Cruise: GU1804, EcoMon Ship: R/V Gordon Gunter Expo Code: 33GG20180822

Dates: August 22, 2018 - August 31, 2018

Chief Scientist: Harvey Walsh

Equipment: CTD Rosette & Ship's Flow Thru (FT) **Total number of stations:** 23 (16 CTD and 7 FT)

Location: U.S. Mid-Atlantic and New England coastal region

The samples were run for Chris Melrose of the NEFSC as part of our coastal ocean acidification monitoring project.

Sample Collection

The discrete samples were collected from Niskin bottles attached to a 24 bottle configured rosette onboard the R/V Gordon Gunter by the survey tech Christopher Taylor. The date and time listed in the data file are UTC when each sample bottle was collected.

DIC:

23 locations, 60 samples each 500-ml, 5 duplicate samples.

Sample_ID#: 90101, etc.; Station, cast number and Niskin bottle number

PI: Dr. Rik Wanninkhof

Analyzed by: Charles Featherstone and Patrick Mears

pH:

23 locations, 60 samples each 500-ml, 5 duplicate samples.

Sample ID#: 90101, etc.; Station, cast number and Niskin bottle number

PI: Dr. Rik Wanninkhof

Analyzed by: Charles Featherstone and Patrick Mears

TAlk:

23 locations, 60 samples each 500-ml, 5 duplicate samples.

Sample ID#: 90101, etc.; Station, cast number and Niskin bottle number

PI: Dr. Rik Wanninkhof

Analyzed by: Leticia Barbero, Charles Featherstone and Patrick Mears

Sample Analysis

DIC:

Instrument	Date	Certified	CRM	CRM	Blank	Avg.
ID		CRM	Value	Offset	(Counts)	Sample
		(µmol/kg)	(µmol/kg)	(µmol/kg)		Analysis
						Time
AOML 5	09/24/2018	2017.88	2020.34	2.46	12.0	7.0
AOML 5	09/25/2018	2017.88	2017.18	0.70	16.0	7.0

AOML 6	09/24/2018	2017.88	2021.15	3.27	12.0	14.0
AOML 6	09/24/2018	2017.88	2019.50	1.62	22.0	10.0

Analysis date: 09/24/2018

Coulometer used: DICE-CM5011- AOML 5

Blanks: 12.0 counts/min

CRM # 1036 was used and with an assigned value of (includes both DIC and salinity):

Batch 150, c: 2017.88 µmol/kg, S: 33.343

CRM values measured: AOML 5: offset 2.46 µmol/kg (2020.34 µmol/kg). Average run time, minimum run time, maximum run time: 7, 7 and 8 min.

Analysis date: 09/25/2018

Coulometer used: DICE-CM5011- AOML 5

Blanks: 16.0 counts/min

CRM # 180 was used and with an assigned value of (includes both DIC and salinity):

Batch 150, c: 2017.88 µmol/kg, S: 33.343

CRM values measured: AOML 5: offset 0.70 µmol/kg (2017.18 µmol/kg). Average run time, minimum run time, maximum run time: 7, 7 and 7 min.

Analysis date: 09/25/2018

Coulometer used: DICE-CM5011- AOML 6

Blanks: 12.0 counts/min

CRM # 1092 was used and with an assigned value of (includes both DIC and salinity):

Batch 150, c: 2017.88 μmol/kg, S: 33.343

CRM values measured: AOML 6: offset 3.27 µmol/kg (2021.15 µmol/kg). Average run time, minimum run time, maximum run time: 14, 8 and 20 min.

Analysis date: 09/25/2018

Coulometer used: DICE-CM5011- AOML 6

Blanks: 22.0 counts/min

CRM # 486 was used and with an assigned value of (includes both DIC and salinity):

Batch 150, c: 2017.88 µmol/kg, S: 33.343

CRM values measured: AOML 6: offset 1.62 µmol/kg (2019.50 µmol/kg). Average run time, minimum run time, maximum run time: 10, 7 and 15 min.

