Cruise: EQNX_20161030
Ship: Royal Caribbean Equinox
Expo Code: MLCE20161030
Dates: October 30th – November 11th, 2016
Chief Scientist: Dr. Denis Pierrot
Equipment: TSG-Flow thru system
Total number of stations: 35
Location: Ft. Lauderdale, FL to Lisbon, Portugal (Trans-Atlantic)

Sample Collection

The discrete samples were collected from the TSG-flow thru system onboard the ship of opportunity Royal Caribbean Equinox by Dr. Denis Pierrot. The date and time listed in the data file are UTC when each sample bottle was collected.

DIC:
35 locations, 38 samples each 500-ml, 3 duplicate samples.
Sample_ID#: 301, etc.; Sample bottle number
PI: Dr. Rik Wanninkhof
Analyzed by: Charles Featherstone

pH:
35 locations, 38 samples each 500-ml, 3 duplicate samples.
Sample_ID#: 301, etc.; Sample bottle number
PI: Dr. Rik Wanninkhof
Analyzed by: Charles Featherstone

TAlk:
35 locations, 38 samples each 500-ml, 3 duplicate samples.
Sample_ID#: 301, etc.; Sample 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 3	11/09/2016	2022.04	2023.53	1.49	28.0	20
AOML 4	11/08/2016	2022.04	2021.29	0.75	26.0	17
AOML 4	11/09/2016	2022.04	2020.94	1.10	28.0	17
AOML 4	11/10/2016	2022.04	2022.90	0.86	35.0	12

Analysis date: 11/09/2016
Coulometer used: DICE–CM5015- AOML 3
Blanks: 23.2 counts/min and raised to 28.0 counts/min before CRM analysis
CRM # 625 was used and with an assigned value of (includes both DIC and salinity):
Batch 123, c: 2022.4 µmol/kg, S: 33.384
CRM values measured: AOML 3: offset 1.49 µmol/kg (2023.53 µmol/kg).
Average run time, minimum run time, maximum run time: 20, 19 and 20 min.

Analysis date: 11/08/2016
Coulometer used: DICE–CM5015- AOML 4
Blanks: 10.4 counts/min and raised to 26.0 counts/min before CRM analysis
CRM # 560 was used and with an assigned value of (includes both DIC and salinity):
Batch 123, c: 2202.04 µmol/kg, S: 33.384
CRM values measured: AOML 4: offset 0.75 µmol/kg (2021.29 µmol/kg).
Average run time, minimum run time, maximum run time: 17, 11 and 20 min.

Analysis date: 11/09/2016
Coulometer used: DICE–CM5015- AOML 4
Blanks: 12.3 counts/min and raised to 28.0 counts/min before CRM analysis
CRM # 292 was used and with an assigned value of (includes both DIC and salinity):
Batch 123, c: 2202.04 µmol/kg, S: 33.384
CRM values measured: AOML 4: offset 1.10 µmol/kg (2020.94 µmol/kg).
Average run time, minimum run time, maximum run time: 17, 11 and 20 min.

Analysis date: 11/10/2016
Coulometer used: DICE–CM5015- AOML 4
Blanks: 27.4 counts/min and raised to 35.0 counts/min before CRM analysis
CRM # 18 was used and with an assigned value of (includes both DIC and salinity):
Batch 123, c: 2022.04 µmol/kg, S: 33.384
CRM values measured: AOML 4: offset 0.86 µmol/kg (2022.90 µmol/kg).
Average run time, minimum run time, maximum run time: 12, 9 and 15 min.

Reproducibility: (# samples and average difference): 3 sets of duplicate samples, average difference 4.52 µmol/kg (1.14-7.54), average STDEV of 3.19 (0.81-5.33).

Instrument ID	Sample ID	Bottle #	Corrected DIC (µmol/kg)	Average	Difference	STDEV
AOML4	620000	62	2112.27			
AOML4	630000	63	2117.14	2114.71	4.87	3.44
AOML4	730000	73	2114.45			
AOML4	740000	74	2115.59	2115.02	1.14	0.81
AOML3	1770000	177	2078.62			

AOML3	1780000	178	2086.16	2082.39	7.54	5.33
Average					4.52	3.19

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 samples were analyzed using the DICE (AOML 3 & AOML 4) and a new coulometer from UIC, Inc. CM5015 with CM5011 emulation software.

Duplicates were sampled 1 to 2 minutes apart from the ships TSG flow thru system.

pH:

Analysis date: 11/08/2016,11/09/2016 & 11/10/2016
Spectrophotometer used: HP Agilent 8453

CRM Batch 123 pH results

System	Analysis Date	Certified CRM pH	CRM Value pH	CRM Offset
HP Agilent 8453	11/08/2016	8.00	7.9082	0.0910
HP Agilent 8453	11/09/2016	8.00	7.9199	0.0801
HP Agilent 8453	11/10/2016	8.00	7.9242	0.0758

Reproducibility: (# samples and average difference): 3 sets of duplicate samples, average difference 0.0053 (0.0022-0.0105), average STDEV of 0.0038 (0.0016-0.0074).

