

Cruise: GU1902
Ship: R/V Gordon Gunter
Expo Code: 33GG20190815
Dates: August 15th, 2019 – August 30th, 2019
Chief Scientist: Harvey Walsh
Equipment: CTD Rosette & Ship's Flow Thru (FT)
Total number of stations: 23
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:

23 locations, 86 samples each 500-ml, 9 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, 86 samples each 500-ml, 9 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, 86 samples each 500-ml, 9 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 5	09/12/2019	2042.41	2042.84	0.43	18.0	8
AOML 5	09/13/2019	2042.41	2048.15	5.74	12.3	9

AOML 6	09/12/2019	2050.56	2052.21	1.65	12.8	8
AOML 6	09/13/2009	2042.41	2045.74	3.33	12.0	8

Analysis date: 09/12/2019
 Coulometer used: DICE–CM5011- AOML 5
 Blanks: 18.0 counts/min
 CRM # 261 was used and with an assigned value of (includes both DIC and salinity):
 Batch 173, c: 2042.41 $\mu\text{mol/kg}$, S: 33.414
 CRM values measured: AOML 5: offset 0.43 $\mu\text{mol/kg}$ (2042.84 $\mu\text{mol/kg}$).
 Average run time, minimum run time, maximum run time: 8, 7 and 10 min.

Analysis date: 09/13/2019
 Coulometer used: DICE–CM5011- AOML 5
 Blanks: 12.3 counts/min
 CRM # 942 was used and with an assigned value of (includes both DIC and salinity):
 Batch 173, c: 2042.41 $\mu\text{mol/kg}$, S: 33.414
 CRM values measured: AOML 5: offset 5.74 $\mu\text{mol/kg}$ (2048.15 $\mu\text{mol/kg}$).
 Average run time, minimum run time, maximum run time: 9, 7 and 12 min.

Analysis date: 09/12/2019
 Coulometer used: DICE–CM5011- AOML 6
 Blanks: 12.8 counts/min
 CRM # 278 was used and with an assigned value of (includes both DIC and salinity):
 Batch 174, c: 2050.56 $\mu\text{mol/kg}$, S: 33.408
 CRM values measured: AOML 6: offset 1.65 $\mu\text{mol/kg}$ (2052.21 $\mu\text{mol/kg}$).
 Average run time, minimum run time, maximum run time: 8, 7 and 10 min.

Analysis date: 09/13/2019
 Coulometer used: DICE–CM5011- AOML 6
 Blanks: 12.0 counts/min
 CRM # 1001 was used and with an assigned value of (includes both DIC and salinity):
 Batch 173, c: 2042.41 $\mu\text{mol/kg}$, S: 33.414
 CRM values measured: AOML 6: offset 3.33 $\mu\text{mol/kg}$ (2045.75 $\mu\text{mol/kg}$).
 Average run time, minimum run time, maximum run time: 8, 7 and 9 min.

Reproducibility: (# samples and average difference): 9 duplicate samples were collected with an average difference 0.48 $\mu\text{mol/kg}$ (0.07-1.89) and an average STDEV of 0.34 (0.05-1.33).

System	Sample ID	DIC	Average	Difference	STDEV
AOML 6	270501	2188.81			
AOML 6	270501	2189.67	2189.24	0.86	0.61
AOML 5	490801	2170.90			

AOML 5	490801	2171.67	2171.29	0.77	0.54
AOML 5	811505	2023.35			
AOML 5	811505	2021.46	2022.40	1.89	1.33
AOML 5	811501	2056.68			
AOML 5	811501	2056.61	2056.64	0.07	0.05
AOML 6	861601	2009.54			
AOML 6	861601	2009.64	2009.59	0.10	0.07
AOML 6	861605	2009.57			
AOML 6	861605	2009.49	2009.53	0.08	0.06
AOML 5	861612	2009.53			
AOML 5	861612	2009.75	2009.64	0.22	0.15
AOML 5	1302308	2038.82			
AOML 5	1302308	2038.75	2038.79	0.07	0.05
AOML 5	1302312	1953.99			
AOML 5	1302312	1953.68	1953.83	0.31	0.22
Average				0.48	0.34

