

ARKXXII/2 Carbon Measurements

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Abstract

This document outlines the procedures followed in collection and analysis for DIC and TALK of seawater samples during Polarstern cruise ARKXXII/2 and the subsequent processing of the results. Some of the various considerations during data processing are discussed, as well as the basic workings of the MATLAB-routines that were programmed specifically to facilitate rapid but thorough and well-documented processing of the measurements. Scripts are included verbatim, as are several figures and an extensive table containing raw and processed results. Briefly, sampling was performed according to DOE1994, but analysis follows DOE1994 less stringent. An assessment of data quality is presented at the end of this document. Although the measurement system was not absolutely calibrated, resulting data is very well correctable through the use of CRM, after which data is deemed to be of reasonably high quality.

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1 Metadata

Name of cruise: ARKXXII/2

Research vessel: F/S Polarstern

Time: 28 July (Tromsø) to 10 October 2007 (Bremerhaven)

Working area: Eurasian Arctic

Parameters: Total alkalinity (TAlk) and dissolved inorganic carbon (DIC)

Analyst: Sven Ober (RoyalNIOZ, The Netherlands)

Analyzer: VINDTA #14 (owned by NIOZ)

Data processing: Steven van Heuven (University of Groningen, The Netherlands)

of samples analyzed: 453

of stations sampled: 40

of CRM analyses: 140 (70 bottles, two subsequent runs from each bottle).

2 Analytical methods

2.1 Sampling procedure

Samples were collected in 250ml borosilicate bottles following DOE1994. Samples were poisoned with HgCl, closed with ground glass stoppers, using grease and rubber bands and stored dark and cold until analysis. All samples were analyzed on board, within 8 weeks after sampling. A correction for the diluting effect of adding HgCl is performed, but the headspace equilibration correction (ΔD) is not, because the atmospheric concentration of CO₂ in the rosette tapping room was not known. Since headspace volume was consistently very low ($\sim 1\%$ of sample volume), no influence on DIC of more than $.5 \mu\text{mol/kg}$ is expected.

2.2 Analyzer description

Samples were analyzed on a VINDTA 3C (Versatile Instrument for Determination of Titration Alkalinity) type 3C, developed and built by Dr. Ludger Mintrop, MARIANDA, Kiel, Germany. This device concurrently performs a potentiometric alkalinity titration and a coulometric DIC titration (see DOE1994 and references therein). Calculations performed by the VINDTA at time of measurement were considered to be preliminary, because of a lack of accurate salinity and nutrient values, which are required for these calculations. Storage of all raw titration results allowed for post-cruise recalculation of all results.

2.3 Analysis procedure

Samples were allowed to reach analysis temperature by being placed in a waterbath of 25.0°C for ~ 1 hour. Sample bottle stoppers were removed immediately prior to insertion of the sampling line to the machine. Samples were drawn towards the machine by a peristaltic pump. Although a slight underpressure is generated in the sampling line in this way, no excessive bubble formation (dissolved gas being ‘pulled out of solution’) was observed. Sample was first used to rinse and fill the DIC pipette, and after that to rinse and fill the TAlk pipette. Care was taken to avoid sample carry-over (by separating subsequent samples by a small volume of air). Measurements were not performed around the clock, but mainly during daytime. In order to set the measurement accuracy, Certified Reference Material was analyzed at least twice during a measurements day: after the coulometric cell was successfully started (i.e., after a suitable number of dummy runs were performed and coulometer blank level was stable), and shortly before the end of the day. Occasionally CRM was analyzed halfway the day as well.

2.4 DIC-specific remarks

DIC determinations were performed using the standard coulometric method, using a UIC model 5011 coulometer. No current-to-frequency calibration has been performed either pre- or post-cruise, and an inaccuracy may be present in the coulometric data, up to 0.5% (i.e., $10 \mu\text{mol/kg}$) in either direction. Also, no highly accurate determination of pipette volume has been performed, but pipette is known to have been 19.5 ± 0.1 ml (accuracy thus $\sim 0.5\%$ i.e., $\sim 10 \mu\text{mol/kg}$). These errors are expected to have been very constant during the course of the cruise, and both have a linear effect on the measured values and are therefore exactly correctable by the use of CRM. No gas-loop calibration was used.

2.5 TAlk-specific remarks

TAlk determinations were performed by an acid titration that combines aspects from both the commonly used ‘closed cell’ method and the ‘open cell’ method, following the VINDTA’s standard settings. Batches of acid were carefully prepared to be 0.1M, but no determinations of the exact acid strengths were performed (error assumed to be $< 0.25\%$ i.e., $\sim 6 \mu\text{mol/kg}$). Also, no highly accurate determination of pipette volume has been performed, but pipette is known to have been 97.0 ± 0.5 ml (accuracy $\sim 0.5\%$ i.e., $\sim 12 \mu\text{mol/kg}$). Burette (on a Metrohm Titrino model 719) volume was determined post cruise to be exactly 5.00ml to within 0.1% (i.e., $\sim 0.2 \mu\text{mol/kg}$). New electrodes from Metrohm (reference) and

Orion (measurement) were used, but no formal assessment of their quality (E^0 , Nernst response) was performed¹. Significant and unquantifiable inaccuracies may therefore be present in the final dataset.

¹Please note that even when correcting values to CRM-results, a non-Nernstian electrode will yield inaccurate values on samples with TAlk values different from those of the CRM!

