Cruise: GU1608 , EcoMon
Ship: R/V Gordon Gunter
Dates: 05/21/2016 – 06/03/2016 Leg1 and 06/07/2016 – 06/16/2016 Leg2
Expo Code: 33GG20160521 (Leg1) and 33GG20160616 (Leg2)
Chief Scientist: J. Prezioso (Leg1); Chris Melrose (Leg2)
Equipment: CTD Rosette
Total number of stations: 36
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:
36 locations, 120 samples each 500-ml, 13 duplicate samples.
Sample_ID#: 90101, etc.; Station, cast number and Niskin bottle number
PI: Dr. Rik Wanninkhof
Analyzed by: Charles Featherstone

pH:
36 locations, 120 samples each 500-ml, 13 duplicate samples.
Sample_ID#: 90101, etc.; Station, cast number and Niskin bottle number
PI: Dr. Rik Wanninkhof
Analyzed by: Charles Featherstone

TAlk:
36 locations, 120 samples each 500-ml, n13 duplicate samples.
Sample_ID#: 90101, etc.; Station, cast number and Niskin bottle number
PI: Dr. Rik Wanninkhof
Analyzed by: Dr. Leticia Barbero 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 4	07/19/2016	2031.53	2026.12	5.41	28.0	15

AOML 3	07/20/2016	2031.53	2031.15	0.38	26.0	13
AOML 4	07/20/2016	2031.53	2027.03	4.50	28.0	12
AOML 3	07/21/2016	2031.53	2029.12	2.41	26.0	15
AOML 4	07/21/2016	2031.53	2025.97	5.56	28.0	13
AOML 3	07/22/2016	2031.53	2030.00	1.53	26.0	17
AOML 4	07/22/2016	2031.53	2028.59	2.94	28.0	13
AOML 3	07/25/2016	2031.53	2032.03	1.50	26.0	17
AOML 4	07/25/2016	2031.53	2025.30	6.23	28.0	12

Analysis date: 07/19/2016
Coulometer used: DICE–CM5015- AOML 4
Blanks: 28.0 counts/min
CRM # 236 was used and with an assigned value of (includes both DIC and salinity):
Batch 144, c: 2031.53 µmol/kg, S: 33.571
CRM values measured: AOML 4: offset 5.41 µmol/kg (2026.12 µmol/kg).
Average run time, minimum run time, maximum run time: 15, 12 and 20 min.

Analysis date: 07/20/2016
Coulometer used: DICE–CM5015- AOML 3
Blanks: 26.0 counts/min
CRM # 483 was used and with an assigned value of (includes both DIC and salinity):
Batch 144, c: 2031.53 µmol/kg, S: 33.571
CRM values measured: AOML 3: offset 0.38 µmol/kg (2031.15 µmol/kg).
Average run time, minimum run time, maximum run time: 13, 9 and 20 min.

Analysis date: 07/20/2016
Coulometer used: DICE–CM5015- AOML 4
Blanks: 28.0 counts/min
CRM # 1406 was used and with an assigned value of (includes both DIC and salinity):
Batch 144, c: 2031.53 µmol/kg, S: 33.571
CRM values measured: AOML 4: offset 4.50 µmol/kg (2027.03 µmol/kg).
Average run time, minimum run time, maximum run time: 12, 9 and 18 min.

Analysis date: 07/21/2016
Coulometer used: DICE–CM5015- AOML 3
Blanks: 26.0 counts/min
CRM # 366 was used and with an assigned value of (includes both DIC and salinity):
Batch 144, c: 2031.53 µmol/kg, S: 33.571
CRM values measured: AOML 3: offset 2.41 µmol/kg (2029.12 µmol/kg).
Average run time, minimum run time, maximum run time: 15, 8 and 20 min.

Analysis date: 07/21/2016
Coulometer used: DICE–CM5015- AOML 4
Blanks: 28.0 counts/min
CRM # 304 was used and with an assigned value of (includes both DIC and salinity):
Batch 144, c: 2031.53 µmol/kg, S: 33.571
CRM values measured: AOML 4: offset 5.56 µmol/kg (2025.97 µmol/kg).

Average run time, minimum run time, maximum run time: 13, 10 and 20 min.

