README FOR DISCRETE DATA MEASUREMENTS ON THE SOOP SKOGAFOSS

Cruise: Skogafoss, SKO0406 Dates: June 4 - 11, 2004

Chief Scientists: not applicable

Equipment: Surface samples collected next to TSG from ship's engine cooling water.

Total number of stations: VOS Underway Cruise

Chemical measurements:

DIC: 12 locations, 20 samples each 500-ml, 16 duplicate samples

PI: Dr. Rik Wanninkhof Collected by: Denis Pierrot Analyzed by: Esa Peltola

Salinity: Salinity from the ship's thermosalinograph on the Practical

Salinity Scale

Details:

DIC:

Analysis date: April 27-28, 2004

Coulometers used: AOML1 and AOML2

Blank range: 13.4-23.3 counts/min

CRM # used and assigned value (include both DIC and salinity): Batch 45, c:1994.17

umol/kg,S:33.487

CRM value measured: AOML 1: offset 4.9umol/kg (1999.0 umol/kg)

AOML-2: offset 10.2 umol/kg (2004.4 umol/kg)

Average run time, minimum run time, maximum run time: 9 min, 8 min, 14 min

Reproducibility: (# samples and average difference): 8 sets of duplicate samples, average

difference 1.4 umol/kg

CRM, salinity and HgCl2 correction applied: yes

Cruise: SKO0406 Ship: M/V Skogafoss Dates: April 4 - 11, 2004 Chief Scientist: not applicable

Equipment: Surface samples collected.

Total number of stations: VOS Underway Cruise

Sample Collection

The discrete samples were collected by Denis Pierrot at a tap on the side of the TSG enclosure in the engine room. The underway pCO2 instrument and the TSG were supplied with water from the flow used for engine cooling. The water flowing through the TSG is believed to be 0.2 degrees C warmer than in-situ SST. The date and time listed in the data file are UTC when each sample bottle was collected.

DIC:

12 locations, 20 samples each 500-ml, 8 duplicate samples

Sample_ID#: 1 – 20 PI: Dr. Rik Wanninkhof Collected by: Denis Pierrot Analyzed by: Esa Peltola

Salinity 1:

8 locations, 24 samples each 180-ml

Sample_ID#: 745 - 768
PI: Dr. Hedinn Valdimarsson
Collected by: Denis Pierrot

Analyzed by: Magnus Danielsen, Icelandic Marine Research Institute

Sample Analysis

DIC:

Analysis date: April 27-28, 2004

Coulometers used: AOML1 and AOML2 Blank range: 13.4-23.3 counts/min

CRM # used and assigned value (include both DIC and salinity): Batch 45, c:1994.17

umol/kg,S:33.487

CRM value measured: AOML 1: offset 4.9umol/kg (1999.0 umol/kg)
AOML-2: offset 10.2 umol/kg (2004.4 umol/kg)

Average run time, minimum run time, maximum run time: 9 min, 8 min, 14 min

Reproducibility: (# samples and average difference): 8 sets of duplicate samples, average

difference 1.4 umol/kg

CRM, salinity and HgCl2 correction applied: yes

Comments

A GPS transducer was connected to the underway pCO2 instrument as well as a thermosalinograph (TSG). The GPS and the TSG, a Seabird SBE-21, were maintained by the Ship of Opportunity Program at AOML

(http://www.aoml.noaa.gov/phod/tsg/soop/index.php).

The latitude, longitude, temperature and salinity reported with the DIC and TAlk measurements were taken from the raw TSG data file. The merging of the discrete measurements with the TSG data was done on the basis of date and time. The TSG values are provided for reference; no post-cruise assurance of accuracy has been done to this data. The results of the analyses of discrete salinity bottles appear on separate lines.

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

Cruise: Skogafoss, SKO0410

Dates: June 26 - July 2, 2004

Chief Scientists: not applicable

Equipment: Surface samples collected next to TSG from ship's engine cooling water.

