Cruise: PC2106 Ship: R/V Pisces Expo Code: 334B20211015 Dates: October 15th – October 25th, 2021 Chief Scientist: Harvey Walsh Equipment: CTD Rosette & Ship's Flow Thru (FT) Total number of stations: 30 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 Pisces by the survey tech. The date and time listed in the data file are UTC when each sample bottle was collected.

DIC:

30 locations, 78 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:

30 locations, 78 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:

30 locations, 78 samples each 500-ml, 6 duplicate samples. Sample_ID#: 90101, etc.; Station, cast number and Niskin bottle number PI: Dr. Rik Wanninkhof Analyzed by: Dr. Leticia Barbero and Dismey Sosa-Rodriguez

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	12/08/2021	1952.65	1949.03	3.62	24.2	8
AOML 5	12/09/2021	1952.65	1954.77	2.12	20.0	8

AOML 6	12/08/2021	1952.65	1950.24	2.41	24.0	8
AOML 6	12/09/2021	1952.65	1954.35	1.70	20.0	9

Analysis date: 12/08/2021 Coulometer used: DICE–CM5011- AOML 5 Blanks: 24.2 counts/min CRM # 691 was used and with an assigned value of (includes both DIC and salinity): Batch 178, c: 1952.65 µmol/kg, S: 33.782 CRM values measured: AOML 5: offset 3.62 µmol/kg (1949.03 µmol/kg). Average run time, minimum run time, maximum run time: 8, 7 and 8 min. Analysis date: 12/09/2021 Coulometer used: DICE–CM5011- AOML 5 Blanks: 20.0 counts/min CRM # 270 was used and with an assigned value of (includes both DIC and salinity): Batch 178, c: 1952.65 µmol/kg, S: 33.782

CRM values measured: AOML 5: offset 2.12 µmol/kg (1954.77 µmol/kg).

Average run time, minimum run time, maximum run time: 8, 7 and 11 min.

Analysis date: 12/08/2021 Coulometer used: DICE–CM5017O- AOML 6 Blanks: 24.0 counts/min CRM # 392 was used and with an assigned value of (includes both DIC and salinity): Batch 178, c: 1952.65 μmol/kg, S: 33.782 CRM values measured: AOML 6: offset 2.41 μmol/kg (1950.24 μmol/kg). Average run time, minimum run time, maximum run time: 8, 8 and 9 min.

Analysis date: 12/09/2021 Coulometer used: DICE–CM5017O- AOML 6 Blanks: 20.0 counts/min CRM # 205 was used and with an assigned value of (includes both DIC and salinity): Batch 178, c: 1952.65 µmol/kg, S: 33.782 CRM values measured: AOML 6: offset 1.70 µmol/kg (1954.35 µmol/kg). Average run time, minimum run time, maximum run time: 9, 8 and 11 min.

Reproducibility: (# samples and average difference): 6 duplicate samples were collected with an average difference 1.40 µmol/kg (0.39-2.09) and an average STDEV of 0.99(0.28-1.48).

Instrument	Sample ID	Bottle #	DIC (µmol/kg)	Average	STDEV	Difference
AOML5	150301	14	2082.47			
AOML5	150301	15	2082.86	2082.9	0.28	0.39
AOML5	350701	29	2193.46			
AOML5	350701	30	2194.48	2194.5	0.72	1.02

AOML6	360811	35	2193.46				
AOML6	360811	36	2194.48	2194.5	0.72	1.02	
AOML6	621304	156	2162.64				
AOML6	621304	226	2160.57	2160.6	1.47	2.08	
AOML6	721601	235	2042.21				
AOML6	721601	236	2044.01	2044.0	1.28	1.80	
AOML5	872112	273	1987.87				
AOML5	872112	274	1985.78	1985.8	1.48	2.09	_
Average					0.99	1.40	-

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: 12/08/2021 and 12/09/2021 Spectrophotometer used: HP Agilent 8453 No CRMs run.

Reproducibility: pH at 20° C (# samples, average difference, average STDEV): 6 duplicate samples were collected with an average difference 0.00467 (0.00067 – 0.01773) and an average STDEV of 0.00331 (0.000467 – 0.01254).

Instrument	Sample ID	Bottle #	pH @20 ⁰ C	Average	STDEV	Difference
HP Agilent 8453	150301	14	7.8507818			
HP Agilent 8453	150301	15	7.8500216	7.85040	0.00054	0.00076
HP Agilent 8453	350701	29	7.7470408			
HP Agilent 8453	350701	30	7.7507658	7.74890	0.00263	0.00372
HP Agilent 8453	360811	35	8.1448032			
HP Agilent 8453	360811	36	8.1480555	8.14643	0.00230	0.00325

HP Agilent 8453	621304	156	7.8955400			
HP Agilent 8453	621304	226	7.8936278	7.89458	0.00135	0.00191
HP Agilent 8453	721601	235	7.9061131			
HP Agilent 8453	721601	236	7.9054458	7.90578	0.00047	0.00067
HP Agilent 8453	872112	273	7.9059751			
HP Agilent 8453	872112	274	7.9237078	7.91484	0.01254	0.01773
Average					0.00331	0.00467

Temperatures measured during pH analysis.