Analysis date: 07/22/2016
Coulometer used: DICE–CM5015- AOML 3
Blanks: 26.0 counts/min
CRM # 967 was used and with an assigned value of (includes both DIC and salinity):
Batch 144, c: 2031.53 µmol/kg, S: 33.571
CRM values measured: AOML 3: offset 1.53 µmol/kg (2030.00 µmol/kg).
Average run time, minimum run time, maximum run time: 17, 13 and 20 min.

Analysis date: 07/22/2016
Coulometer used: DICE–CM5015- AOML 4
Blanks: 28.0 counts/min
CRM # 617 was used and with an assigned value of (includes both DIC and salinity):
Batch 144, c: 2031.53 µmol/kg, S: 33.571
CRM values measured: AOML 4: offset 2.94 µmol/kg (2028.59 µmol/kg).
Average run time, minimum run time, maximum run time: 13, 9 and 20 min.

Analysis date: 07/25/2016
Coulometer used: DICE–CM5015- AOML 3
Blanks: 26.0 counts/min
CRM # 782 was used and with an assigned value of (includes both DIC and salinity):
Batch 144, c: 2031.53 µmol/kg, S: 33.571
CRM values measured: AOML 3: offset 1.50 µmol/kg (2032.03 µmol/kg).
Average run time, minimum run time, maximum run time: 17, 14 and 20 min.

Analysis date: 07/25/2016
Coulometer used: DICE–CM5015- AOML 4
Blanks: 28.0 counts/min
CRM # 176 was used and with an assigned value of (includes both DIC and salinity):
Batch 144, c: 2031.53 µmol/kg, S: 33.571
CRM values measured: AOML 4: offset 6.23 µmol/kg (2025.30 µmol/kg).
Average run time, minimum run time, maximum run time: 12, 9 and 16 min.

Reproducibility: (# samples and average difference): 13 duplicate samples were collected with an average difference 2.90 µmol/kg (0.23 – 6.60) and an average STDEV of 2.05 (0.16 – 4.67).

System	ID	Corr. DIC	Avg	Difference	STDEV
AOML 4	140101	2068.73			
AOML 4	140101	2069.19	2068.96	0.46	0.33
AOML 4	260404	2110.06			
AOML 4	260404	2116.65	2113.36	6.60	4.67
AOML 4	360709	2008.63			

AOML 4	360709	2009.37	2009.00	0.75	0.53
AOML 3	561101	2060.98			
AOML 3	561101	2067.12	2064.05	6.14	4.34
AOML 4	751511	1997.37			
AOML 4	751511	1992.94	1995.15	4.43	3.14
AOML 3	941901	2034.22			
AOML 3	941901	2030.24	2032.23	3.98	2.82
AOML 3	1132205	2043.09			
AOML 3	1132205	2047.41	2045.25	4.32	3.05
AOML 3	1603401	2175.94			
AOML 3	1603401	2171.59	2173.77	4.35	3.07
AOML 3	1603404	2140.96			
AOML 3	1603404	2140.41	2140.68	0.55	0.39
AOML 4	1603411	2020.34			
AOML 4	1603411	2020.57	2020.45	0.23	0.16
AOML 4	1683901	2100.10			
AOML 4	1683901	2101.04	2100.57	0.94	0.66
AOML 4	1683904	2078.50			
AOML 4	1683904	2082.86	2080.68	4.36	3.08
AOML 4	1683911	1962.35			
AOML 4	1683911	1962.89	1962.62	0.54	0.38
Overall Average				2.90	2.05

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 4 (07/19/2016) was raised from 23.9 to 28.0 before running the CRM.

The blank on AOML 3 (07/20/2016) was raised from 17.3 to 26.0 before running the CRM.

The blank on AOML 4 (07/20/2016) was raised from 12.0 to 28.0 before running the CRM.

The blank on AOML 3 (07/21/2016) was raised from 12.0 to 26.0 before running the CRM.

The blank on AOML 4 (07/21/2016) was raised from 19.2 to 28.0 before running the CRM.

The blank on AOML 3 (07/22/2016) was raised from 12.0 to 26.0 before running the CRM.

The blank on AOML 4 (07/22/2016) was raised from 12.0 to 28.0 before running the CRM.

The blank on AOML 3 (07/25/2016) was raised from 18.1 to 26.0 before running the CRM.