3 Post-cruise data processing

A suite of flexible MATLAB scripts was developed to assist in thorough though rapid processing of CO₂-system data gathered during oceanographic expeditions. The scripts as they are detailed here are a customized version (specific to the particular format of the data gathered on this cruise) of the more general scripts. The following subsection will explain the basic workings of each routine

3.1 `vindta222_loadvindtafile`

This scripts loads the dataset output by the VINDTA CO₂-analyzer. This contains such variables as runname, runtime, the sample's station, cast and depth values, CRM batch numbers, etc. The DIC and TALK values calculated by the VINDTA at the end of analysis runs are loaded as well, although these will later on be overwritten with values recalculated from the raw coulometer and titration results and the final salinity and nutrients data.

3.2 `vindta222_loadbottlefile`

This scripts simply loads a cruise's bottlefile, which in this case formatted as an ODV spreadsheet. For each oceanographic sample that was collected during the cruise, station-, cast- and bottle numbers and values of salinity, phosphate and silicate are stored in memory.

3.3 `vindta222_loadlogfile`

This script loads the coulometric logfile generated by the VINDTA's software, associated with DIC-related actions performed by the VINDTA. It contains all coulometer readings that were acquired during the cruise and some associated values (runname, time, etc.). This information was used to calculate the coulometer's blank level (and standarddeviation of that) for each run, by averaging the coulometer increments that were recorded after the carbon peak had been titrated away. To be sure none of the titration peak was accidentally taken into this calculation, averaging was performed for minutes 6 through 14 (which was always the end of each DIC run, roughly coinciding with the end of the TALK determination of the same sample). For each run, the calculated values for blank and blank_std are stored.

3.4 `vindta222_findrawtitfiles`

This scripts browses through the VINDTA's output directories, storing names and dates of these files. This information will be used to match the raw titration data to the data that was collected earlier in the process.

3.5 `vindta222_matchbottledata`

This scripts matches to each of the CO₂-system analyses performed on the VINDTA, the associated chemical and physical parameters (that were loaded in the previous step) by comparing station- cast- and bottlenumber between the two datasets. After this step, accurate salinity, phosphate, silicate, are thus associated with the VINDTA runs.

3.6 `vindta222_matchblanks`

Somewhat analogous to the previous step, this scripts matches the information about per-run coulometer blank level (collected in the first step), to the VINDTA runs.

3.7 `vindta222_matchrawtitdata`

Again analogous to earlier steps, this scripts matches the raw potentiometric titration results to the VINDTA runs, this time on the basis of the timestamp that is known for each run, assuming that the raw results were be written approximately 20 minutes after the start of an analysis. If the software cannot make a definitive match, user input confirmation is required.

3.8 vindta222_setbaseline

Plotting the calculated per-run baseline (see 4.3) against time, clearly reveals both trends and noise in the coulometer's per-run blank value. Some of this noise is of course associated with the stochasticity of the per-minute increments. It was determined preferable to set the per-run level manually, smoothing out that variability, but remaining close the actually observed values. Note that this is different from the standard method of setting a blank level prior to doing the actual runs, in which case the set blank may not correspond closely to the actual values observed during the day. This script plots observed blank levels (and blank_std) against time and allows the user to graphically define a line that overrules the observed values. This level is allowed to gradually increase or decrease with time if the per-run blank level strongly suggests this to reflect the actual coulometer behavior (as is for instance visible at the third measurement series. This step does require some understanding of (or rather experience with) the behavior of coulometric systems. DIC-results are flagged as questionable when they are obtained in a run that had a baseline that was more than one standard deviation away from the user-set baseline *or* that was higher than a certain threshold (set to 160cpm) *or* that had a standard deviation higher than a certain threshold (set to 80cpm). Please refer to figure 1 for an overview of the observed blanks, and the user-set blank that were used for calculations.

3.9 vindta222_recalculatedic

Since the original calculations of DIC, performed by the VINDTA upon completing each analysis, are invalid since the user manually set the baseline levels (see 4.8), a recalculation is required. Pipette volume, electronic calibration of the coulometer and the gas loop calibration are set in this script, all potentially as a (stepwise) function of time. The script subsequently performs the DIC calculation using pipette volume, sample density, rawcounts, blank level, run duration and coulometer- and gas loop calibration.

3.10 vindta222_recalculatedtalk

For each run, raw titration data is read from disk. Now that for each run all information required to precisely (re-)calculate TALK is available (salinity, pipette volume, sample temperature, PO₄, Si, electrode readings, acid volumes, acid salinity, acid concentration, etc.), a recalculation of TALK is performed using the VINDTA.CALC_ALK routine, which is not covered here. The output of these routines is stored.

3.11 vindta222_flagbadcrms

Although care is taken to waste as little CRM as possible, these runs do occasionally fail. If the failure is obvious (caused by analyzer breakdown for instance) a rerun may be performed, but not-so-obvious runs may end up as valid in the dataset. This script graphically displays results from all CRM runs (as deviations from the certified values) vs. time. Slow drifts through time are easily observed this way (for instance caused by the slow weakening of titration acid will slowly alter the TALK's deviation). Obvious outliers are assumed not to represent the actual long term-deviation of the analytical setup but rather result from problems with sample handling. The script allows the user to graphically indicate these runs, upon which they will be flagged as bad and not subsequently used.