Reproducibility: (# samples and average difference): 5 duplicate samples were collected with an average difference 1.02 μ mol/kg (0.24 – 2.35) and an average STDEV of 0.72 (0.17 – 1.66).

System	Sample ID	DIC	Average	Difference	STDEV
AOML5	230501	1998.66			
AOML5	230501	1996.31	1997.48	2.35	1.66
AOML5	290705	2152.51			

AOML5	290705	2153.02	2152.76	0.51	0.36
AOML5	300801 300801	2180.28 2180.04	2180.16	0.24	0.17
A OMI 5	511201	2101.50			
AOML5	511201 511201	2181.59 2182.31	2181.95	0.72	0.51
AOML5	541411	1899.79			
AOML5	541411	1901.06	1900.43	1.27	0.90
Average				1.02	0.72

CRM, salinity and HgCl2 correction applied: Salinity correction was applied using TSG salinity.

Remarks

The volume correction was applied due to added HgCl₂ (Measured DIC*1.00037). The first CRM of each cell was used for a CRM correction.

The DIC instruments were stable: the gas loop and CRM values did not change significantly throughout the life span of each cell.

The blank on AOML 6 (09/25/2018) was raised from 12.0 to 22.0 after running a new CRM.

pH:

Analysis date: 09/24/2018 and 09/25/2018 Spectrophotometer used: HP Agilent 8453

09/24/2018 CRM #798, Batch 150 had a pH value of 7.9412 09/25/2018 CRM #1170, Batch 150 had a pH value of 7.9420

Reproducibility: (# samples and average difference): 5 duplicate samples were collected with an average difference 0.0014 (0.0004 - 0.0027) and an average STDEV of 0.0010 (0.0003 - 0.0019).

	Sample		_			
Instrument	ID	Bottle #	pH @20deeg C	Average	STDEV	Difference
HP Agilent 8453	230501	92	7.9499			
HP Agilent 8453	230501	93	7.9521	7.9510	0.0016	0.0022
HP Agilent 8453	290705	100	7.8632			
HP Agilent 8453	290705	101	7.8632	7.8632	0.0000	0.0001

Average					0.0010	0.0014
HP Agilent 8453	541411	127	8.0525	8.0538	0.0019	0.0027
HP Agilent 8453	541411	126	8.0551			
HP Agilent 8453	511201	118	7.7614	7.7607	0.0010	0.0014
HP Agilent 8453	511201	117	7.7600			
HP Agilent 8453	300801	104	7.7619	7.7622	0.0003	0.0004
HP Agilent 8453	300801	103	7.7624			

Temperatures measured during pH analysis

Sample ID	Station	Botlle #	Temp. ⁰ C
CRM150_798	CRM798	CRM798	20.032
CRM150_1170	CRM 1170	CRM 1170	20.055
80101	8	81	20.035
80102	8	82	20.040
80112	8	83	20.036
110201	11	85	20.050
110203	11	86	20.043
110210	11	87	20.048
150301	15	91	20.055
150305	15	90	20.051
150312	15	89	20.060
230501	23	92	20.061
230501	23	93	20.067
230504	23	94	20.061
230508	23	95	20.065
270601	27	96	20.065
270605	27	97	20.068
270612	27	98	20.058
290701	29	99	20.039
290705	29	100	20.040
290705	29	101	20.033
290712	29	102	20.045
300801	30	103	20.044
300801	30	104	20.045
300804	30	105	20.045
300812	30	106	20.046
360902	36	109	20.055

360905	36	110	20.057
360912	36	111	20.061
371001	37	112	20.058
371004	37	113	20.059
371012	37	114	20.070
511201	51	117	20.051
511201	51	118	20.067
511202	51	119	20.066
511211	51	120	20.060
521301	52	121	20.060
521303	52	122	20.065
521310	52	123	20.060
541401	54	124	20.062
541405	54	125	20.067
541411	54	126	20.064
541411	54	127	20.068
561501	56	128	20.055
561504	56	129	20.051
561509	56	130	20.048
691701	69	132	20.042
691703	69	134	20.043
691706	69	133	20.049
701801	70	135	20.048
701804	70	136	20.047
701811	70	137	20.038
721901	72	138	20.047
721903	72	139	20.037
721911	72	140	20.040
840000	84	84	20.044
880000	88	88	20.050
1070000	107	107	20.046
1080000	108	108	20.049
1150000	115	115	20.063
1160000	116	116	20.060
1310000	131	131	20.048