System	Sample ID	Bottle #	pH	Average	Difference	STDEV
HP Agilent 8453	620000	62	8.0729			
HP Agilent 8453	630000	63	8.0834	8.0782	0.0105	0.0074
HP Agilent 8453	730000	73	8.1077			
HP Agilent 8453	740000	74	8.1055	8.1066	0.0022	0.0016

HP Agilent 8453	1770000	177	8.1446			
HP Agilent 8453	1780000	178	8.1413	8.1429	0.0033	0.0023
Average					0.0053	0.0038

Temperature 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)
610000	61	20.230	21.125	21.258	0.133
620000	62	20.030	21.088	21.463	0.375
630000	63	19.978	20.544	21.207	0.663
640000	64	20.130	21.205	21.898	0.693
650000	65	19.839	20.773	21.308	0.535
660000	66	20.096	21.162	21.655	0.493
670000	67	20.055	21.181	21.939	0.758
680000	68	20.079	21.165	21.864	0.699
690000	69	20.306	21.246	21.994	0.748
700000	70	20.049	20.679	21.459	0.780
710000	71	19.829	20.389	20.990	0.601
720000	72	19.983	20.965	21.510	0.545
730000	73	20.048	20.783	21.662	0.879
740000	74	19.978	20.857	21.530	0.673
750000	75	19.925	20.882	21.699	0.817
760000	76	19.858	20.678	21.501	0.823
770000	77	19.893	20.505	21.305	0.800
780000	78	19.962	20.766	21.343	0.577
790000	79	19.975	20.829	21.551	0.722
800000	80	19.984	20.550	21.271	0.721
1750000	175	20.055	20.689	21.554	0.865
1760000	176	20.015	20.776	21.737	0.961
1770000	177	20.078	20.982	21.865	0.883
1780000	178	19.865	20.769	21.371	0.602
1790000	179	20.051	20.856	21.698	0.842
1800000	180	19.924	20.594	21.436	0.842
1810000	181	19.836	20.613	21.309	0.696
1820000	182	19.941	20.839	21.160	0.321
1830000	183	20.202	21.338	21.727	0.389
1840000	184	19.811	20.330	20.874	0.544
1850000	185	19.868	20.530	20.873	0.343
1860000	186	19.827	20.502	21.035	0.533
1870000	187	19.828	20.515	21.007	0.492

1880000	188	19.904	20.651	21.568	0.917
1890000	189	19.844	20.837	21.359	0.522
1900000	190	19.982	21.628	22.258	0.630
1910000	191	19.78	20.407	21.017	0.610
1920000	192	19.761	20.287	20.850	0.563
CRM 350	CRM 350	19.831	20.672	21.415	0.743
CRM 568	CRM 568	19.87	20.543	21.486	0.943
CRM 75	CRM 75	19.809	20.143	20.443	0.300
Average			20.777	21.426	0.648

Remarks

Duplicates were sampled 1 to 2 minutes apart from the ships TSG flow thru system.

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: 11/17/2016, 11/18/2016 & 11/22/2016
Titration system used: Open cell
CRM Batch 123, Salinity = 33.384, cert. TA = 2225.21 µmol/kg.

On 11/17/2016, 11/18/2016 & 11/22/2016 one CRM was analyzed before the samples and another CRM or same CRM was run at the end of analysis 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|
2	11/17/2016	08:49:58	185	2227.46	
2	11/17/2016	16:05:32	185	2222.63	4.83
2	11/18/2016	09:03:06	129	2222.31	
2	11/18/2016	16:39:16	1062	2217.03	5.28
2	11/22/2016	08:21:52	953	2223.31	

2	11/22/2016	17:14:52	953	2224.52	1.21

Reproducibility: (# samples and average difference): 3 duplicate samples were collected with an average difference 2.03 µmol/kg (0.80 – 2.75) and an average STDEV of 1.44 (0.57 – 1.95).

System	Bottle #	Sample ID	TAlk	Average	Difference	STDEV
System 2	62	190504	2418.77	2417.49	2.55	1.80
System 2	63	190504	2416.22			
System 2	73	200601	2423.59	2424.97	2.75	1.95
System 2	74	200601	2426.34			
System 2	177	200611	2412.48	2412.88	0.80	0.57
System 2	178	200611	2413.28			
Average					2.03	1.44

Remarks

The CRM measurement for each day was used to correct the data for that day only. Both systems worked well.

Duplicates were sampled 1 to 2 minutes apart from the ships TSG flow thru system.

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 bottle number for the discrete samples.

The salinity and temperature were taken from the UW pCO2 system. The salinities were used in the DIC, Talk and pH calculations.

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

UPDATE:
Between March and May 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.