3.12 vindta222_correctcrmsdic

This script is probably the one that is of most influence to the final DIC results. The user is presented a figure displaying the CRM deviations (that is, the ratio between the CRM measurement and its certified value) versus time, three subsequent measurement periods (i.e., three days) at a time. This gives a quick overview of the changing response of the setup through time.

Because CRM's were only run early and late in the day (occasionally halfway, too), the changing response cannot be traced exactly, but will have to be interpolated between the 2 (or 3) known values. Various formal ways of doing this exist, from simply averaging the two (or three) value and assuming no change during the day, through linear interpolations, to complicated curve fits taken the average behavior of the system into account. This routine is potentially flexible in that it allow the user to define *any* curve he can come up with. Of course, the user must try to follow his expert's judgement when

define this curve. To avoid goal-seeking by the user, no feedback on the proposed correction of the final DIC values is given.

After a curve is satisfactorily defined for a particular day, the figure shifts sideways and input for the next period is asked. See figure (2) for the final result for this particular dataset. User-defined correction curves are subsequently used to calculate the final DIC values.

3.13 vindta222_correctcrmstalk

This script is identical to the previous one, except that it works on the TAlk data.

3.14 vindta222_flagbadsamples

This script presents the user with two figures displaying the final values of DIC (or TAlk) vs. depth profiles of all samples that have not already been flagged as bad. Obvious outliers can then be selected by the user and be flagged as bad, which removes them from the figure, which makes for a highly convenient way of flagging data,

3.15 vindta222_updatebottlefile

This script appends the final DIC and TAlk values, their quality flags and a lot of associated data (correction factors, TAlk calculation details, etc.) to the already existing cruise dataset ('bottlefile'). This file is easily imported into programs such as Microsoft's Excel or ODV for further analysis or graphing of the data.

4 Analytical quality assessment

Because not all components of the system were accurately calibrated, a significant systematic error was expected to present in the results. On top of that, medium-term drift in the VINDTA's response were expected, for instance due to changing coulometric cell chemistry or variations in room temperature over the course of a day. To determine (and correct for) these accuracy errors, CRM was analyzed. During the course of the cruise, two subsequent samples were drawn and analyzed from each of a total of 70 bottles of CRM. Running two analyses from one bottle also allows for an assessment of the the precision of measurements, by means of calculating the standard deviation of all differences between these duplicates².

4.1 CRM DIC results: accuracy

See figure 2. Results of analyses of CRM were consistently (only) around 0.25% (i.e., $\sim 5\mu\text{mol/kg}$) higher than the certified value. Apparently, errors in pipette volume calibration and coulometer current-to-counts calibration were smaller than feared or cancelled each other out to some extent. There were, however, significant trends during days (up to $\sim 5\mu\text{mol/kg}$), and a less pronounced day-to-day variation. Both short- and medium term variation are considered to have been quite captured through the use of CRM and corrected for to a final accuracy of $\sim 2\mu\text{mol/kg}$.

4.2 CRM DIC results: precision

See figure 3. Precision for DIC, defined as the standard deviation of differences between duplicate analyses of CRM³, is $\sim 1.5\mu\text{mol/kg}$.

NOTE: All DIC data from runs performed on the following days should be mistrusted due to high coulometer noise (see figure 1): 10–14, 17–22 (first half of the day), 26, 28, 30 and 31 of August. All other days the coulometer displayed regular behavior and data may be considered accurate and precise.

4.3 CRM TALK results: accuracy

See figure 2. Results for CRM can be seen to vary quite smoothly through time (except during measurement days 26/08 and 29/08, which display unexplainable high drifts and off-trend values, respectively). Within-day drift of up to $\sim 4\mu\text{mol/kg}$ are also clearly visible. Also shown in the figure are the correction factors applied to the oceanographic samples. Instrument drift is considered to have been corrected by use of CRM to within 0.1%-0.2%, i.e., to within $\sim 2\text{-}4\mu\text{mol/kg}$.

4.4 CRM TALK results: precision

See figure 4. Precision for TALK, defined as the standard deviation of differences between duplicate analyses of CRM⁴, is $\sim 1.5\mu\text{mol/kg}$.

²Admittedly, for DIC, duplicate analyses from a single bottle is not an optimal solution due to potential gas exchange between the CRM and the opened headspace in the 20 minutes that it takes to run the first sample. However, this effect seems to be of limited size as evident from the histogram, which suggests an average loss of CO_2 to the headspace of $\sim 1\mu\text{mol/kg}$ during those 20 minutes. It needs to be pointed out that any potential variation in this rate of outgassing will lead to an overestimation of the DIC measurement precision.

³For DIC, 19 obviously bad measurements were excluded. 56 usable pairs of duplicates remain.

⁴For TALK, 2 obviously bad measurements were excluded. 68 usable pairs of duplicates remain.

