Cruise: GU1905
Ship: R/V Gordon Gunter
Expo Code: 33GG20191015
Dates: October 15, 2019 – November 1, 2019
Chief Scientist: Jerry Prezioso
Equipment: CTD Rosette & Ship's Flow Thru (FT)
Total number of stations: 24
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 and the TSG flow thru system onboard the R/V Gordon Gunter by the survey tech. The date and time listed in the data file are UTC when each sample bottle was collected.

DIC:
24 locations, 106 samples each 500-ml, 10 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:
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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 5	11/08/2019	2050.56	2050.77	0.21	25	11
AOML 5	11/12/2019	2050.56	2054.28	3.72	20	7

AOML 5	11/13/2019	2019.91	2017.88	2.03	23	10
AOML 6	11/08/2019	2053.41	2050.56	2.85	15	8
AOML 6	11/12/2019	2049.49	2050.56	1.07	16	9
AOML 6	11/13/2009	2018.96	2017.88	1.08	12	8

Analysis date: 11/08/2019
Coulometer used: DICE–CM5011- AOML 5
Blanks: 25.0 counts/min
CRM # 876 was used and with an assigned value of (includes both DIC and salinity):
Batch 174, c: 2050.56 µmol/kg, S: 33.408
CRM values measured: AOML 5: offset 0.21 µmol/kg (2050.77 µmol/kg).
Average run time, minimum run time, maximum run time: 11, 8 and 13 min.

Analysis date: 11/12/2019
Coulometer used: DICE–CM5011- AOML 5
Blanks: 20.0 counts/min
CRM # 578 was used and with an assigned value of (includes both DIC and salinity):
Batch 174, c: 2050.56 µmol/kg, S: 33.408
CRM values measured: AOML 5: offset 3.72 µmol/kg (2054.28 µmol/kg).
Average run time, minimum run time, maximum run time: 7, 7 and 10 min.

Analysis date: 11/13/2019
Coulometer used: DICE–CM5011- AOML 5
Blanks: 23.0 counts/min
CRM # 841 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 2.03 µmol/kg (2019.91 µmol/kg).
Average run time, minimum run time, maximum run time: 10, 9 and 12 min.

Analysis date: 11/08/2019
Coulometer used: DICE–CM5017O- AOML 6
Blanks: 15.0 counts/min
CRM # 949 was used and with an assigned value of (includes both DIC and salinity):
Batch 174, c: 2050.56 µmol/kg, S: 33.408
CRM values measured: AOML 6: offset 2.85 µmol/kg (2053.41 µmol/kg).
Average run time, minimum run time, maximum run time: 8, 7 and 9 min.

Analysis date: 11/12/2019
Coulometer used: DICE–CM5017O- AOML 6
Blanks: 16.0 counts/min
CRM # 37 was used and with an assigned value of (includes both DIC and salinity):
Batch 174, c: 2042.41 µmol/kg, S: 33.408
CRM values measured: AOML 6: offset 1.07 µmol/kg (2049.49 µmol/kg).
Average run time, minimum run time, maximum run time: 9, 7 and 11 min.

Analysis date: 11/13/2019
Coulometer used: DICE–CM5017O- AOML 6
Blanks: 12.0 counts/min
CRM # 913 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 1.08 µmol/kg (2018.96 µmol/kg).
Average run time, minimum run time, maximum run time: 8, 7 and 9 min.

Reproducibility: (# samples and average difference): 10 duplicate samples were collected with an average difference 0.54 µmol/kg (0.03-1.28) and an average STDEV of 0.38 (0.02-0.90).

System	Sample ID	DIC	Average	Difference	STDEV
AOML 6	130101	1964.25			
AOML 6	130101	1964.28	1964.27	0.03	0.02
AOML 6	180312	2067.31			
AOML 6	180312	2067.46	2067.38	0.15	0.10
AOML 6	380604	1959.04			
AOML 6	380604	1958.32	1958.68	0.72	0.51
AOML 5	430801	2197.72			
AOML 5	430801	2196.45	2197.09	1.28	0.90
AOML 6	491112	1971.55			
AOML 6	491112	1972.34	1971.95	0.80	0.56
AOML 6	621301	2170.89			
AOML 6	621301	2169.79	2170.34	1.10	0.78
AOML 5	651505	2008.89			
AOML 5	651505	2008.37	2008.63	0.52	0.37
AOML 5	791601	2038.24			
AOML 5	791601	2038.41	2038.33	0.18	0.13
AOML 5	1001903	2139.04			
AOML 5	1001903	2138.86	2138.95	0.18	0.13
AOML 6	1102101	2062.57			

