Cruise: GU1701
Ship: R/V Gordon Gunter
Expo Code: 33GG20170516 (Leg 1) and 33GG20170530 (Leg 2)
Dates: Leg 1 (05/16/2017 – 05/26/2017) and Leg 2 (05/30/2017 – 06/06/2017)
Chief Scientist: J. Prezioso (Leg 1); D. Richardson (Leg 2)
Equipment: CTD Rosette & Ship's Flow Thru (FT)
Total number of stations: 42
Location: U.S. Mid-Atlantic and New England coastal region

The samples were run for Dr. Jon Hare 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:
42 locations, 132 samples each 500-ml, 11 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:
42 locations, 132 samples each 500-ml, 11 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:
42 locations, 132 samples each 500-ml, 11 duplicate samples.
Sample_ID#: 90101, etc.; Station, cast number and Niskin bottle number
PI: Dr. Rik Wanninkhof
Analyzed by: Dr. Leticia Barbero, Patrick Mears and Charles Featherstone

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	06/08/2017	2017.88	2018.85	0.97	26.0	11

AOML 4	06/08/2017	2017.88	2012.15	5.73	37.0	13
AOML 3	06/09/2017	2017.88	2019.74	1.86	36.0	13
AOML 4	06/09/2017	2017.88	2013.14	4.74	47.0	14
AOML 3	06/12/2017	2017.88	2016.60	0.73	18.0	14
AOML 3	06/12/2017	2017.88	2021.52	3.64	27.0	14
AOML 4	06/12/2017	2017.88	2014.18	3.70	28.0	16
AOML 3	06/13/2017	2017.88	2017.38	0.50	28.0	13
AOML 4	06/13/2017	2017.88	2017.93	0.05	38.0	16

Analysis date: 06/08/2017
Coulometer used: DICE–CM5015- AOML 3
Blanks: 26.0 counts/min
CRM # 1027 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 3: offset 0.97 µmol/kg (2018.85 µmol/kg).
Average run time, minimum run time, maximum run time: 11, 8 and 16 min.

Analysis date: 06/08/2017
Coulometer used: DICE–CM5015- AOML 4
Blanks: 37.0 counts/min
CRM # 730 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 4: offset 5.73 µmol/kg (2012.15 µmol/kg).
Average run time, minimum run time, maximum run time: 13, 9 and 17 min.

Analysis date: 06/09/2017
Coulometer used: DICE–CM5015- AOML 3
Blanks: 36.0 counts/min
CRM # 675 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 3: offset 1.86 µmol/kg (2019.74 µmol/kg).
Average run time, minimum run time, maximum run time: 13, 7 and 20 min.

Analysis date: 06/09/2017
Coulometer used: DICE–CM5015- AOML 4
Blanks: 47.0 counts/min
CRM # 34 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 4: offset 4.74 µmol/kg (2013.14 µmol/kg).
Average run time, minimum run time, maximum run time: 14, 12 and 16 min.

Analysis date: 06/12/2017
Coulometer used: DICE–CM5015- AOML 3
Blanks: 18.0 and 27.0 counts/min
CRM # 173 and #857 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 3: offset 0.73 µmol/kg (2016.60 µmol/kg).

CRM values measured: AOML 3: offset 3.64 µmol/kg (2021.52 µmol/kg).
Average run time, minimum run time, maximum run time: 14, 10 and 15 min.

Analysis date: 06/12/2017
Coulometer used: DICE–CM5015- AOML 4
Blanks: 28.0 counts/min
CRM # 480 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 4: offset 3.70 µmol/kg (2014.18 µmol/kg).
Average run time, minimum run time, maximum run time: 16, 13 and 16 min.

Analysis date: 06/13/2017
Coulometer used: DICE–CM5015- AOML 3
Blanks: 28.0 counts/min
CRM # 547 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 3: offset 0.50 µmol/kg (2017.38 µmol/kg).
Average run time, minimum run time, maximum run time: 13, 10 and 15 min.

Analysis date: 06/13/2017
Coulometer used: DICE–CM5015- AOML 4
Blanks: 38.0 counts/min
CRM # 223 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 4: offset 0.05 µmol/kg (2017.93 µmol/kg).
Average run time, minimum run time, maximum run time: 16, 13 and 20 min.