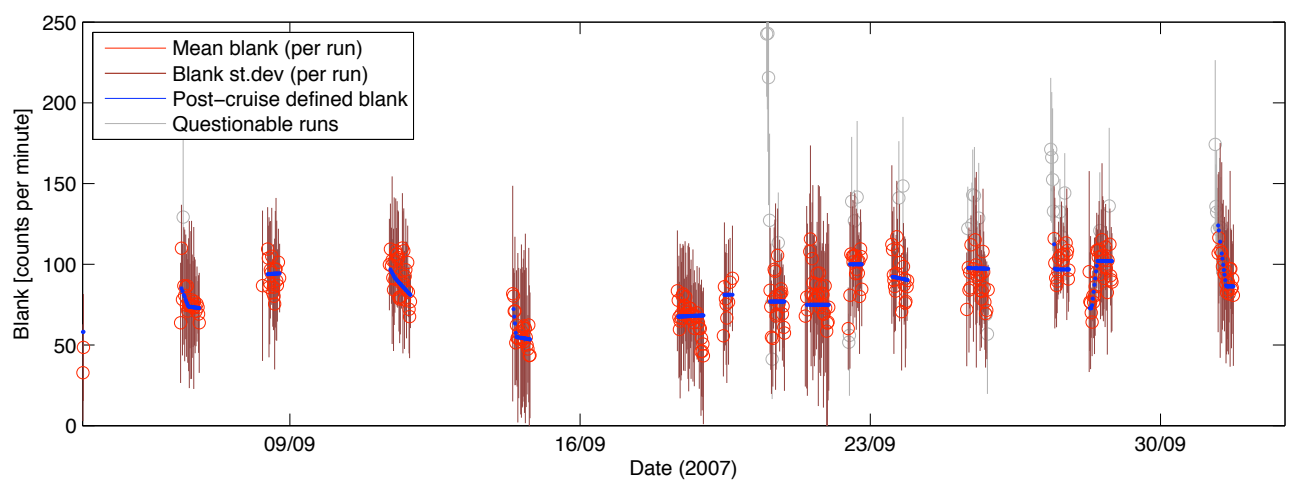
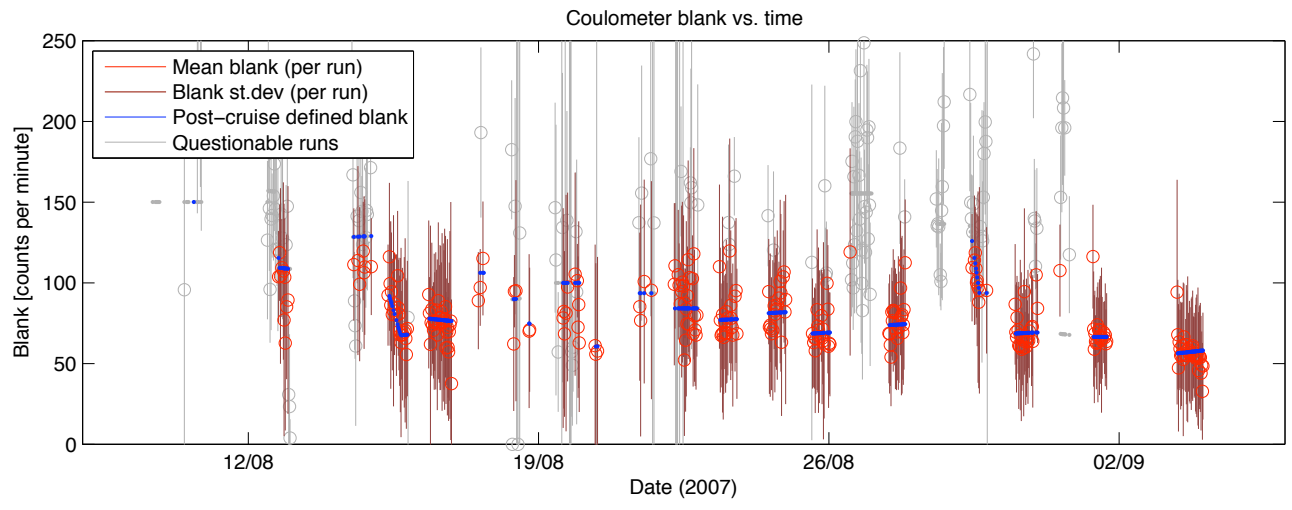


Figure 1: Timeseries of per-run- and user-set-coulometer blank levels.