AOML 6	1102101	2062.11	2062.34	0.46	0.33
Average				0.54	0.38

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.

pH:

Analysis date: 11/08/2019, 11/12/2019 and 11/13/2019
Spectrophotometer used: HP Agilent 8453
11/08/2019 CRM #79, Batch 174 had a pH value of 7.85894
11/12/2019 CRM #1214, Batch 150 had a pH value of 7.9397244
11/13/2019 CRM #1150, Batch 150 had a pH value of 7.93667

Reproducibility: (# samples and average difference): 9 duplicate samples were collected with an average difference 0.0006 (0.0001 – 0.0016) and an average STDEV of 0.0004 (0.00005 – 0.0012).

System	Sample ID	Sample Bottle #	Salinity	T ^0C	pH	Average	STDEV	Difference
HP Agilent 8453	130101	1	31.6428	20.039	7.93429			
HP Agilent 8453	130101	2	31.6428	20.048	7.93465	7.93447	0.0003	0.0004
HP Agilent 8453	180312	12	35.8641	20.044	8.09295			
HP Agilent 8453	180312	13	35.8641	20.048	8.09301	8.09298	0.0000	0.0001
HP Agilent 8453	380604	24	31.9512	20.045	8.00871			
HP Agilent 8453	380604	25	31.9512	20.047	8.00906	8.00889	0.0003	0.0004
HP Agilent 8453	430801	32	35.2517	20.041	7.74453			

HP Agilent 8453	430801	33	35.2517	20.042	7.74470	7.74461	0.0001	0.0002
HP Agilent 8453	491112	47	32.0828	20.026	7.95350			
HP Agilent 8453	491112	48	32.0828	20.027	7.95406	7.95378	0.0004	0.0006
HP Agilent 8453	621301	54	35.7517	20.041	7.86214			
HP Agilent 8453	621301	55	35.7517	20.030	7.86186	7.86200	0.0002	0.0003
HP Agilent 8453	651505	64	32.2512	20.028	7.89704			
HP Agilent 8453	651505	65	32.2512	20.021	7.89774	7.89739	0.0005	0.0007
HP Agilent 8453	791601	68	32.3843	20.033	7.85308			
HP Agilent 8453	791601	69	32.3843	20.035	7.85423	7.85366	0.0008	0.0011
HP Agilent 8453	1001903	82	34.7418	20.040	7.84520			
HP Agilent 8453	1001903	83	34.7418	20.046	7.84453	7.84486	0.0005	0.0007
HP Agilent 8453	1102101	90	32.6907	20.028	7.82096			
HP Agilent 8453	1102101	91	32.6907	20.034	7.82260	7.82178	0.0012	0.0016
Average							0.0004	0.0006

Temperatures measured during pH analysis

Sample ID	Station	Sample Bottle #	Temp. at Analysis
CRM174_79	CRM174_79	CRM174_79	20.035
CRM150_1214	CRM150_1214	CRM150_1214	19.998
CRM150_1150	CRM150_1150	CRM150_1150	20.025
130100	13	5	20.041
130101	13	1	20.039
130101	13	2	20.048

130104	13	3	20.044
130112	13	4	20.039
160200	16	9	20.046
160201	16	6	20.046
160205	16	7	20.042
160212	16	8	20.043
180300	18	14	20.054
180301	18	10	20.049
180302	18	11	20.049
180312	18	12	20.044
180312	18	13	20.048
190400	19	18	20.045
190401	19	15	20.042
190404	19	16	20.044
190412	19	17	20.046
240500	24	22	20.040
240501	24	19	20.050
240505	24	20	20.043
240512	24	21	20.042
380600	38	27	20.027
380601	38	23	20.056
380604	38	24	20.045
380604	38	25	20.047
380612	38	26	20.047
410700	41	31	20.033
410701	41	28	20.041
410705	41	29	20.050
410712	41	30	20.045
430800	43	36	20.036
430801	43	32	20.041
430801	43	33	20.042
430803	43	34	20.037
430812	43	35	20.043
440900	44	40	20.045
440901	44	37	20.051
440902	44	38	20.031
440912	44	39	20.047
481000	48	44	20.045
481001	48	41	20.045
481005	48	42	20.046
481012	48	43	20.043