Reproducibility: (# samples and average difference): 11 duplicate samples were collected with an average difference 4.28 µmol/kg (0.91 – 8.02) and an average STDEV of 3.03 (0.0.65 – 5.67).

Instrument	Sample ID	Corrected DIC (umol/kg)	Average	STDEV	Difference
AOML3	180101	1992.06			
AOML3	180101	1988.13	1990.10	2.78	3.93
AOML3	280205	1967.32			
AOML3	280205	1970.97	1969.14	2.58	3.65
AOML4	370505	2027.98			
AOML4	370505	2027.06	2027.52	0.65	0.91
AOML4	390601	2202.49			
AOML4	390601	2206.39	2204.44	2.76	3.90
AOML3	561111	2061.19			
AOML3	561111	2067.72	2064.46	4.62	6.54

AOML3	641304	2120.42			
AOML3	641304	2124.83	2122.63	3.11	4.40
AOML4	731401	2191.22			
AOML4	731401	2192.93	2192.08	1.21	1.71
AOML3	891911	2003.81			
AOML3	891911	2008.01	2005.91	2.97	4.20
AOML4	1212211	2027.50			
AOML4	1212211	2032.85	2030.18	3.79	5.35
AOML4	1222304	2143.32			
AOML4	1222304	2147.78	2145.55	3.16	4.46
AOML4	1272404	2163.68			
AOML4	1272404	2171.70	2167.69	5.67	8.02
Average				3.03	4.28

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 (06/08/2017) was raised from 16.9 to 26.0 before running the CRM.

The blank on AOML 4 (06/08/2017) was raised from 33.0 to 37.0 before running the CRM.

The blank on AOML 3 (06/09/2017) was raised from 24.6 to 36.0 before running the CRM.

The blank on AOML 4 (06/09/2017) was raised from 24.5 to 37.0 before running the CRM. Raised blank to 47.0 and re-ran CRM.

The blank on AOML 3 (06/12/2017) was raised from 12.0 to 18.0 before running the CRM. After sample bottle 79 raised blank to 27.0 and ran another CRM.

The blank on AOML 4 (06/12/2017) was raised from 13.0 to 28.0 before running the CRM.

The blank on AOML 3 (06/13/2017) was raised from 12.0 to 28.0 before running the CRM.

The blank on AOML 4 (06/13/2017) was raised from 25.2 to 38.0 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: 06/08/2017 to 06/09/2017 and 06/12/2017 to 06/13/2017
Spectrophotometer used: HP Agilent 8453

CRMs measured before each sample run

CRM #	Analysis Date	Salinity	pH Value
967	6/8/17	33.343	7.9422
423	6/9/17	33.343	7.9434
361	6/12/17	33.343	7.9429
1168	6/13/17	33.343	7.9403

Average	7.9422
STDEV	0.0014

Reproducibility: (# samples and average difference): 11 duplicates were collected.

System	Sample ID	pH	Average	Difference	STDEV
HP Agilent 8453	180101	7.851			
HP Agilent 8453	180101	7.850	7.851	0.0010	0.0007
HP Agilent 8453	280205	7.986			
HP Agilent 8453	280205	7.986	7.986	0.0005	0.0004
HP Agilent 8453	370505	7.918			
HP Agilent 8453	370505	7.919	7.919	0.0009	0.0006
HP Agilent 8453	390601	7.726			
HP Agilent 8453	390601	7.727	7.727	0.0010	0.0007

HP Agilent 8453	561111	8.040			
HP Agilent 8453	561111	8.041	8.040	0.0007	0.0005
HP Agilent 8453	641304	7.9063			
HP Agilent 8453	641304	7.9066	7.906	0.0003	0.0002
HP Agilent 8453	731401	7.7666			
HP Agilent 8453	731401	7.7664	7.766	0.0002	0.0002
HP Agilent 8453	891911	7.9306			
HP Agilent 8453	891911	7.9397	7.935	0.0091	0.0064
HP Agilent 8453	1212211	7.928			
HP Agilent 8453	1212211	7.928	7.928	0.0002	0.0002
HP Agilent 8453	1222304	7.852			
HP Agilent 8453	1222304	7.853	7.853	0.0008	0.0006
HP Agilent 8453	1272404	7.7913			
HP Agilent 8453	1272404	7.7907	7.791	0.0006	0.0004
Average				0.0014	0.0010

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).