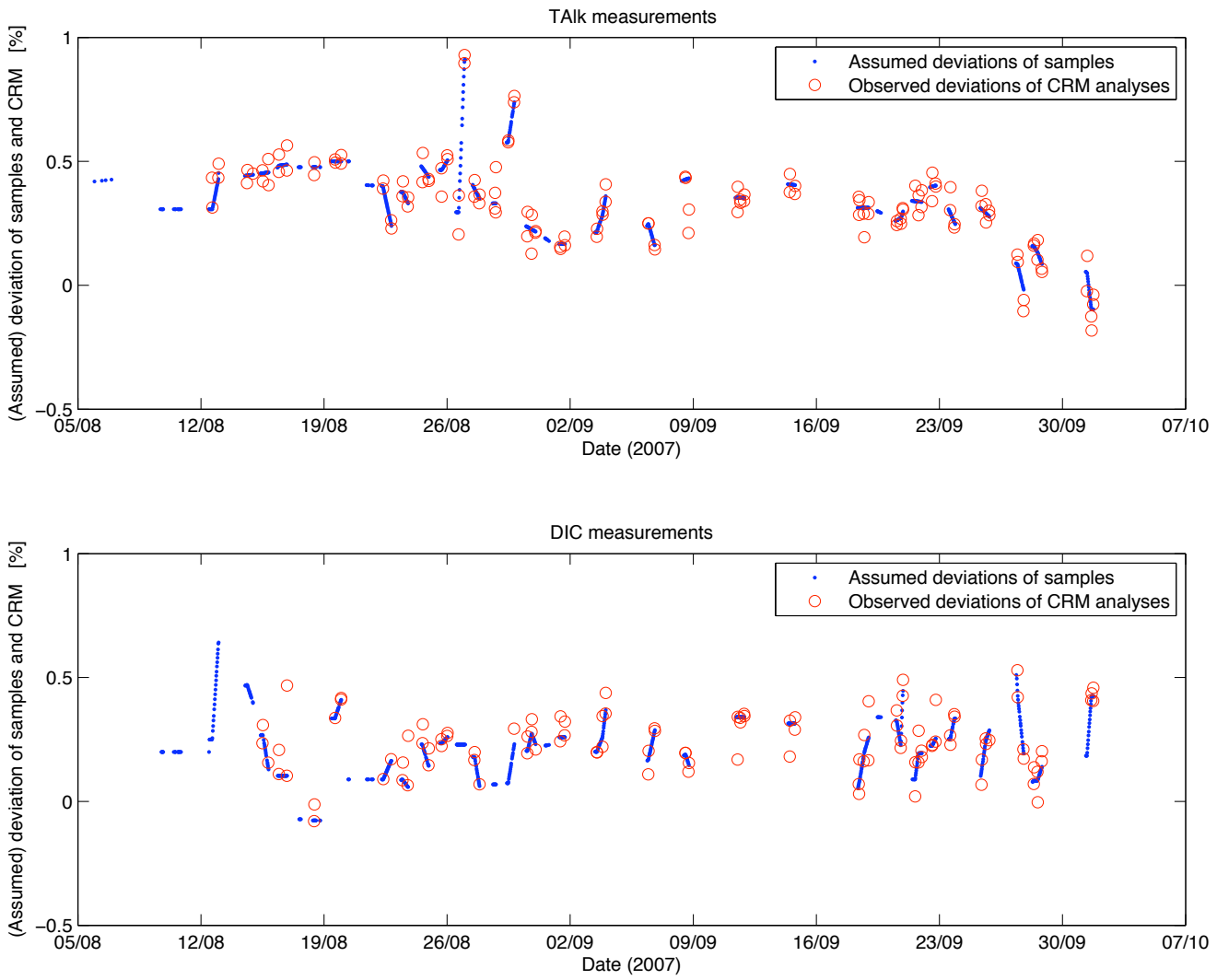


Figure 2: Timeseries of TALK and DIC CRM deviations and user-set correction factors for samples.

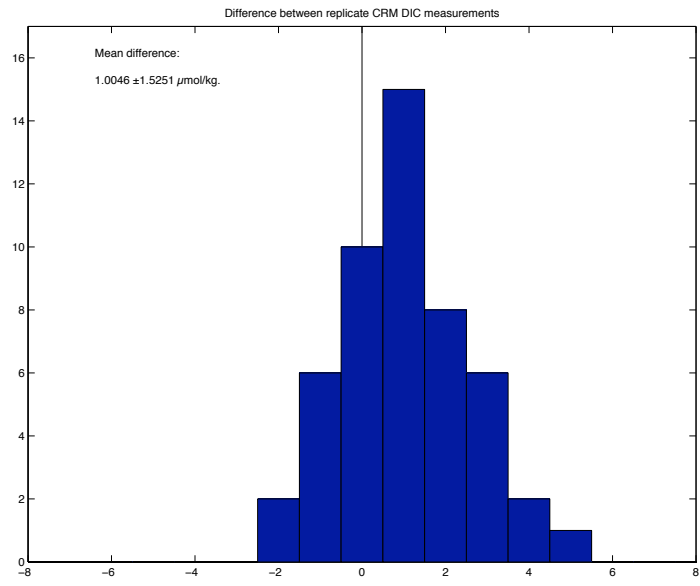


Figure 3: Histogram of differences between duplicate DIC analyses of the same CRM.

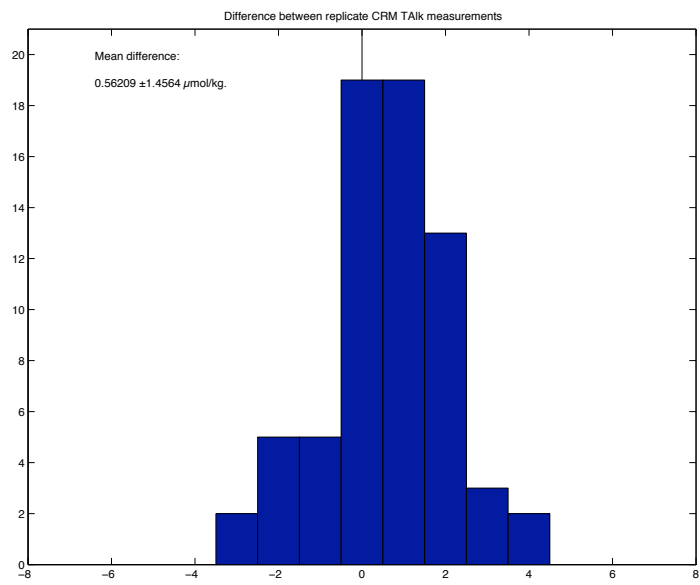


Figure 4: Histogram of differences between duplicate TALK analyses of the same CRM.

A Appendix: Scripts

This appendix lists the scripts used in processing.