Total number of stations: VOS Underway Cruise

Chemical measurements:

DIC: 14 locations, 20 samples each 500-ml, 12 duplicate samples

PI: Dr. Rik Wanninkhof Collected by: Denis Pierrot Analyzed by: Esa Peltola

Salinity: 14 locations, 20 samples each 180-ml, 12 duplicates

PI: Dr. Gustavo Goni Collected by: Denis Pierrot

Analyzed by: Magnus Danielsen, Icelandic Marine Research Institute

Details:

DIC:

Analysis date: November 9-10, 2004

Coulometer used: AOML1

Blank range: 12.0-12.0 counts/min

CRM # used and assigned value (include both DIC and salinity): Batch 59, c:2007.1

umol/kg,S:33.316

CRM value measured: AOML 1: offset 1.0 umol/kg (2006.1 umol/kg)

Average run time, minimum run time, maximum run time: 10 min, 8 min, 11 min Reproducibility: (# samples and average difference): 6 sets of duplicate samples, average difference 0.7 umol/kg

CRM, salinity and HgCl2 correction applied: yes

Cruise: Skogafoss, SKO0414

Dates: October 16 - 22, 2004

Chief Scientists: not applicable

Equipment: Surface samples collected next to TSG from ship's engine cooling water.

Total number of stations: VOS Underway Cruise

Chemical measurements:

DIC: 10 locations, 20 samples each 500-ml, 20 duplicate samples

PI: Dr. Rik Wanninkhof Collected by: Kevin Sullivan Analyzed by: Esa Peltola

Salinity: Salinity from the ship's thermosalinograph on the Practical

Salinity Scale

Details:

DIC:

Analysis date: Nov 12, 2004

Coulometers used: AOML1 and AOML2 Blank range: 17.7-24.3 counts/min

CRM # used and assigned value (include both DIC and salinity): Batch 59, c:2007.1

umol/kg,S:33.316

CRM value measured: AOML 1: offset 4.1 umol/kg (2003.1 umol/kg)

AOML-2: offset 0.5 umol/kg (2006.7 umol/kg)

Average run time, minimum run time, maximum run time: 15 min, 9 min, 20 min Reproducibility: (# samples and average difference): 10 sets of duplicate samples,

average difference 1.2 umol/kg

CRM, salinity and HgCl2 correction applied: yes

Cruise: Skogafoss, SKO0510

Dates: September 17 - 23, 2005

Chief Scientists: not applicable

Equipment: Surface samples collected next to TSG from ship's engine cooling water.

Total number of stations: VOS Underway Cruise

Chemical measurements:

DIC: 10 locations, 20 samples each 500-ml, 20 duplicate samples

PI: Dr. Rik Wanninkhof Collected by: Denis Pierrot Analyzed by: Esa Peltola

Salinity: Salinity from the ship's thermosalinograph on the Practical

Salinity Scale

TALK: 10 locations, 10 samples each 500-ml

PI: Dr. Frank Millero Collected by: Denis Pierrot Analyzed by: Fen Huang

Details:

DIC:

Analysis date: October 3, 2005

Coulometers used: AOML1 and AOML2 Blank range: 12.0-25.0 counts/min

CRM # used and assigned value (include both DIC and salinity): Batch 59, c:2007.1

umol/kg,S:33.316

CRM value measured: AOML 1: offset 5.8 umol/kg (2001.3 umol/kg)

AOML-2: offset 9.3 umol/kg (1997.8 umol/kg)

Average run time, minimum run time, maximum run time: 11 min, 8 min, 19 min Reproducibility: (# samples and average difference): 10 sets of duplicate samples,

average difference 1.4 umol/kg

CRM, salinity and HgCl2 correction applied: yes

Cruise: Skogafoss, SKO604

Dates: April 19-28, 2006

Chief Scientists: N/A

Equipment: N/A

Total number of stations: UW

Chemical measurements:

DIC: 23 samples each 500-ml, 10 duplicates

PI: Wanninkhof;

Collected by: Sullivan,

Analyst: Peltola

Details: **DIC-**

Analysis dates: May 15, 2006

Coulometers used: AOML1 and AOML2

Blank range: 18.8-26.5 counts/min

CRM # used and assigned value (include both DIC and salinity): Batch 66, c:1969.57

umol/kg,S:32.997

CRM value measured: AOML 1: offset 8.0 umol/kg (1961.5 umol/kg)

AOML-2: offset 6.3 umol/kg (1963.3 umol/kg)

Average run time, minimum run time, maximum run time: 13 min, 9 min, 20 min Reproducibility: (# samples and average difference): 22 duplicate samples, average

difference 1.6 umol/kg

CRM Salinity and HgCl2 correction applied: yes

Remarks-

A density correction was applied for all the samples.

The volume correction was applied due to added HgCl2 (Measured DIC*1.00037).

The average CRM correction was 7.1 umol/kg and was run in the beginning and end of the cell.

The first CRM of each cell was used for a CRM correction.