Temperature for each sample was measured before analysis using a Hart Scientific Fluke 1523 reference thermometer.

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

pH was measured with an automated system and water bath for constant temperature.

TAlk:

Analysis date: 06/12/2017 - 06/14/2017 and 06/19/2017 – 06/22/2017
Titration system used: Open cell

CRM Batch 129, Salinity = 33.361, cert. TA = 2237.32 µmol/kg (06/12/2017 Sys1).
CRM Batch 150, Salinity = 33.343, cert. TA = 2214.71 µmol/kg.

The 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|
1	06/12/2017	12:22:54	588	2219.41	
1	06/12/2017	19:36:20	588	2220.40	0.99
1	06/13/2017	11:52:24	927	2221.62	
1	06/13/2017	17:35:14	927	2220.22	1.40
1	06/19/2017	12:59:51	1109	2220.70	
1	06/19/2017	18:54:44	1109	2219.25	1.47
1	06/20/2017	10:36:11	47	2217.59	
1	06/20/2017	15:50:31	47	2118.41	0.82
1	06/21/2017	10:56:48	973	2220.14	
1	06/21/2017	15:28:53	973	2222.60	2.46
1	06/22/2017	10:22:03	654	2217.10	
1	06/22/2017	15:11:47	654	2218.92	1.82
2	06/12/2017	12:45:57	784	2220.64	
2	06/12/2017	19:32:23	784	2223.14	2.50
2	06/13/2017	11:41:22	1229	2220.38	
2	06/13/2017	17:41:01	1229	2217.97	2.41
2	06/14/2017	08:29:20	604	2218.38	
2	06/14/2017	19:09:49	604	2217.03	1.77
2	06/19/2017	11:16:12	300	2216.16	
2	06/19/2017	18:50:2	300	2219.61	3.45

Reproducibility: (# samples and average difference): 11 duplicate samples were collected with an average difference 2.96 µmol/kg (0.15 – 10.14) and an average STDEV of 2.09 (0.11 – 7.17).

System	Sample ID	TAlk	Average	Difference	STDEV
System 2	180101	2115.06	2117.60	5.09	3.60
System2	180101	2120.15			
System 1	280205	2186.50	2181.86	9.29	6.57
System 1	280205	2177.22			
System 2	370505	2192.06	2192.40	0.68	0.48
System2	370505	2192.74			
System 1	390601	2317.78	2317.19	1.19	0.84
System 1	390601	2316.59			
System2	561111	2304.59	2304.66	0.15	0.11
System 2	561111	2304.74			
System2	641304	2313.67	2314.28	1.22	0.86
System 2	641304	2314.89			
System 2	731401	2324.75	2325.59	1.68	1.19
System2	731401	2326.43			
System 2	891911	2178.84	2183.91	10.14	7.17
System2	891911	2188.98			
System2	1212211	2205.17	2204.47	1.40	0.99
System 2	1212211	2203.77			
System 1	1222304	2307.56	2307.91	0.70	0.50
System 1	1222304	2308.26			
System 1	1272404	2302.14	2301.60	1.06	0.75
System 1	1272404	2301.07			
Average				2.96	2.09

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.

Salinity values for the flow thru (FT) samples were taken from the UW pCO2 system.

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

Cruise: GU1702

Cruise: GU1702
Ship: R/V Gordon Gunter
Expo Code: 33GG20170610
Dates: 06/10/2017 – 06/21/2017
Chief Scientist: Harvey Walsh
Equipment: Niskin bottle & Ship's Flow Thru (FT)
Total number of stations: 18
Location: U.S. Mid-Atlantic and New England coastal region

The samples were run as part of our coastal ocean acidification monitoring project.

Sample Collection

The discrete samples were collected from an old fashioned Niskin bottle triggered with a messenger onboard the R/V Gordon Gunter by H. Walsh and E. Broughton. Depths are approximate, there is no digital information about bottle trip depths. The date and time listed in the data file are UTC when each sample bottle was collected.