The blank on AOML 4 (07/25/2016) was raised from 12.5 to 28.0 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: 07/19/2016 to 07/22/2016 and 07/25/2016
Spectrophotometer used: HP Agilent 8453

Reproducibility: (# samples and average difference): 13 duplicates were collected.

Instrument	Sample_ID	Bottle #	pH @20deeg C	Average	STDEV	Difference
HP Agilent 8453	140101	1	7.8460			
HP Agilent 8453	140101	2	7.8383	7.8422	0.0055	0.0078
HP Agilent 8453	260404	13	7.9535			
HP Agilent 8453	260404	14	7.9586	7.9561	0.0036	0.0051
HP Agilent 8453	360709	23	7.8884			
HP Agilent 8453	360709	24	7.8899	7.8891	0.0011	0.0015

HP Agilent 8453	561101	34	7.7615			
HP Agilent 8453	561101	35	7.7651	7.7633	0.0025	0.0036
HP Agilent 8453	751511	48	7.9333			
HP Agilent 8453	751511	49	7.9311	7.9322	0.0016	0.0022
HP Agilent 8453	941901	59	7.9132			
HP Agilent 8453	941901	60	7.9061	7.9096	0.0050	0.0070
HP Agilent 8453	1132205	70	7.8895			
HP Agilent 8453	1132205	71	7.8966	7.8931	0.0050	0.0071
HP Agilent 8453	1603401	103	7.7147			
HP Agilent 8453	1603401	104	7.7105	7.7126	0.0029	0.0041
HP Agilent 8453	1603404	105	7.7021			
HP Agilent 8453	1603404	106	7.6993	7.7007	0.0020	0.0029
HP Agilent 8453	1603411	107	7.9393			
HP Agilent 8453	1603411	108	7.9386	7.9389	0.0005	0.0008
HP Agilent 8453	1683901	115	7.7063			
HP Agilent 8453	1683901	116	7.7100	7.7081	0.0026	0.0037
HP Agilent 8453	1683904	117	7.7272			
HP Agilent 8453	1683904	118	7.7234	7.7253	0.0027	0.0039
HP Agilent 8453	1683911	119	7.9606			
HP Agilent 8453	1683911	120	7.9605	7.9606	0.0001	0.0001
Average					0.0027	0.0038

Temperatures measured during pH analysis

Sample ID	Sample BTL #	Btl. Temp	Start Cell (^{0}C)	End Cell (^{0}C)	Differ Start to End Cell (^{0}C)
140101	1	19.942	20.778	21.770	0.992
140101	2	20.059	20.992	21.968	0.976
140105	5	20.129	20.959	21.988	1.029
140107	3	20.103	20.857	21.816	0.959
140110	4	20.204	20.938	21.905	0.967
170202	6	19.954	20.771	21.855	1.084
170205	7	19.961	20.789	21.822	1.033

170210	8	19.990	20.995	21.775	0.780
180301	9	20.127	21.114	21.932	0.818
180302	10	20.087	21.326	21.893	0.567
180310	11	20.031	20.854	21.754	0.900
260401	12	19.947	20.825	21.720	0.895
260404	13	20.023	20.879	21.838	0.959
260404	14	20.214	21.307	22.126	0.819
260411	15	20.027	20.681	21.581	0.900
310501	16	19.874	20.769	21.946	1.177
310503	17	20.111	20.994	21.933	0.939
330601	18	20.183	21.024	21.712	0.688
330602	19	20.034	20.989	21.816	0.827
330612	20	20.020	21.104	21.933	0.829
360701	21	19.977	20.975	21.892	0.917
360705	22	19.935	20.813	21.585	0.772
360709	23	20.024	20.880	21.834	0.954
360709	24	19.935	20.729	21.550	0.821
370801	25	20.127	20.978	21.816	0.838
370809	26	20.003	20.922	21.658	0.736
370812	27	20.070	20.764	21.447	0.683
460902	28	20.149	21.008	21.711	0.703
460906	29	20.065	21.133	21.767	0.634
460910	30	19.934	20.882	21.567	0.685
471001	31	20.246	21.087	21.914	0.827
471004	32	20.115	21.008	21.785	0.777
471008	33	20.050	21.050	21.998	0.948
561101	34	20.346	21.035	21.969	0.934
561101	35	20.080	21.070	21.627	0.557
561105	36	19.915	20.828	21.653	0.825
661201	37	19.995	20.894	21.990	1.096
661202	38	19.936	20.739	21.575	0.836
661211	39	20.133	20.979	21.787	0.808
671301	40	19.985	20.954	21.731	0.777
671304	41	20.064	21.104	21.814	0.710
671311	42	20.186	21.010	21.900	0.890
711401	43	19.839	20.356	20.824	0.468
711407	44	20.121	20.784	21.326	0.542
711411	45	20.022	20.671	21.335	0.664
751501	46	20.092	20.645	21.369	0.724
751507	47	20.022	20.929	21.367	0.438
751511	48	19.994	20.721	21.504	0.783
751511	49	20.070	20.676	21.511	0.835
851601	50	20.046	20.886	21.612	0.726