There was a good agreement between the duplicate samples, except samples S09 and S10. Also S13 differs from samples S11 and S12. No reason for these differences were found due to analysis. All 23 samples were sent to Millero's lab for alkalinity analysis

Cruise: SKO0611

Dates: October 15 - 23, 2006 **Chief Scientists:** not applicable

Equipment: Surface samples collected.

Total number of stations: VOS Underway Cruise

Chemical measurements:

DIC: 10 locations, 24 samples each 500-ml, 24 duplicate samples (some of them

triplicates)

PI: Dr. Rik Wanninkhof Collected by: Kevin Sullivan Analyzed by: Esa Peltola

Salinity: Salinity from the ship's thermosalinograph on the Practical

Salinity Scale

TALK:

PI: Dr. Frank Millero

Collected by Kevin Sullivan Analyzed by: Fen Huang

Details:

DIC:

Analysis date: December 5, 2006

Coulometers used: AOML1 and AOML2 Blank range: 12.0-20.0 counts/min

CRM # used and assigned value (include both DIC and salinity): Batch 59, c: 2007.1

umol/kg, S: 33.316

CRM value measured: AOML 1: offset 6.5 umol/kg (2013.6 umol/kg) AOML-2: offset 3.4 umol/kg (2010.5 umol/kg)

Average run time, minimum run time, maximum run time: 11 min, 8 min, 20 min Reproducibility: (# samples and average difference): 11 sets of duplicate (triplicate) samples, average difference 1.8 umol/kg

CRM, salinity and HgCl2 correction applied: Salinity correction was applied for the AOML1 samples, the AOML2 samples were calculated using TSG salinity; CRM and HgCl2 volume correction was applied

Location of analyses files: Esa's computer file/directory/name: My

Documents/SOMMA/Lab Studies/2006 (12) Skogafoss /

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.

There was a good agreement between the duplicate samples 101-120. The samples 121-124 were marked questionable. All 20 samples were sent to Millero's lab for alkalinity analysis

Cruise: SKO0721

Dates: May 26 – June 2, 2007 **Chief Scientists:** not applicable

Equipment: Surface samples collected.

Total number of stations: VOS Underway Cruise

Chemical measurements:

DIC: 19 locations, 21 samples each 500-ml, 2 duplicate samples

PI: Dr. Rik Wanninkhof Collected by: Denis Pierrot Analyzed by: Esa Peltola

Salinity: Salinity from the ship's thermosalinograph on the Practical

Salinity Scale

TALK:

PI: Dr. Frank Millero

Collected by Denis Pierrot Analyzed by: Fen Huang

Details:

DIC:

Analysis date: September 24, 2007 Coulometers used: DICE3 and DICE4 Blank range: 14.3-25.0 counts/min

CRM # used and assigned value (include both DIC and salinity): Batch 59, c: 2007.1

umol/kg, S: 33.316

CRM value measured: DICE3: offset 1.6 umol/kg (2008.7 umol/kg) DICE4: offset 3.2 umol/kg (2010.3 umol/kg)

Average run time, minimum run time, maximum run time: 8 min, 8 min, 8 min

Reproducibility: (# samples and average difference): 2 sets of duplicate samples, average

difference 0.5 umol/kg

CRM, salinity and HgCl2 correction applied: Salinity correction was applied for all the samples using TSG salinity; CRM and HgCl2 volume correction was applied

Location of analyses files: Esa's computer file/directory/name: My

Documents/SOMMA/Lab Studies/2007 (09) Skogafoss 721 /

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.

There was a good agreement between the duplicate samples. All 20 samples were sent to Millero's lab for alkalinity analysis

Cruise: Skogafoss 1406

Ship: Skogafoss

Dates: June 20th – June 28th, 2014 **Chief Scientist:** Christopher Taylor

Equipment: TSG-Underway **Total number of stations**: 33 **Location**: North atlantic transect

The samples were run as part of our ocean acidification monitoring project.

Sample Collection

The discrete samples were collected from the TSG underway (UW) system onboard the ship by Christopher Taylor. The date and time listed in the data file are UTC when each sample bottle was collected.

DIC:

33 locations, 33 samples each 500-ml, no duplicate samples.

Sample ID#: 10000, etc.; Sample bottle number, no Niskin or cast number

PI: Dr. Rik Wanninkhof

Analyzed by: Charles Featherstone

pH:

33 locations, 33 samples each 500-ml, no duplicate samples.

