Cruise: Selfoss846
Ship: Cargo Ship Selfoss
Expocode: 46SL20181115
Dates: Nov. 15th – Nov. 23rd, 2018
Chief Scientist: Dr. Denis Pierrot
Equipment: Flow thru
Total number of stations: 40
Location: North Atlantic, transit between Portland, Maine (United States) and
Reykjavik, Iceland

Samples were collected for Dr. Leticia Barbero for the Ocean Acidification Program
during the Ships of Opportunity Project (SOOP) transit of the cargo ship Selfoss by Dr.
Denis Pierrot.

Sample Collection

The discrete samples were collected from the flow thru system onboard the container ship
Selfoss by Denis Pierrot. The date and time listed in the data file are UTC when each
sample bottle was collected.

DIC:
40 locations, 40 samples each 500-ml, 3 duplicate samples.
Sample ID#: 10000, etc.; Sample bottle number, Station, cast number and Niskin bottle
number
PI: Dr. Rik Wanninkhof
Analyzed by: Charles Featherstone and Patrick Mears

pH:
40 locations, 40 samples each 500-ml, 3 duplicate samples.
Sample ID#: 10000, etc.; Sample bottle number, Station, cast number and Niskin bottle
number
PI: Dr. Rik Wanninkhof
Analyzed by: Charles Featherstone and Patrick Mears

TAlk:
40 locations, 40 samples each 500-ml, 3 duplicate samples.
Sample ID#: 10000, etc.; Sample bottle number, 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	CRM Value (µmol/kg)	CRM Offset (µmol/kg)	Blank (Counts)	Avg. Sample

		(μmol/kg)				Analysis Time
AOML 5	02/05/2019	2020.88	2025.37	4.49	18	7
AOML 6	02/05/2019	2020.88	2026.07	5.19	16	7

Analysis date: 02/05/2019
Coulometer used: DICE–CM5011- AOML 5
Blanks: 18 counts/min
CRM # 623 was used and with an assigned value of (includes both DIC and salinity):
Batch 152, c: 2020.88 μmol/kg, S: 33.371
CRM values measured: AOML 5: offset 4.49 μmol/kg (2025.37 μmol/kg).
Average run time, minimum run time, maximum run time: 7, 7 and 8 min.

Analysis date: 02/05/2019
Coulometer used: DICE–CM5011- AOML 6
Blanks: 16.0 counts/min
CRM # 469 was used and with an assigned value of (includes both DIC and salinity):
Batch 152, c: 2020.88 μmol/kg, S: 33.371
CRM values measured: AOML 6: offset 5.19 μmol/kg (2026.07 μmol/kg).
Average run time, minimum run time, maximum run time: 7, 7 and 9 min.

Reproducibility: (# samples and average difference/STDEV): 3 duplicate samples were collected. The average difference was 0.90 μmol/kg and average STDEV of 0.64 μmol/kg

Sample ID	Bottle #	DIC	Average	Difference	STDEV
19	19	2102.80			
20	20	2102.71	2102.75	0.09	0.06
29	29	2053.99			
30	30	2051.74	2052.87	2.25	1.59
35	35	2024.41			
36	36	2024.78	2024.59	0.36	0.26
Average				0.90	0.64

Remarks
CRM, salinity and HgCl2 correction applied: Salinity correction was applied using TSG salinity.

The volume correction was applied due to added $HgCl_2$ (Measured DIC*1.0004).
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: 02/05/2019
A CRM was analyzed before sample analysis.
CRM #869, Batch 152 pH = 7.9400

Spectrophotometer used: HP Agilent 8453

Salinity and temperature of pH samples analyzed.

Sample ID	Sample Bottle #	Temp	Salinity
CRM152_869	CRM152_869	20.030	33.371
1	1	20.028	34.926
2	2	20.033	34.997
3	3	20.034	34.997
4	4	20.026	34.832
5	5	20.038	34.765
6	6	20.036	34.825
7	7	20.046	34.727
8	8	20.040	34.751
9	9	20.025	34.759
10	10	20.047	34.735
11	11	20.042	34.714
12	12	20.041	34.776
13	13	20.041	34.649
14	14	20.042	34.650
15	15	20.041	34.645
16	16	20.047	34.456
17	17	20.036	34.294
18	18	20.037	34.266
19	19	20.044	34.075
20	20	20.040	34.079
21	21	20.030	34.108
22	22	20.033	34.021
23	23	20.032	32.378
24	24	20.044	31.888
25	25	20.047	32.026
26	26	20.049	31.626

27	27	20.036	31.674
28	28	20.033	31.904
29	29	20.043	31.839
3	30	20.030	31.844
31	31	20.041	31.532
32	32	20.044	30.765
33	33	20.036	31.126
34	34	20.038	30.768
35	35	20.042	30.845
36	36	20.048	30.759
37	37	20.043	30.250
38	38	20.037	30.182
39	39	20.042	30.291
40	40	20.039	30.145

Reproducibility: (# samples and average difference/STDEV): 3 duplicates were collected. The average difference was 0.0009 pH Units and average STDEV was 0.0006 pH units. The pH values below are reported analyzed at 20^0C.