491100	49	49	20.035
491101	49	45	20.031
491105	49	46	20.021
491112	49	47	20.026
491112	49	48	20.027
611200	61	53	20.022
611201	61	50	20.029
611202	61	51	20.033
611212	61	52	20.032
621300	62	58	20.041
621301	62	54	20.041
621301	62	55	20.030
621304	62	56	20.035
621312	62	57	20.042
641400	64	62	20.036
641401	64	59	20.035
641404	64	60	20.036
641412	64	61	20.032
651500	65	67	20.010
651501	65	63	20.026
651505	65	64	20.028
651505	65	65	20.021
651512	65	66	20.025
791600	79	72	20.034
791601	79	68	20.033
791601	79	69	20.035
791605	79	70	20.032
791612	79	71	20.030
841700	84	76	20.035
841701	84	73	20.040
841704	84	74	20.035
841712	84	75	20.030
851800	85	80	20.035
851801	85	77	20.029
851804	85	78	20.035
851812	85	79	20.031
1001900	100	85	20.042
1001901	100	81	20.042
1001903	100	82	20.040
1001903	100	83	20.046
1001912	100	84	20.041

1072000	107	89	20.041
1072001	107	86	20.045
1072004	107	87	20.043
1072012	107	88	20.040
1102100	110	94	20.061
1102101	110	90	20.028
1102101	110	91	20.034
1102105	110	92	20.047
1102112	110	93	20.040
1142200	114	98	20.065
1142201	114	95	20.054
1142204	114	96	20.047
1142212	114	97	20.060
1152300	115	102	20.059
1152301	115	99	20.054
1152304	115	100	20.055
1152312	115	101	20.061
1162400	116	106	20.055
1162401	116	103	20.060
1162404	116	104	20.051
1162412	116	105	20.057

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 and pH at analysis temperature in the data spreadsheet.

TAlk:

Analysis date: 11/13/2019, 11/14/2019 and 11/15/2019
Titration system used: Open cell
CRM Batch 150, Salinity = 33.343, cert. TA = 2214.71µmol/kg.

On 11/14/2019 and 11/15/2019 one CRM was analyzed before the samples and the same CRM was run at the end of analysis each day for each system, except on 11/13/2019 two different CRMs were run 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	11/13/2019	11:13:00	913	2217.89	
1	11/13/2019	17:34:34	605	2218.80	0.91
1	11/14/2019	09:10:27	542	2211.28	
1	11/14/2019	19:06:18	542	2214.31	3.03
1	11/15/2019	09:36:08	220	2214.96	
1	11/15/2019	09:36:08	220	2214.96	0.00
2	11/13/2019	11:23:46	1150	2216.09	
2	11/13/2019	17:22:41	841	2213.86	2.23
2	11/14/2019	09:22:16	279	2216.00	
2	11/14/20019	19:18:55	279	2212.11	4.11
2	11/15/2019	10:06:51	186	2214.07	
2	11/15/2019	17:03:50	186	2214.01	0.06

Reproducibility: (# samples and average difference): 10 duplicate samples were collected with an average difference µmol/kg 4.10 (0.80-17.91) and an average STDEV of 2.90 (0.57-12.66).

Instrument	Sample ID	Bottle #	TA (µmol/kg)	Average	Difference	STDEV
System 1	130101	1	2133.27			
System 1	130101	2	2135.73	2134.50	2.45	1.73
System 2	180312	12	2352.62			
System 2	180312	13	2357.52	2355.07	4.90	3.46
System 2	380604	24	2165.09			
System 2	380604	25	2167.42	2166.25	2.34	1.65

System 1	430801	32	2322.77			
System 2	430801	33	2326.20	2324.48	3.43	2.43
System 2	491112	47	2159.69			
System 2	491112	48	2163.24	2161.46	3.55	2.51
System 1	621301	54	2346.05			
System 1	621301	55	2347.27	2346.66	1.22	0.86
System 1	651505	64	2175.64			
System 1	651505	65	2172.12	2173.88	3.51	2.48
System 2	791601	68	2189.15			
System 2	791601	69	2188.24	2188.69	0.91	0.64
System 1	1001903	82	2300.06			
System 1	1001903	83	2282.15	2291.11	17.91	12.66
System 1	1102101	90	2202.15			
System 1	1102101	91	2201.35	2201.75	0.80	0.57
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.

Only one CRM was run at the beginning of analysis on System 1 on 11/15/2019. No CRM was run at the end of analysis.

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.

Final data – the sample ID number of the flow through (FT) samples is the sample station, cast number and 0 for Niskin bottle number (example 260400).

CTD surface sample temperature and salinity was used for the FT samples.

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