Sample ID#: 10000, etc.; Sample bottle number, no Niskin or cast number

PI: Dr. Rik Wanninkhof

Analyzed by: Charles Featherstone

TAlk:

33 locations, 33 samples each 500-ml, no duplicate samples.

Sample ID#: 10000, etc.; Sample bottle number, no Niskin or cast number

PI: Dr. Rik Wanninkhof

Analyzed by: Leticia Barbero and Denis Pierrot

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 2 | 07/17/14 | 2016.65 | 2018.57 | 1.92 | 13.7 | 8 |
| AOML 2 | 07/18/14 | 2016.65 | 2018.40 | 1.75 | 12.0 | 8 |

Analysis date: 07/17/2104

Coulometer used: SOMMA –AOML 2

Blanks: 13.7 counts/min

CRM # 0967 was used and with an assigned value of (includes both DIC and salinity):

Batch 129, c: 2016.65 µmol/kg, S: 33.361

CRM values measured: AOML 2: offset 1.92 μ mol/kg (2018.57 μ mol/kg). Average run time, minimum run time, maximum run time: 8, 8 and 8 min.

Analysis date: 07/18/2104

Coulometer used: SOMMA –AOML 2

Blanks: 12.0 counts/min

CRM # 0090 was used and with an assigned value of (includes both DIC and salinity):

Batch 129, c: 2016.65 µmol/kg, S: 33.361

CRM values measured: AOML 2: offset 1.75 µmol/kg (2018.40 µmol/kg). Average run time, minimum run time, maximum run time: 8, 8 and 8 min.

Reproducibility: (# samples and average difference): No duplicate samples were

collected.

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 instrument was stable: CRM values did not change significantly throughout the life span of each cell.

pH:

Analysis date: July 17th and 18th, 2014 Spectrophotometer used: HP Agilent 8453

Reproducibility: (# samples and average difference): No duplicates were collected.

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^oC 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:

The results posted are analyses from the same sample bottles used for DIC.

Analysis date: 08/05/2014 – 08/06/2014

Titration system used: Open cell CRM analysis (values in μmol/kg):

CRM analyzed:

Batch 123, Salinity = 33.384, cert. TA = $2225.21 \mu mol/kg$.

2 CRM samples were run daily on each cell, before (CRM-1) and after (CRM-2) the seawater samples. The TA for the water samples was corrected using the daily averaged

ratios between the certified and measured values of the 2 CRMs run on each cell. The following table shows the CRM measurements for each day and cell.

| | | | | | SYSTEM 1 | | | SYST EM 2 | |
|-----|----------|-------|-------------|----------|-----------------|---------------------|-----------------|---------------------|--------------------------|
| CRM | Date | Batch | Bottle # | meas. TA | meascert. TA | Diff. in Offsets | meascert. TA | meas cert. TA | Diff. in Offsets |
| 1 | 08/05/14 | 123 | 10 | 2223.51 | -1.7 | 0.89 | 2214.09 | -11.12 | 3.41 |
| 2 | 08/05/14 | 123 | 505 | 2222.62 | -2.59 | | 2210.68 | -14.53 | |
| 1 | 08/06/14 | 123 | 787 | 2220.04 | -5.17 | 0.56 | 2215.29 | -9.92 | 1051 was not |
| 2 | 08/06/14 | 123 | 1051 | 2220.60 | -4.61 | 0.56 | 2208.08 | -17.13 | used in the calculations |
| | | | | | | | | | |

Reproducibility: No duplicates were collected.

Remarks

System 1 behaved well during the analyses. System 2 was more inconsistent. On August 6th, the value for the second CRM used on system 2 was considered suspicious based on the normal values obtained for CRMs from batch 123 and was not used for the correction of the few samples run on system 2 on that day.

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

Comments

Sample ID # is the sample bottle number. No station or niskin bottle numbers with underway sampling. 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.

Cruise: Skogafoss1501

Ship: Skogafoss

Expo Code: AGFO20141217

Dates: December 12th, 2014 – January 15th, 2015

Chief Scientist: Dr. Denis Pierrot **Equipment**: TSG-Flow thru system

Total number of stations: 9 **Location:** Iceland to Argentia

Sample Collection

The discrete samples were collected from the TSG-flow thru system onboard the ship of opportunity Skogafoss by Benjamin Rumeau. The date and time listed in the data file are UTC when each sample bottle was collected.

DIC:

9 locations, 9 samples each 500-ml, no duplicate samples.