851603	51	19.937	20.827	21.380	0.553
851611	52	20.014	20.618	21.484	0.866
861701	53	20.022	20.888	21.682	0.794
861703	54	19.993	20.865	21.830	0.965
861711	55	19.947	20.450	21.097	0.647
911801	56	19.943	20.908	21.597	0.689
911805	57	19.965	20.904	21.566	0.662
911811	58	20.055	21.156	21.698	0.542
941901	59	19.869	20.649	21.065	0.416
941901	60	20.082	20.674	21.293	0.619
941905	61	20.174	20.769	21.520	0.751
941911	62	20.032	20.981	21.577	0.596
1022001	63	19.925	20.515	21.282	0.767
1022002	64	20.154	21.182	21.791	0.609
1022011	65	19.969	20.828	21.419	0.591
1042101	66	20.134	21.297	21.988	0.691
1042103	67	19.959	20.732	21.372	0.640
1042111	68	19.971	20.960	21.634	0.674
1132201	69	20.091	20.796	21.609	0.813
1132205	70	19.954	20.882	21.543	0.661
1132205	71	19.929	20.596	21.337	0.741
1132211	72	19.958	21.128	21.694	0.566
1192301	73	19.853	20.836	21.537	0.701
1192305	74	20.041	20.946	21.847	0.901
1192311	75	19.928	20.726	21.523	0.797
1312401	76	20.118	20.994	21.779	0.785
1312404	77	20.107	20.989	21.845	0.856
1312411	78	20.182	20.844	21.657	0.813
1322501	79	19.904	20.624	21.510	0.886
1322505	80	20.066	20.716	21.448	0.732
1322511	81	20.193	21.118	21.807	0.689
1332602	82	19.851	20.644	21.495	0.851
1332604	83	20.067	20.900	21.574	0.674
1332611	84	19.942	20.807	21.626	0.819
1352801	85	19.800	20.647	21.531	0.884
1352804	86	20.179	21.088	21.869	0.781
1352811	87	19.962	20.872	21.674	0.802
1412901	88	20.140	21.094	21.998	0.904
1412904	89	20.312	21.121	21.838	0.717
1412911	90	20.185	21.453	21.973	0.520
1453001	91	20.014	20.828	21.654	0.826
1453004	92	19.954	20.844	21.616	0.772
1453011	93	20.138	21.220	21.844	0.624

1513101	94	19.903	20.815	21.534	0.719
1513104	95	19.920	20.874	21.743	0.869
1513111	96	20.038	21.041	21.792	0.751
1563201	97	19.925	20.761	21.372	0.611
1563204	98	20.125	20.975	21.684	0.709
1563211	99	20.066	21.075	21.982	0.907
1583301	100	20.255	21.115	21.989	0.874
1583304	101	20.096	20.946	21.790	0.844
1583311	102	19.937	20.760	21.460	0.700
1603401	103	19.873	20.725	21.336	0.611
1603401	104	20.001	20.808	21.417	0.609
1603404	105	20.005	20.933	21.575	0.642
1603404	106	20.028	20.813	21.445	0.632
1603411	107	19.971	20.808	21.592	0.784
1603411	108	19.967	20.641	21.251	0.610
1613501	109	19.903	20.625	21.255	0.630
1613504	110	20.082	21.078	21.787	0.709
1613511	111	20.061	21.158	22.014	0.856
1633601	112	20.091	20.994	21.774	0.780
1633604	113	20.014	20.889	21.563	0.674
1633611	114	19.946	20.928	21.569	0.641
1683901	115	19.973	20.883	21.629	0.746
1683901	116	19.952	20.669	21.462	0.793
1683904	117	20.079	20.849	21.560	0.711
1683904	118	19.960	20.825	21.647	0.822
1683911	119	19.951	20.748	21.423	0.675
1683911	120	20.062	20.647	21.368	0.721
Average		20.031	20.890	21.655	0.766

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.

