Cruise: GU1706
Ship: R/V Gordon Gunter
Expo Code: 33GG20171031
Dates: 10/31/2017 – 11/09/2017
Chief Scientist: Harvey Walsh
Equipment: CTD Rosette & Ship's Flow Thru (FT)
Total number of stations: 13
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:
13 locations, 45 samples each 500-ml, 6 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:
13 locations, 45 samples each 500-ml, 6 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:
13 locations, 45 samples each 500-ml, 6 duplicate samples.
Sample_ID#: 90101, etc.; Station, cast number and Niskin bottle number
PI: Dr. Rik Wanninkhof
Analyzed by: Charles Featherstone and Patrick Mears

Sample Analysis
DIC:

Instrument ID	Date	Certified CRM (μmol/kg)	CRM Value (μmol/kg)	CRM Offset (μmol/kg)	Blank (Counts)	Avg. Sample Analysis Time
AOML 3	11/29/2017	2017.95	2018.60	0.65	25.0	11
AOML 4	11/29/2017	2017.95	2015.10	2.85	25.0	11

Analysis date: 11/29/2017
Coulometer used: DICE–CM5015- AOML 3
Blanks: 25.0 counts/min
CRM # 214 was used and with an assigned value of (includes both DIC and salinity):
Batch 153, c: 2017.95 µmol/kg, S: 33.357
CRM values measured: AOML 3: offset 0.65 µmol/kg (2018.60 µmol/kg).
Average run time, minimum run time, maximum run time: 11, 8 and 14 min.

Analysis date: 11/29/2017
Coulometer used: DICE–CM5015- AOML 4
Blanks: 25.0 counts/min
CRM # 519 was used and with an assigned value of (includes both DIC and salinity):
Batch 153, c: 2017.95 µmol/kg, S: 33.357
CRM values measured: AOML 4: offset 2.85 µmol/kg (2015.10 µmol/kg).
Average run time, minimum run time, maximum run time: 11, 8 and 19 min.

Reproducibility: (# samples and average difference): 6 duplicate samples were collected with an average difference 1.21 µmol/kg (0.05 – 2.38) and an average STDEV of 0.86 (0.03 – 1.68).

Instrument	Sample ID	DIC (umol/kg)	Average	STDEV	Difference
AOML3	20111	2033.25			
AOML3	20111	2034.31	2033.78	0.75	1.06
AOML3	60404	2137.72			
AOML3	60404	2135.77	2136.74	1.37	1.94
AOML4	260901	2194.08			
AOML4	260901	2194.23	2194.15	0.11	0.15
AOML4	391406	2018.32			
AOML4	391406	2018.83	2018.58	0.36	0.51
AOML4	441510	2060.58			
AOML4	441510	2062.96	2061.77	1.68	2.38
AOML4	591605	1970.61			
AOML4	591605	1970.56	1970.58	0.03	0.05
Average				0.86	1.21

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

Remarks
The volume correction was applied due to added $HgCl_2$ (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 3 (11/29/2017) was raised from 12.0 to 25.0 before running the CRM.

The blank on AOML 4 (09/28/2017) was raised from 12.0 to 25.0 before running the CRM.

The samples were analyzed using the DICE (AOML 3 and 4) and a new coulometer from UIC, Inc. CM5015 with CM5011 emulation software.

pH:

Analysis date: 11/29/2017
Spectrophotometer used: HP Agilent 8453
CRM #838, Batch 153 had a pH value of 7.9864

Reproducibility: (# samples and average difference): 6 duplicate samples were collected with an average difference 0.0011 (0.0000 – 0.0025) and an average STDEV of 0.0008 (0.0000 – 0.0018).