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.

pH:

Analysis date: 09/12/2019 and 09/13/2019

Spectrophotometer used: HP Agilent 8453

09/12/2019 CRM #632, Batch 173 had a pH value of 7.8734

09/13/2019 CRM #570, Batch 173 had a pH value of 7.8729

Reproducibility: (# samples and average difference): 9 duplicate samples were collected with an average difference 0.0008 (0.0002 – 0.0019) and an average STDEV of 0.0006 (0.0001 – 0.0013).

Instrument	Sample ID	Bottle #	pH @20deeg C	Average	STDEV	Difference
HP Agilent 8453	270501	14	7.7537			
HP Agilent 8453	270501	15	7.7548	7.7542	0.0007	0.0010
HP Agilent 8453	490801	29	7.8611			
HP Agilent 8453	490801	28	7.8592	7.8601	0.0013	0.0019
HP Agilent 8453	811505	53	7.8995			
HP Agilent 8453	811505	54	7.9007	7.9001	0.0008	0.0012
HP Agilent 8453	811501	55	7.8355			
HP Agilent 8453	811501	56	7.8351	7.8353	0.0002	0.0003
HP Agilent 8453	861601	57	7.9002			
HP Agilent 8453	861601	58	7.8994	7.8998	0.0006	0.0008
HP Agilent 8453	861605	59	7.8999			
HP Agilent 8453	861605	60	7.8990	7.8994	0.0007	0.0010
HP Agilent 8453	861612	61	7.9005			
HP Agilent 8453	861612	62	7.9001	7.9003	0.0003	0.0004
HP Agilent 8453	1302308	83	7.8407			
HP Agilent 8453	1302308	84	7.8405	7.8406	0.0001	0.0002
HP Agilent 8453	1302312	85	7.9698			
HP Agilent 8453	1302312	86	7.9690	7.9694	0.0006	0.0008
Average					0.0006	0.0008

Temperatures measured during pH analysis

Sample ID	Station	Sample Bottle #	Temperature at Analysis
CRM173_632	CRM 632	632	19.998
CRM173_570	CRM 570	570	19.996
90112	9	1	19.989

90104	9	2	20.007
90101	9	3	20.016
100201	10	4	20.012
100203	10	5	20.016
100212	10	6	20.019
170301	17	7	20.012
170306	17	8	20.013
170309	17	9	20.006
260400	26	13	20.020
260401	26	12	20.014
260403	26	11	20.016
260412	26	10	20.010
270501	27	14	20.021
270501	27	15	20.015
270502	27	16	20.023
270512	27	17	20.019
310601	31	18	20.011
310607	31	19	20.022
310612	31	20	20.013
310600	31	21	20.012
350710	35	22	20.016
350707	35	23	20.024
350701	35	24	20.021
490800	49	25	20.024
490801	49	29	20.016
490801	49	28	20.020
490803	49	27	20.022
490812	49	26	20.011
500900	50	30	20.014
500901	50	31	20.014
500902	50	32	20.018
500912	50	33	20.023
541001	54	34	20.016
541005	54	35	20.017
541012	54	36	20.021
681101	68	37	20.028
681102	68	38	20.009
681112	68	39	20.024
701200	70	40	20.012
701201	70	41	20.009

701204	70	42	20.009
701212	70	43	20.009
761300	76	44	20.019
761301	76	45	20.016
761302	76	46	20.012
761312	76	47	20.015
791401	79	48	20.022
791403	79	49	20.020
791412	79	50	20.018
811512	81	51	20.026
811512	81	52	20.023
811505	81	53	20.024
811505	81	54	20.024
811501	81	55	20.015
811501	81	56	20.017
861601	86	57	20.026
861601	86	58	20.011
861605	86	59	20.024
861605	86	60	20.025
861612	86	61	20.024
861612	86	62	20.022
931701	93	63	20.007
931706	93	64	20.011
931712	93	65	20.016
981801	98	66	20.018
981805	98	67	20.018
981812	98	68	20.018
1061912	106	69	20.004
1061903	106	70	20.014
1061901	106	71	20.015
1152001	115	72	20.016
1152005	115	73	20.025
1152012	115	74	20.016
1162101	116	75	20.018
1162105	116	76	20.021
1162112	116	77	20.017
1172201	117	78	20.008
1172206	117	79	20.020
1172212	117	80	20.015
1302301	130	82	20.005