TAlk:

Analysis date: 7/29/2016, 8/11/2016, 8/12/2016 and 8/15/2016
Titration system used: Open cell
CRM Batch 120, Salinity = 33.072, cert. TA = 2208.34 µmol/kg.
CRM Batch 144, Salinity = 33.571, cert. TA = 2238.60 µmol/kg (8/12/2016).

On 7/29, 8/11, 8/12 and 8/15 one CRM was analyzed before the samples and another 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	07/29/2016	10:02:57	156	2211.40	
1	07/29/2016	17:24:01	156	2208.76	2.64
1	08/11/2016	09:15:27	213	2211.13	
1	08/11/2016	16:27:55	213	2210.74	0.39
1	08/12/2016	09:06:19	54	2242.35	
1	08/12/2016	16:05:49	54	2239.71	2.64
1	08/15/2016	08:38:38	705	2213.50	
1	08/15/2016	14:23:21	705	2211.77	1.73
2	07/29/2016	11:30:04	536	2185.34	
2	07/29/2016	17:36:40	536	2182.04	3.30
2	08/11/2016	09:34:57	486	2183.41	
2	08/11/2016	16:21:22	486	2181.61	1.80
2	08/12/2016	09:14:26	117	2216.01	
2	08/12/2016	16:20:31	117	2212.94	3.07
2	08/15/2016	10:34:37	972	2186.41	
2	08/15/2016	14:19:17	972	2184.32	2.09

Reproducibility: (# samples and average difference): 13 duplicate samples were

collected with an average difference 2.60 µmol/kg (0.33 – 7.08) and an average STDEV of 1.61 (0.23 – 5.01).

System	Sample ID	TAlk	Average	Difference	STDEV
System 1	140101	2214.53	2214.03	1.00	0.71
System 1	140101	2213.52			
System 2	260404	2322.10	2321.93	0.33	0.23
System 2	260404	2321.77			
System 1	360709	2153.04	2152.65	0.77	0.55
System 1	360709	2152.27			
System 1	561101	2170.28	2168.80	2.96	2.09
System 1	561101	2167.32			
System 2	751511	2159.00	2159.23	0.45	0.32
System 2	751511	2159.45			
System 2	941901	2201.50	2201.33	0.33	0.23
System 2	941901	2201.16			
System 1	1132205	2203.28	2202.05	2.47	1.75
System 1	1132205	2200.81			
System 1	1603401	2270.35	2271.87	3.05	2.15
System 1	1603401	2273.40			
System 1	1603404	2233.58	2231.98	3.20	2.26
System 1	1603404	2230.38			
System 1	1603411	2176.04	2176.53	0.98	0.69
System 1	1603411	2177.02			
System 2	1683901	2186.24	2189.78	7.08	5.01
System 2	1683901	2193.32			
System 2	1683904	2166.75	2169.73	5.95	4.20
System 2	1683904	2172.70			

System 2	1683911	2128.25	2125.63	5.25	3.71
System 2	1683911	2123.00			
Overall Average				2.60	1.61

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

This carbon dataset has been merged with nutrient data from the same cruise, provided by Dr. Jon Hare's group. Where samples for carbon parameters and nutrients were drawn from different Niskin bottles, merging has been done based on sample depth, assuming all Niskin bottles tripped at the same depth would have the same nutrient values.

The following columns have been imported from the nutrients file:

Date_UTC, Depth_station, Depth_sampling, CTDPRS, CTDOXY, CTDOXYMOL, SILCAT, NITRIT+NITRAT, AMMONIA, PHSPHT

An additional column named Niskin_nuts has been added to reflect the niskin that nutrient samples were drawn from (which sometimes is different from the niskin used for carbon samples).

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.