A.1 vindta222_loadvindtafile.m

```
1 % Load the main VINDTA file (concatenated by user in e.g. Excel)
2
3 CO2file = 'VINDTADATA222.csv';
4
5 % Read VINDTA data...
6 [runname station cast niskin depth salinity rawcounts runlength blank...
7 tct crmCT crmAT crmbatch at rms machine ctgood atgood rundatetimestr] = ...
8 textread(CO2file, '%*q%q%d%d%d%*q%f%d%d%*q%*q%d%f%*q%f%*q%f%*q%f%*q%f%*q%*q%*q%*q%*q%*q%*q%*q%u%u%u%s', ...
9 'headerlines',1,'delimiter','.',',','emptyvalue',NaN);
10 nos=length(at); % Number of Samples
11 disp(cat(2,'VINDTA data loaded. Length: ',int2str(nos))); disp(' ');
12
13 % ...and create sensible dates from/for it...
14 rundatetime=datenum(rundatetimestr,'yyyy-mm-dd-HH-MM');
15
16 % Define sampletypes - These are the criteria as valid during ANT24-3
17 samplotype = nan(nos,1);
18 F=station==9;          samplotype(F)=1; % i.e., junk
19 F=station>9;          samplotype(F)=3; % i.e., regular sample
20 F=station==0;         samplotype(F)=4; % i.e., CRM
21
22 % Generate some vectors
23 pipvolct = nan(length(at),1);
24 pipvolat = nan(length(at),1);
25 acidconc = nan(length(at),1);
26 coulcalcfacs = ones(length(rawcounts),1); % Set coulometer calc factor to 1. (since not known)
27 piptemptp = ones(length(at),1).*25; % Assume that sample in pipette was 25deg (which it was!)
28 piptempat = ones(length(at),1).*25; % Assume that sample in pipette was 25deg (which it was!)
29 acidsalt = ones(length(at),1).*35; % TAlk titration acid salinity (g/L)
30
31 % Set pipette volumes
32 pipvolat(:)=97.0;
33 pipvolct(:)=19.5;
34
35 %Set acid strength
36 acidconc(:)=0.1;
37
38 clear CO2file nos F blank
```

A.2 vindta222_loadbottlefile.m

```
1 % Load the cruises 's bottlefile
2
3 bottlefile='bottlefilegood.csv';
4 fid=fopen(bottlefile);
5
6 A=textscan(fid, '%f%f%f%f%f%f%f%f%f%f%f%f%f%f%f%f%f%f%f%f%f', 'delimiter',' ','headerlines',1);
7 bottlestat = A{1};
8 bottlecast = A{2};
9 bottlebotl = A{18};
10 bottledpth = A{11};
11 bottlesal = A{14};
12 bottlesi = A{22};
13 bottlepo4 = A{21};
14
15 % Generate sensible dates:
16 bottledate = datenum(A{3},A{4},A{5},A{6},A{7},0);
17
18 % Store contents for future use.
19 BOTTLEFILE=A;
20
21 clear bottlefile fid A
```

A.3 vindta222_loadlogfile.m

```
1 % This routine gathers the baseline info from VINDA logfiles.
2
3 logfile = 'logfile.bak';
4 disp('Make sure that the last line of each logfile is the last minute of a run! If not, just delete the rest using a texteditor.');
```

5

```
6
7 % Read the first 4 characters of each line in the file, as well as the
8 disp('Fetching baseline data from logfile.');
```

9

```
10 fid=fopen(logfile); % Open datafile
11 AAA=textscan(fid, '%2c%s%s*[\n]', 'headerlines', 0, 'delimiter', '\t', 'MultipleDelimsAsOne', 1); % Read data
12 A=AAA{1}; % This should contain the first 2 characters of each line. 'Ti' and '16' should be recognisable in this.
13 B=AAA{2}; % This should contain the raw counts
14 C=AAA{3}; % This should contain the run names
15
16 % Find the upper and lower limit of the runs in the file
17 strtpos=strmatch('Ti',A,'exact')+1; % Since the run start one line later than the header
18 stoppos=strmatch('14',A,'exact'); % This will only be used to determine whether a run actually finished
19
20 F=strmatch('14',A(strtpos+13,1:2)); % find those runs that, 13 lines later, reach minute 14, rather than somewhere halfway the next run due to abort...
21
22 % Feedback to user:
23 disp(cat(2,int2str(size(strtpos,1)), ' runs have started. '))
24 disp(cat(2,int2str(size(F,1)), ' runs have finished. '))
25 disp(' ');
26 rr=setdiff((1:length(strtpos)),F);
27 for i = 1:size(rr,1)
28     disp(cat(2,'Removed run no. ',int2str(rr(i)), ' (somewhere near line ',int2str(strtpos(rr(i))+2.02*rr(i)), ' in logfile). Did not finish. '));
29 end
30 strtpos=strtpos(F); % ... and strip them from index string.
31
32 % Set the row IDs where the names, times and counts of the successful runs are to be found
33 namepos=strtpos-3; datepos=strtpos-4;
34
35 BASELINE=cell(size(strtpos,1),6);
36
37 for i=1:length(strtpos)
38     counts=B(strtpos(i):strtpos(i)+13);
39     name=C{namepos(i)};
40     if ~isempty(name)
41         datetime=B{datepos(i)}(end-14:end);
42         datetime=datetime(datetime, 'mm/dd/yy HH:MM');
```