1302308	130	83	19.997
1302308	130	84	19.994
1302312	130	85	19.996
1302312	130	86	20.010

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 25⁰C and pH at analysis temperature in the data spreadsheet.

Talk:

Analysis date: 09/17/2019 and 09/19/2019

Titration system used: Open cell

CRM Batch 174, Salinity = 33.343, cert. TA = 2214.71 μmol/kg.

On 09/17/2019 and 09/18/2019 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 System 2 on 09/17/2019 2 different CRMs were run. 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	09/17/2019	10:16:15	1111	2212.16	
1	09/17/2019	18:01:40	1111	2212.38	0.28
1	09/18/2019	08:22:54	160	2210.44	
1	09/18/2019	16:12:34	160	2210.21	0.23
2	09/17/2019	10:40:07	722	2210.31	
2	09/17/2019	17:56:16	397	2208.01	2.30

2	09/18/2019	08:54:17	215	2209.49	
2	09/18/2019	16:06:17	215	2206.57	2.92

Reproducibility: (# samples and average difference): 9 duplicate samples were collected with an average difference $\mu\text{mol/kg}$ 2.65 (0.09-6.56) and an average STDEV of 1.87 (0.06-4.64).

Instrument	Sample ID	Bottle #	TA		Difference	STDEV
			($\mu\text{mol/kg}$)	Average		
System 2	270501	14	2314.55			
System 2	270501	15	2318.64	2316.59	4.09	2.89
System 1	490801	29	2345.35			
System 1	490801	28	2351.91	2348.63	6.56	4.64
System 1	811505	53	2191.02			
System 1	811505	54	2190.48	2190.75	0.54	0.38
System 1	811501	55	2200.93			
System 1	811501	56	2200.84	2200.89	0.09	0.06
System 1	861601	57	2175.87			
System 1	861601	58	2176.90	2176.38	1.03	0.73
System 1	861605	59	2180.34			
System 1	861605	60	2175.60	2177.97	4.74	3.35
System 2	861612	61	2176.65			
System 2	861612	62	2177.21	2176.93	0.56	0.40
System 1	1302308	83	2182.08			
System 1	1302308	84	2178.09	2180.09	4.00	2.83
System 1	1302312	85	2141.79			
System 1	1302312	86	2144.01	2142.90	2.22	1.57
Average					2.65	1.87

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.

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).

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

Sample bottle #81 was broken during shipment of samples and was not analyzed. It was the duplicate sample for the bottom at station 130 cast 23.

Sample bottle #24 was analyzed but no data could be reduced because the CTD salinity and temperature values were not available (sample ID 350710-Surface sample).

Sample ID 811501-Sample bottle #51 a duplicate for the surface at station 81 was thrown out and not averaged with the other surface sample collected. The DIC, TA and pH values matched up with the bottom sample values. The other sample collected from the surface, bottle #52 was good and reported with a flag of 2 instead of 6. A sampling error may have occurred since Niskin 1 and 12 are right next to each other.

The hand written log was changed from Station 14 to 17. Station 14 was a bongo net tow station with no water sample collection.

The bottom and surface values for the carbon data were switched with each other at stations 10, 17, 26 and 35. A sampling error may have occurred with not writing down the correct sample bottle number or picking the wrong sample bottle when sampling. The bottom sample values for these stations were very similar to other surface values and a FT sample collected at the same station, based on this the values were switched. Station 79 had the same problem but with the mid and bottom depth.

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

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.