DIC:
18 locations, 20 samples each 500-ml, 2 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:
18 locations, 20 samples each 500-ml, 2 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:
18 locations, 20 samples each 500-ml, 2 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	09/28/2017	2017.95	2018.67	0.72	28.0	11
AOML 4	09/28/2017	2017.95	2010.87	7.07	28.0	20
AOML 4	09/28/2017	2017.95	2010.85	7.10	40.0	15

Analysis date: 09/28/2017
Coulometer used: DICE–CM5015- AOML 3
Blanks: 28.0 counts/min
CRM # 948 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 0.72 µmol/kg (2018.67 µmol/kg).
Average run time, minimum run time, maximum run time: 11, 8 and 14 min.

Analysis date: 09/28/2017
Coulometer used: DICE–CM5015- AOML 4
Blanks: 28.0 and 40.0 counts/min
CRM # 651 and 707 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 7.07 and 7.10 µmol/kg (2010.87 and 2010.85 µmol/kg).
Average run time, minimum run time, maximum run time: 16, 8 and 20 min.

Reproducibility: (# samples and average difference): 2 duplicate samples were collected with an average difference 41.46 µmol/kg (5.07 – 88.00) and an average STDEV of 41.46 (3.59 – 62.22). **The first sample for 440101 (1953.78) was marked as bad**

which resulted in such a large difference with its duplicate.

Instrument	Sample ID	DIC (umol/kg)	Average	STDEV	Difference
AOML4	440101	1953.78			
AOML4	440101	2041.78	1997.78	62.22	88.00
AOML4	970101	2054.92			
AOML4	970101	2059.99	2057.45	3.59	5.07
Average				41.46	41.46

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 first sample for 440101 (1953.78) was marked as bad which resulted in such a large difference with its duplicate.

The blank on AOML 3 (09/28/2017) was raised from 18.3 to 28.0 before running the CRM.

The blank on AOML 4 (09/28/2017) was raised from 21.2 to 28.0 before running the CRM. The blank was also raised again to 40.0 after running another CRM and before sample 13.

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: 09/28/2017
Spectrophotometer used: HP Agilent 8453

Reproducibility: (# samples and average difference): 2 duplicate samples were collected with an average difference 0.0006 (0.0003 – 0.0009) and an average STDEV of 0.0004 (0.0002 – 0.0006).

System	Sample Bottle #	Sample ID	S	t	Corrected pH	Average	Difference	STDEV
HP Agilent 8453	11	440101	35.07	19.743	8.0944			
HP Agilent 8453	10	440101	35.07	19.788	8.0935	8.094	0.0009	0.0006
HP Agilent 8453	17	970101	36.35	19.778	8.164			
HP Agilent 8453	18	970101	36.35	19.762	8.164	8.164	0.0003	0.0002
Average							0.0006	0.0004

Temperatures measured during pH analysis

Sample ID	Station	Bottle #	Temperature Deg C
60101	6	1	19.742
180101	18	2	19.736
190000	0	19	19.756
190101	19	3	19.749
200000	0	20	19.760
260101	26	4	19.740
270101	27	5	19.746
330101	33	6	19.756
340101	34	7	19.769
420101	42	8	19.758
430101	43	9	19.767
440101	44	11	19.744
440101	44	10	19.778
530101	53	12	19.771
550101	55	13	19.777
830101	83	14	19.769
850101	85	15	19.783
930101	93	16	19.751
970101	97	17	19.742
970101	97	18	19.755

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.

TAlk:

Analysis date: 10/17/2017
Titration system used: Open cell
CRM Batch 153, Salinity = 33.357, cert. TA = 2225.59µmol/kg.

On 10/17/2017 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|
1	10/17/2017	13:17:29	593	2222.72	
1	10/17/2017	21:33:19	593	2222.42	0.30
2	10/17/2017	13:39:01	683	2222.94	
2	10/17/2017	21:29:46	683	2223.37	0.43

Reproducibility: (# samples and average difference): 2 duplicate samples were collected with an average difference 4.10 µmol/kg (0.56 – 7.65) and an average STDEV of 2.90 (0.40 – 5.41).

System	Sample ID	TAlk	Average	Difference	STDEV
System 2	440101	2299.40	2299.12	0.56	0.40
System 2	440101	2298.84			
System 2	970101	2366.78	2370.60	7.65	5.41
System 2	970101	2374.43			
Average				4.10	2.90

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.
One of the samples from the flow-through line was considered bad and flagged 4 for DIC, TA and pH. This sample is not reported in the final data file.

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