (the highest frequency sampled).

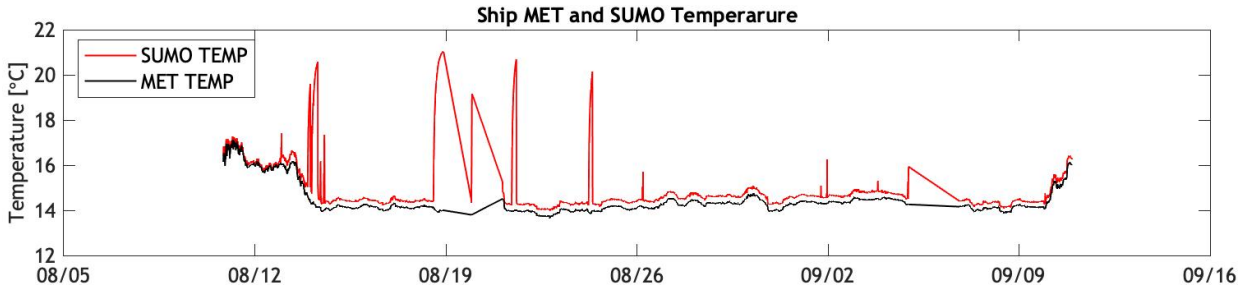

Figure 1. Ship (MET) and BGC-SUMO TSG temperature records.

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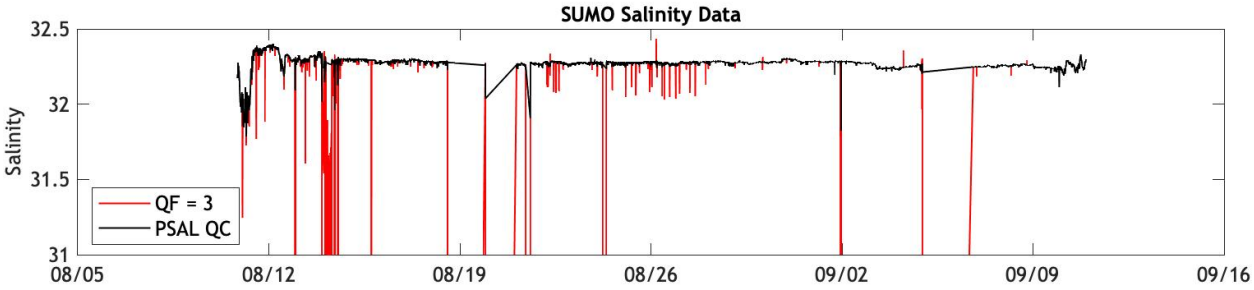

Figure 2. Raw salinity data from the BGC-SUMO TSG (red line) and salinity data deemed acceptable after QC (black line). Flagged salinity values were used to flag spikes in the BGC-SUMO nitrate and pH time series.

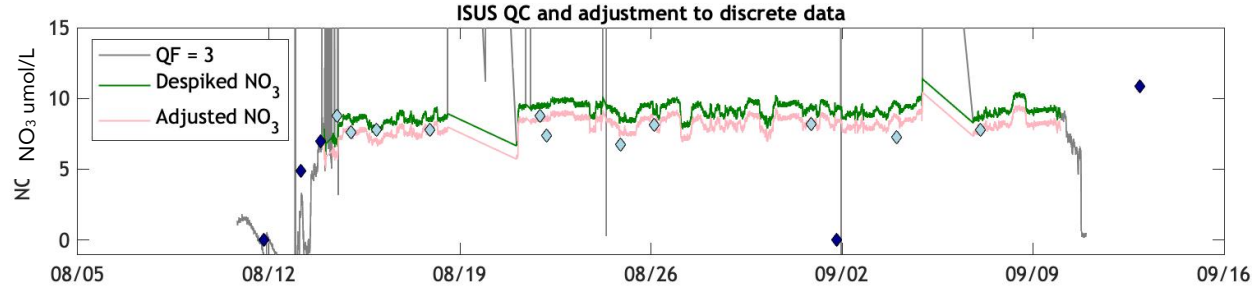

Figure 3. Underway (lines) and discrete (diamonds) nitrate data. Discrete observations collected during the sensor warm up phase or near shore (as well as one outlier) were omitted from the quality control analysis (black diamonds). Underway data shown in green were de-spiked and adjusted based on the mean offset between the underway data and discrete observations shown with light blue diamonds. Final, QC'd nitrate values are shown with a pink line.

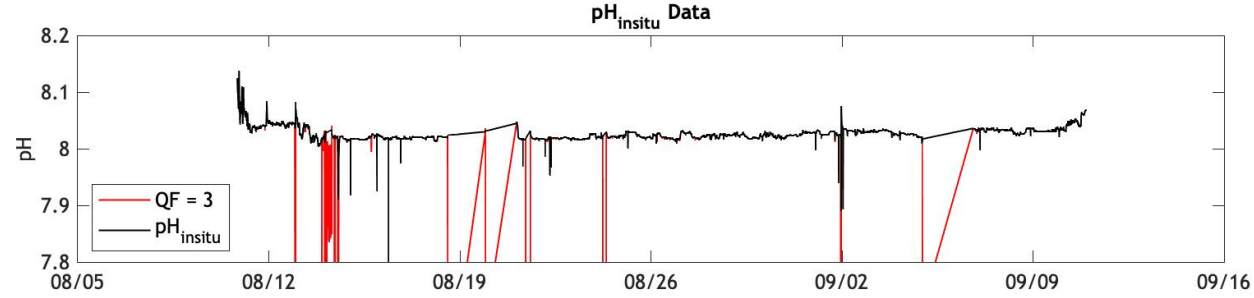

Figure 4. Raw pH data calculated at in situ (MET) temperature (red) and pH at in situ (MET) temperature deemed acceptable after QC.

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Bittig H. C., T. Steinhoff, H. Claustre, B. Fiedler, N. L. Williams, R. Sauzède, A. Körtzinger and J.-P.Gattuso, 2018: An Alternative to Static Climatologies: Robust Estimation of Open Ocean CO2 Variables and Nutrient Concentrations From T, S, and O2 Data Using Bayesian Neural Networks. Front. Mar. Sci. 5:328. doi: 10.3389/fmars.2018.00328.

Johnson, K. S., and L. J. Coletti (2002), In situ ultraviolet spectrophotometry for high resolution and long-term monitoring of nitrate, bromide and bisulfide in the ocean, Deep Sea Res. Part I Oceanogr. Res. Pap., 49(7), 1291–1305, doi:10.1016/S0967-0637(02)00020-1.

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