Sample ID#: 61, etc.; Sample bottle number

PI: Dr. Rik Wanninkhof

Analyzed by: Charles Featherstone

pH:

9 locations, 9 samples each 500-ml, no duplicate samples.

Sample ID#: 61, etc.; Sample bottle number

PI: Dr. Rik Wanninkhof

Analyzed by: Charles Featherstone

TAlk:

9 locations, 9 samples each 500-ml, no duplicate samples.

Sample ID#: 61, etc.; Sample bottle number

PI: Dr. Rik Wanninkhof

Analyzed by: Dr. Leticia Barbero, Dr. Denis Pierrot 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 | 03/05/2015 | 2016.65 | 2020.35 | 3.70 | 30.0 | 16 |

Analysis date: 03/05/2015

Coulometer used: DICE-CM5015- AOML 4

Blanks: 18.2, 30.0 counts/min

CRM # 0758 was used and with an assigned value of (includes both DIC and salinity):

Batch 129, c: 2016.65 μmol/kg, S: 33.361

CRM values measured: AOML 4: offset 3.70 µmol/kg (2020.35 µmol/kg). Average run time, minimum run time, maximum run time: 16, 11 and 19 min.

Reproducibility: (# samples and average difference): No duplicate samples were collected.

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. The end blank (AOML 4 = 33.4) slightly higher at the end of sample analysis.

The blank on AOML 4 (03/05/2015) was raised from 18.2 to 30.0 before running the CRM.

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

pH:

Analysis date: 03/05/2015

Spectrophotometer used: HP Agilent 8453

Reproducibility: (# samples and average difference): No duplicates were collected.

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^oC 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:

The results posted are analyses from the same sample bottles used for DIC and pH.

Analysis dates: 03/10/2015

Titration system used: Open cell

CRM batch: 129, S = 33.361, certified TA = $2237.32 \mu mol/kg$

2 CRM samples were run on the cell, before and after the seawater samples. The TA for the water samples was corrected using the averaged ratios between the certified and measured values of the 2 CRMs run on the cell. The following table shows the CRM measurements for the cell.

| Cell Syster | Date | Time | Bottle # | TA | \Delta CRM |
|----------------|-----------|----------|----------|---------|------------|
| 2 | 3/10/2015 | 09:59:22 | 533 | 2214.91 | |
| 2 | 3/10/2015 | 16:26:57 | 601 | 2214.36 | 0.55 |

Reproducibility: No duplicates were collected.

Remarks

The system behaved well during the analyses.

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.

Exact salinity values were not recorded at the time of sampling. Values have been extracted from the TSG values available in the underway pCO2 file. The salinity used is an average of the values measured between the start and end time of sampling, which ranged from 10 to 45 minutes. Thus, salinity is approximated. However, based on the actual salinity values measured and the standard deviations during the sampling periods, the averaged salinity is considered appropriate for the DIC, and TA calculations.

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

Cruise: Skogafoss 1506

Ship: Skogafoss

Expo Code: AGFO20150530 **Dates:** June 25th – June 28th, 2015 **Chief Scientist:** Dr. Gilles Reverdin

Equipment: TSG-Underway **Total number of stations**: 20

Location: Reykjavik, Iceland to Argentia

Samples were collected as part of the SOOP (Ships of Opportunity Program)

Sample Collection

The discrete samples were collected from the TSG underway (UW) system onboard the ship by Antoine Petrelli. The date and time listed in the data file are UTC when each sample bottle was collected.

DIC:

20 locations, 20 samples each 500-ml, no duplicate samples.

Sample ID#: 220000, etc.; Sample bottle number, no Niskin or cast number

PI: Dr. Rik Wanninkhof Analyzed by: Robert Castle

TAlk:

20 locations, 20 samples each 500-ml, no duplicate samples.

Sample ID#: 220000, etc.; Sample bottle number, no Niskin or cast number

PI: Dr. Rik Wanninkhof

Analyzed by: Leticia Barbero and Denis Pierrot

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 | 07/27/15 | 2031.53 | 2032.25 | 0.72 | 24 | 11 |

Analysis date: 07/27/2015

Coulometer used: DICE-CM5015- AOML 3

Blanks: 12.0 raised to 24.0 before analysis of CRM counts/min

CRM # 715 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 0.72 µmol/kg (2032.25 µmol/kg). Average run time, minimum run time, maximum run time: 11, 9 and 13 min.