43

```
44     else
45         disp(cat(2,'Problem with reading header of run no. ',int2str(i), ' (somewhere near line ',int2str(strtpos(i)+2.02*i), ' in logfile. '));
46         datetime=NaN;
47         name='NONAME';
48     end
49     cnts=nan(length(counts),1);
50     for j=1:length(counts)
51         cnts(j)=str2double(counts{j});
52     end
53     incr=diff([0;cnts]);
54     BASELINE(i,:)={name cnts incr mean(incr(6:end)) std(incr(6:end)) datetime};
55 end
56
57 fclose(fid); disp(' '); disp('Done!'); disp(' ');
58 clear counts namepos strtpos rr F stoppos A B C incr cnts datetime name datepos AAA fid logfile
```


A.4 vindta222_findrawtitfiles.m

```
1 % Find the available raw titration data files and store info about them.
2
3 basedir='/Users/Steven/Documents/-WORK/CarboOcean/CarboOcean Cruises/ARK22-2 - Arctic Ocean/vindta222/VINDTA DATA/';
4
5 A=dir(basedir)';
6 dirnames={A.name}';
7 dirnames=dirnames(4:end);
8 nod=length(dirnames);
9 DATFILESHORTNAMESA = {};
10 DATFILEFULLNAMESA = {};
11 DATFILEDATESA     = [];
12 for i = 1:nod
13     datadiri = cat(2,basedir,dirnames{i});
14     query    = cat(2,datadiri,'/*.dat');
15     B=dir(query);
16     datfilesshortnames={B.name}';
17     datfiledates=cell2mat({B.datenum})';
18     nof=size(datfilesshortnames,1);
19     datfilefullnames=cell(nof,1);
20     for j=1:nof
21         datfilefullnames{j,1}=cat(2,datadiri,'/',datfilesshortnames{j});
22     end
23     [datfiledates ,F]=sort(datfiledates);
24     DATFILESHORTNAMESA = [DATFILESHORTNAMESA; datfilesshortnames(F)]; % Not preallocated!
25     DATFILEFULLNAMESA  = [DATFILEFULLNAMESA ; datfilefullnames(F) ]; % Not preallocated!
26     DATFILEDATESA     = [DATFILEDATESA      ; datfiledates      ]; % Not preallocated!
27 end
28
29 format long
30 nofa=size(DATFILESHORTNAMESA,1);
31 disp('Number of datafiles found:');
32 disp(nofa); disp(' ');
```

A.5 vindta222_matchbottledata.m

```
1 % Match bottle data to vindta runs
2
3 format short g
4
5 realsamples = find(sampletype==3);
6 noas = length(sampletype); % Number of runs (all samples)
7 nors = length(realsamples); % Number of real samples
8
9 matchedsal = nan(noas,1);
10 matchedsi = nan(noas,1);
11 matchedpo4 = nan(noas,1);
12 matcheddep = nan(noas,1);
13 V2Bindex = nan(noas,1);
14
15 for i=1:nors
16
17     sid=realsamples(i);
18
19     vstat = station(sid);
20     vcast = cast(sid);
21     vbotl = niskin(sid);
22     %     vdpth = depth(sid);
23     %     vsali = salinity(sid);
24
25     F = bottlestat==vstat & bottlecast==vcast & bottlebotl==vbotl;
26
27     %     bstat = bottlestat(F);
28     %     bcast = bottlecast(F);
29     %     bbotl = bottlebotl(F);
30     %     bdpth = bottledpth(F);
31     %     bsali = bottlesal(F);
32     %     bpo4 = bottlepo4(F);
33     %     bsi = bottlesi(F);
34
35     matchedsal(sid) = bottlesal(F);
36     matchedpo4(sid) = bottlepo4(F);
37     matchedsi(sid) = bottlesi(F);
38     matcheddep(sid) = bottledpth(F);
39
40     V2Bindex(sid)=find(F); % The location in the bottlefile where the later calculated ct and at values should be written to.
41
42 end
43
44 matchedsal(matchedsal<0) = nan; % Salinities of -9999 to be replaced with nan (but not '0', so as not to overwrite the CRM's salinities later on)
45 matchedpo4(matchedpo4<0) = 0; % When nutrients are from a different cast then the co2 data, 0 is better then -9999
46 matchedsi(matchedsi <0) = 0; % When nutrients are from a different cast then the co2 data, 0 is better then -9999
47
48 F=~isnan(matchedsal); salinity(F) = matchedsal(F);
49 F=~isnan(matchedsi); si(F) = matchedsi(F);
50 F=~isnan(matchedpo4); po4(F) = matchedpo4(F);
51 F=~isnan(matcheddep); depth(F) = matcheddep(F);
52
53
54
55 % Set properties of CRMs
56 crmCT=nan(size(at));
57 crmAT=nan(size(at));
58 F=sampletype==4 & crmbatch==53; po4(F) = 0.41; si(F) = 2.1; salinity(F) = 33.453; crmCT(F)=2012.03; crmAT(F)=2222.68;
59 F=sampletype==4 & crmbatch==70; po4(F) = 0.36; si(F) = 1.77; salinity(F) = 33.016; crmCT(F)=1989.53; crmAT(F)=2160.46;
60 F=sampletype==4 & crmbatch==71; po4(F) = 0.30; si(F) = 2.1; salinity(F) = 33.923; crmCT(F)=2032.84; crmAT(F)=2254.50;
61 F=sampletype==4 & crmbatch==73; po4(F) = 0.35; si(F) = 1.1; salinity(F) = 34.523; crmCT(F)=2057.30; crmAT(F)=2253.50;
62 F=sampletype==4 & crmbatch==74; po4(F) = 0.22; si(F) = 1.8; salinity(F) = 34.739; crmCT(F)=2085.53; crmAT(F)=2305.34;
63 F=sampletype==4 & crmbatch==76; po4(F) = 0.38; si(F) = 2.23; salinity(F) = 34.835; crmCT(F)=2101.69; crmAT(F)=2314.49;
64
65 clear bottle* vstat vcast vbotl vdpth vsali F bstat bcast bbotl bdpth bsali bpo4 bsi sid i j realsamples noas nors matched*
```