Remarks

The equations of Liu et al, 2011 formulated using the purified m-cresol purple indicator was used to determine pH of the samples. pH samples were analyzed at 20⁰C at Full Scale (pH 0-14).

Samples were run on an automated system where the temperature was kept constant.

Approximately 80 mL of sample was extracted from each DIC sample bottle by syringe before DIC analysis to determine the pH.

A CRM was run for pH before analysis of samples.

pH values are reported at 25°C in the data spreadsheet.

TAlk:

Analysis date: 09/25/2018, 09/26/2018, 09/27/2018 and 09/28/2018

Titration system used: Open cell

CRM Batch 150, Salinity = 33.343, cert. TA = 2214.71μ mol/kg.

On 09/25/2018, 09/26/2018, 09/27/2018 and 09/28/2018 one CRM was analyzed before the samples and the same CRM was run at the end of analysis each day for each system. The TA for the water samples was corrected using the daily averaged ratios between the certified and measured values of the CRMs run on each cell. The following table shows the CRM measurements for each day and cell.

Cell System	Date	Time	Bottle #	TA	ΔCRM
2	09/25/2018	13:03:03	180	2223.96	
2	09/25/2018	16:21:02	180	2223.06	0.90
2	09/26/2018	09:40:09	1216	2211.60	
2	09/26/2018	17:15:03	1216	2221.03	9.43
2	09/27/2018	11:07:17	616	2223.92	
2	09/27/2018	16:24:32	616	2224.78	0.86
2	09/28/2018	08:34:52	292	2215.09	
2	09/28/2018	13:40:41	292	2223.74	8.65

Reproducibility: (# samples and average difference): 5 duplicate samples were collected with an average difference μ mol/kg 9.48 (1.45-38.04) and an average STDEV of 6.71 (1.74-26.90).

System	Sample ID	TA	Average	Difference	STDEV
2	230501	2181.02			
2	230501	2178.56	2179.79	2.47	1.74
2	290705	2332.78			
2	290705	2294.74	2313.76	38.04	26.90

Average				9.48	6.71
2	541411	2132.94	2131.67	2.54	1.80
2	541411	2130.40			
2	511201	2301.01	2302.47	2.92	2.07
2	511201	2303.93			
2	300801	2316.25	2316.97	1.45	1.03
2	300801	2317.70			

Remarks

The CRM measurement for each day was used to correct the data for that day only. Both systems worked well.

The second duplicate with sample ID 290705 had a large difference which contributed to the overall high average for the difference and STDEV of all the samples.

Comments

Sample bottle 121 the titration stopped mid ways thru and could not be recovered. The sample was marked 4-Bad. DIC and pH values were good.

The latitude, longitude, date, and time reported with the DIC, pH and TAlk measurements were taken from the sample field log. The field log values are provided for reference; no post-cruise assurance of accuracy has been done to this data.

The Sample ID is the sample station, cast number and Niskin bottle number for the discrete samples.

Corresponding UW pCO2 data can be found at the following website http://www.aoml.noaa.gov/ocd/ocdweb/occ.html

Final data – the sample ID number of the flow through (FT) samples is the same as the bottle number in which they were collected, example bottle 84 = sample ID of 840000.

The temperature and salinity for the FT samples were taken from the ship's TSG.

UPDATE:

Between March and June of 2021, all of the data for the discrete samples was put into a uniform format. The supporting information was checked for accuracy, especially the expocode, date, time, and positions.

Additionally, pH results were recalculated to 20 and 25 degrees Celsius.