Reproducibility: (# samples and average difference): No duplicate samples were collected.

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 instrument was stable: CRM values did not change significantly throughout the life span of each cell.

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

TAlk:

The results posted are duplicate analyses from the same sample bottles used for DIC.

Analysis dates: 08/04/2015 Titration system used: Open cell

CRM batch: 129, S = 33.361, certified TA = 2237.32 μ mol/kg

2 CRM samples were run daily on each cell, before and after the seawater samples. The TA for the water samples was corrected using the daily averaged ratios between the certified and measured values of the 2 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 | 2/4/2015 | 12:57:04 | 146 | 2223.74 | |
| 1 | 2/4/2015 | 16:10:28 | 756 | 2226.2 | 2.46 |
| | | | | | |
| 2 | 2/5/2015 | 11:54:15 | 146 | 2216.92 | |
| 2 | 2/5/2015 | 16:17:45 | 756 | 2220.46 | 3.54 |
| | | | | Average | 3.00 |
| | | | | Std. Dev. | 0.76 |
| | | | | | |

Reproducibility: No duplicates were collected.

Remarks

The two systems behaved well during the analyses.

Comments

The latitude, longitude, date, and time reported with the DIC 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.

Salinity was measured by Magnus Danielsen after the cruise.

Sample ID # is the sample bottle number. No station or niskin bottle numbers with underway sampling.

Cruise: Skogafoss 1509, Skogafoss 1604

Ship: Skogafoss

Expo Code: AGFO20150903, AGFO20160316

Dates: Sep. 3rd 2015– Mar. 30th, 2016 **Chief Scientist:** Dr. Denis Pierrot **Equipment:** TSG-Underway

Total number of stations: 22

Location: Reykjavik, Iceland to Argentia

Samples were collected as part of the SOOP (Ships of Opportunity Program)

Sample Collection

The discrete samples were collected from the TSG underway (UW) system onboard the ship by Benjamin Rumeau. The date and time listed in the data file are UTC when each sample bottle was collected.

DIC:

22 locations, 22 samples each 500-ml, no duplicate samples.

Sample ID#: 220000, etc.; Sample bottle number, no Niskin or cast number

PI: Dr. Rik Wanninkhof

Analyzed by: Charles Featherstone

pH:

22 locations, 22 samples each 500-ml, no duplicate samples.

Sample ID#: 220000, etc.; Sample bottle number, no Niskin or cast number

PI: Dr. Rik Wanninkhof

Analyzed by: Charles Featherstone

TAlk:

22 locations, 22 samples each 500-ml, no duplicate samples.

Sample ID#: 220000, etc.; Sample bottle number, no Niskin or cast number

PI: Dr. Rik Wanninkhof

Analyzed by: Leticia Barbero and Denis Pierrot

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 | 10/06/2015 | 2031.53 | 2025.74 | 5.79 | 35.0 | 16 |

Analysis date: 10/06/2015

Coulometer used: DICE-CM5015- AOML 4

Blanks: 35.0 counts/min

CRM # 1155 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 5.79 µmol/kg (2025.74 µmol/kg). Average run time, minimum run time, maximum run time: 16, 11 and 20 min.

Reproducibility: (# samples and average difference): No duplicate samples were collected.

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 instrument was stable: CRM values did not change significantly throughout the life span of each cell.

The blank was raised from 24.4 to 35.0 before the analysis of the CRM.

pH:

Analysis date: 10/06/2015

Spectrophotometer used: HP Agilent 8453

Reproducibility: (# samples and average difference): No duplicates were collected.

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^oC 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:

The results posted are duplicate analyses from the same sample bottles used for DIC and pH.

Analysis dates: 12/14/2015 Titration system used: Open cell

CRM batch: 129, S = 33.361, certified TA = 2237.32 μ mol/kg

2 CRM samples were run daily on each cell, before and after the seawater samples. The TA for the water samples was corrected using the daily averaged ratios between the certified and measured values of the 2 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 | 12/14/15 | 10:59:19 | 977 | 2214.23 | |
| 2 | 12/14/15 | 18:57:24 | 369 | 2210.83 | 3.40 |

Reproducibility: No duplicates were collected.

Remarks

Alkalinity system 2 behaved well during the analyses

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. Salinity was measured by Magnus Danielsen after the cruise.

Sample ID # is the sample bottle number. No station or niskin bottle numbers with underway sampling.

Sample bottle #18 had a broken neck and could not run the sample for DIC.