System	Sample ID	Sample Bottle #	S	t	pH	Average	Difference	STDEV
HP Agilent 8453	20111	83	31.8022	19.772	7.794252			
HP Agilent 8453	20111	84	31.8022	19.786	7.794975	7.795	0.0007	0.0005
HP Agilent 8453	60404	92	33.2309	19.784	7.682116			
HP Agilent 8453	60404	93	33.2309	19.767	7.684164	7.683	0.0020	0.0014
HP Agilent 8453	260901	101	35.3047	19.776	7.772782			
HP Agilent 8453	260901	102	35.3047	19.789	7.775322	7.774	0.0025	0.0018
HP Agilent 8453	391406	112	32.3239	19.771	7.908962			
HP Agilent 8453	391406	113	32.3239	19.774	7.908934	7.909	0.0000	0.0000

HP Agilent 8453	441510	117	34.9236	19.774	8.057859			
HP Agilent 8453	441510	118	34.9236	19.749	8.058077	8.058	0.0002	0.0002
HP Agilent 8453	591605	120	31.7665	19.749	7.946792			
HP Agilent 8453	591605	121	31.7665	19.748	7.947652	7.947	0.0009	0.0006
Average							0.0011	0.0008

Temperatures measured during pH analysis

Sample ID	Station	Botlle #	Temp. ^{0}C
CRM 838	CRM 838	CRM 838	19.772
20101	2	81	19.772
20104	2	82	19.776
20111	2	83	19.772
20111	2	84	19.786
30201	3	85	19.782
30205	3	86	19.789
30211	3	87	19.786
40301	4	88	19.795
40303	4	89	19.799
40308	4	90	19.781
60401	6	91	19.777
60404	6	92	19.784
60404	6	93	19.767
60411	6	94	19.772
120601	12	95	19.774
120604	12	96	19.763
120610	12	97	19.748
240802	24	98	19.744
240806	24	99	19.758
240811	24	100	19.759
260901	26	101	19.776
260901	26	102	19.789
260904	26	103	19.79
260911	26	104	19.792
271101	27	105	19.783
271104	27	106	19.774
271111	27	107	19.787
351201	35	108	19.784

351204	35	109	19.776
351208	35	110	19.778
391401	39	111	19.79
391406	39	112	19.771
391406	39	113	19.774
391411	39	114	19.768
441501	44	115	19.766
441505	44	116	19.764
441510	44	117	19.774
441510	44	118	19.749
591602	59	119	19.751
591605	59	120	19.749
591605	59	121	19.748
591611	95	122	19.752
631701	63	123	19.759
631705	63	124	19.764
631711	63	125	19.757

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 20^0C 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 25^0C in the data spreadsheet.

TAlk:

Analysis date: 12/01/2017, 12/04/2017, 12/07/2017 and 12/08/2017
Titration system used: Open cell
CRM Batch 153, Salinity = 33.357, cert. TA = 2225.59µmol/kg.

On 12/01/2017, 12/04/2017, 12/07/2017 and 12/08/2017 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	12/01/2017	15:06:16	1143	2209.54	
2	12/01/2017	20:50:35	1143	2210.90	1.36
2	12/04/2017	13:56:31	892	2208.66	
2	12/04/2017	21:08:05	892	2204.52	4.14
2	12/07/2017	16:19:31	766	2209.25	
2	12/07/2017	21:32:45	766	2197.96	11.29
2	12/08/2017	16:23:14	147	2202.82	
2	12/08/2017	19:38:59	147	2198.37	4.45

Reproducibility: (# samples and average difference): 6 duplicate samples were collected with an average difference μmol/kg 2.66 (0.37-4.46) and an average STDEV of 1.88 (0.26-3.59).

System	Sample ID	TAlk	Average	Difference	STDEV
2	20111	2159.12			
2	20111	2158.55	2158.83	0.57	0.40
2	60404	2233.60			
2	60404	2235.64	2234.62	-2.04	1.44
2	260901	2330.61			
2	260901	2335.07	2332.84	-4.46	3.16
2	391406	2174.00			
2	391406	2177.41	2175.70	-3.42	2.42
2	441510	2312.19			
2	441510	2312.56	2312.38	-0.37	0.26
2	591605	2147.32			
2	591605	2142.25	2144.79	5.07	3.59
Average				2.66	1.88

Remarks

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

Comments

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