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Sample	Sample BTL		Analysis T			
ID	#	Salinity	(⁰ C)			
50500	1	33.148	19.980			
60600	2	33.586	19.964			
70700	3	33.481	19.971			
80800	4	34.093	19.985			
90900	5	34.259	19.974			
101000	6	34.354	19.977			
111100	7	35.203	19.984			
120101	8	35.090	19.988			
120105	9	35.540	19.973			
120112	10	34.860	19.973			
130201	11	35.790	19.973			
130204	12	35.830	19.966			
130212	13	35.140	19.969			
150301	14	33.730	19.962			
150301	15	33.730	19.968			
150306	16	33.850	19.975			
150312	17	33.250	19.963			
200401	18	32.110	19.970			
200406	19	31.930	19.960			
200412	20	31.920	19.966			
300501	21	31.630	19.962			
300506	23	30.730	19.967			
300512	24	30.170	19.960			
322800	25	32.379	19.964			

330601	26	32.650	19.969
330606	27	32.150	19.971
330612	28	32.150	19.966
350701	29	35.310	19.954
350701	30	35.310	19.973
350704	31	35.890	19.966
350712	32	36.010	19.966
360801	33	35.090	19.968
360807	34	35.420	19.973
360811	35	35.970	19.976
360811	36	35.970	19.992
390901	37	35.810	19.982
390906	38	35.340	19.980
390912	39	35.300	19.991
411001	40	33.210	19.977
411008	147	33.410	19.950
411012	148	33.000	19.957
420000	22	33.779	19.963
491101	149	32.620	19.968
491106	150	31.750	19.964
491112	151	31.710	19.977
611201	152	35.070	19.965
611204	153	35.350	19.966
611212	154	35.590	19.970
621301	155	35.680	19.960
621304	156	35.890	19.965
621304	226	35.890	19.965
621312	227	34.910	19.966
661401	228	33.810	19.953
661404	229	34.510	19.961
661412	230	33.600	19.956
691501	231	33.760	19.955
691507	233	32.720	19.967
691512	234	32.470	19.974
721601	235	32.980	19.965
721601	236	32.980	19.978
721604	257	32.890	19.955
721612	258	32.830	19.966
791701	259	34.450	19.966
791704	260	33.570	19.958
791712	261	32.720	19.972

831801	262	33.070	19.966
831806	263	33.050	19.990
831812	264	32.080	19.990
851901	265	32.730	19.972
851906	266	32.490	19.989
851912	267	31.930	19.994
862001	268	32.590	19.977
862006	269	32.530	19.980
862012	270	31.750	19.998
872101	271	32.310	19.976
872105	272	32.180	19.966
872112	273	31.810	19.968
872112	274	31.810	19.981

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.

pH values are reported at 20°C and 25°C.

TAlk:

Analysis date: 12/09/2021 and 12/10/2021 Titration system used: Open cell CRM Batch 178, Salinity = 33.782, cert. TA = 2216.53 µmol/kg.

System 1: On 12/09/2021 CRM #691 was run before analysis and at the end of analysis. On 12/10/2021 CRM #691 was run before analysis and at the end of analysis.

System 2: On 12/092021 CRM #392 was run before analysis and at the end of analysis. On 12/10/2021 CRM #205 was run before analysis and at the end of analysis.

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

Cell System	Date	Time	Bottle #	TA	$ \Delta CRM $	Difference
1	12/09/2021	09:44:20	691	2212.40		4.13
1	12/09/2021	17:52:38	691	2211.86	0.54	4.67
1	12/10/2021	09:09:08	270	2216.36		0.17
1	12/10/2021	17:28:52	270	2212.19	4.17	4.34
2	12/09/2021	09:52:55	392	2215.63		0.90
2	12/09/2021	17:51:49	392	2215.70	0.07	0.83
2	12/10/2021	09:06:04	205	2216.74		0.21
2	12/10/2021	17:38:53	205	2215.75	1.01	0.78

the CRM measurements for each day and cell.

Reproducibility: (# samples and average difference): 6 duplicate samples were collected with an average difference μ mol/kg 3.41 (0.36-8.06) and an average STDEV of 2.41 (0.25-5.70).

			TA			
Station	Sample ID	Bottle #	(umol/kg)	Average	STDEV	Difference
15	150301	14	2247.2			
15	150301	15	2246.9	2247.1	0.25	0.36
35	350701	29	2319.3			
35	350701	30	2325.9	2322.6	4.62	6.54
36	360811	35	2375.1			
36	360811	36	2375.3	2375.2	0.10	0.14
62	621304	156	2357.4			
62	621304	226	2356.9	2357.1	0.37	0.53
72	721601	235	2219.4			
72	721601	236	2211.3	2215.4	5.70	8.06
87	872112	273	2155.0			
87	872112	274	2159.9	2157.4	3.42	4.84
Average					2.41	3.41

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).

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