Sample ID	Sample Btl #	Salinity	Temp	pH@20C	Average	Difference	STDEV
19	19	34.075	20.044	7.8633			
20	20	34.079	20.040	7.8634	7.8633	0.0001	0.0001
29	29	31.839	20.043	7.7698			
30	30	31.844	20.030	7.7712	7.7705	0.0013	0.0009
35	35	30.845	20.042	7.7460			
36	36	30.759	20.048	7.7472	7.7466	0.0011	0.0008
Average						0.0009	0.0006

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). The pH was reported at 25^0C.

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 automatic syringe before DIC analysis to determine the pH.

TAlk:
Analysis date: 02/15/2019
Titration system used: Open cell
CRM #1059 Batch 152, Salinity = 33.371, cert. TA = 2216.94µmol/kg.
CRM #309 Batch 152, Salinity = 33.371, cert. TA = 2216.94µmol/kg

Analysis date: 02/19/2019
Titration system used: Open cell
CRM #672 Batch 152, Salinity = 33.371, cert. TA = 2216.94µmol/kg.
CRM #370 Batch 152, Salinity = 33.371, cert. TA = 2216.94µmol/kg

Analysis date: 02/20/2019
Titration system used: Open cell
CRM #996 Batch 152, Salinity = 33.371, cert. TA = 2216.94 µmol/kg.
CRM #388 Batch 169, Salinity = 33.518, cert. TA = 2207.03 µmol/kg

On 02/15/2019 CRM #1059, Batch 152 was analyzed before the samples and CRM #309, Batch 152 was run at the end of analysis on system 1.

On 02/19/2019 CRM #672, Batch 152 was analyzed before the samples and CRM #370, Batch 152 was run at the end of analysis on system 1.

On 02/20/2019 CRM #996, Batch 152 was analyzed before the samples and CRM #388, Batch 169 was run at the end of analysis on system 1.

The TA for the water samples was corrected using the daily averaged ratios between the certified and measured values of the CRMs run on system 1 cell. The following table shows the CRM measurements for each day and cell.

Cell System	Date	Time	Bottle #	TA	$|\Delta CRM|$
1	02/15/2019	10:44:15	1059	2231.84	14.90
1	02/15/2019	17:51:19	309	2221.23	4.29
1	02/19/2019	11:35:56	672	2232.38	15.44
1	02/19/2019	17:50:41	370	2224.04	7.10
1	02/20/2019	10:31:12	996	2225.66	8.72
1	02/20/2019	16:36:51	388	2207.04	0.01

Reproducibility: (# samples and average difference/STDEV): 3 duplicates were collected. The average difference was 3.61 µmol/kg and average STDEV was 2.56 µmol/kg.

System	Sample ID	TAlk	Average	Difference	STDEV
2	19	2257.09			
2	20	2259.03	2258.06	1.94	1.37
2	29	2165.58			
2	30	2158.41	2162.00	7.18	5.07
2	35	2125.05			
2	36	2126.78	2125.91	1.73	1.22
Average				3.61	2.56

Remarks

The CRM measurement for each day was used to correct the data for that day only.

Nutrients:
Analysis Date: May 12th, 2018

Samples for the determination of phosphate, nitrate (nitrate + nitrite) and silicate concentrations were collected in 250 ML soft low-density polyethylene bottles that were washed with dilute hydrochloric acid prior to the cruise. Samples were refrigerated or frozen until analyzed. An AA3 Seal autoanalyzer was used for nutrient sample analysis. The methods used were those described by Grasshoff (Grasshoff, 1970) except for phosphate where a modified version of the Murphy and Riley method was automated (Murphy and Riley, 1962). A series of five working standards were run along with a batch of samples and the response fitted to concentration with a linear regression. Alice Benoit-Cattin-Breton from the Marine and Freshwater Research Institute was responsible for sample collection and analysis (alice.benoit-cattin@hafogvatn.is).

Comments

The latitude, longitude, date, and time reported with the DIC, pH and TAlk measurements were taken from the sample field log.

The Sample ID and station number is the sample bottle number for the discrete samples.

New clean sampling tube was used after sample bottle 1.

Temperature data from the UW pCO2 was used for the Flow-thru (FT)

samples collected.

Duplicates were reported as individual samples in the data, resulting in 40 data points instead of 37.

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.