A.6 vindta222_matchblanks.m

```

1 % Match the blank data (calculated from logfiles) to the vindta runs
2
3 SRN = runname; % vector of Sample Run Names
4 SDT = rundatetime; % vector of Sample DateTimes
5 perrunblank = nan(length(SDT),1); % preallocate
6 perrunblankstd = nan(length(SDT),1); % preallocate
7
8 LRN = BASELINE(:,1); % LOGRUNNAME
9 LDT = cell2mat(BASELINE(:,6)); % LOGDATETIME
10 BLNK = cell2mat(BASELINE(:,4)); % Blanks previously calc'd from logfile
11 BLNKSTD = cell2mat(BASELINE(:,5)); % Blankstds previously calc'd from logfile
12
13 igood=0; % counter
14
15 for i = 1:length(LDT)
16     F=SDT==LDT(i);
17
18     if sum(F)==0;
19         if isnan(LDT(i)); LDT(i)=0; end
20         disp(cat(2,'0 matches found for ',LRN{i},' at ',datestr(LDT(i),0))); disp(' ');
21         continue
22     end
23
24     % If the found match has the matching names, too, then accept and continue
25     if strcmp(LRN{i},SRN{F})
26         perrunblank(F)=BLNK(i);
27         perrunblankstd(F)=BLNKSTD(i);
28         igood=igood+1;
29         continue
30     else % else ask user input
31         disp(cat(2,'Badly-named match found for ',LRN{i},' at ',datestr(LDT(i),0),' : ',SRN{F}));
32         % xxx1=[i-2:i+2];
33         % xxx2=[(find(F)-2):(find(F)+2)];
34         %
35         % disp(' '); disp('Trying to find a match for the 3rd one of these runs (as from LOGFILE.BAK):')
36         % for j=1:5; disp(cat(2,int2str(j),' : ',LRN{xxx1(j)})); end; disp(' ');
37         %
38         % disp('Files around match:')
39         % for j=1:5; disp(cat(2,int2str(j),' : ',SRN{xxx2(j)})); end; disp(' '); disp(' '); disp(' ');
40         %
41         % answer=input(cat(2,'Please select correct match for ',LRN{i},' (1 through 5) : [3] ','), 's');
42         % answer=str2num(answer);
43         % if isempty(answer)
44         %     disp('no answer, set 3'); answer=3;
45         % elseif answer>5 | answer<1
46         %     disp('bad value, set 3'); answer=3;
47         % end
48         % F=xxx2(answer);
49         disp(cat(2,SRN{F},' selected. '));
50         perrunblank(F)=BLNK(i);
51         perrunblankstd(F)=BLNKSTD(i);
52         igood=igood+1;
53     end
54 end
55
56 disp(cat(2,'Matching succes rate (%): ',num2str((igood/length(LDT))*100),'.'));
57 disp(cat(2,'Matches not found: ',num2str(length(LDT)-igood),'.'));
58
59 clear BLNK igood LDT SRN SDT LRN z i j F

```

A.7 vindta222_matchrawtitdata.m

```
1 % Match the files containing raw titration data (found earlier) to the vindta runs
2
3 format long g
4
5 SRN = runname; % SAMPLERUNNAME
6 SDT = rundatetime; % SAMPLEDATETIME
7
8 MATCHEDFILENAMESSHORT = cell(length(runname),1);
9 MATCHEDFILENAMEFULL = cell(length(runname),1);
10
11 DRNS = DATFILESHORTNAMESA;
12 DRNF = DATFILEFULLNAMESA;
13 DDT = DATFILEDATESA;
14
15 F=samplotype>0; %(samplotype==3 | samplotype==2);
16 SID=find(F); % Sample ID's
17 nos=length(SID);
18
19 % for each of the samples, try to find a matching .dat-file
20 for j = 1:nos
21     sid=SID(j);
22
23     srn=SRN(sid); % name of the sample under consideration
24     sdt=SDT(sid); % datetime at beginning of the run. .dat-file is written 20 minutes later, so ddt is always larger than the associated sdt
25
26     timediff=DDT-sdt-1/(24*6);
27     timediff(timediff<0)=nan;
28     F=find(timediff==min(timediff));
29
30     drns=DRNS{F};
31     drnf=DRNF{F};
32     ddt=DDT(F);
33     dt=(ddt-sdt)*24*60;
34
35     if isempty(strfind(drns,cell2mat(srn))) && dt>23
36         disp(['Unsuccesfully tried to match "' cell2mat(srn) '". Closest match in time was "' drns "''])
37         disp([int2str(dt) ' minutes'])
38         disp(datestr(sdt))
39         disp(datestr(ddt))
40         FF=[F-10:F+10]';
41
42         for k = 1:21
43             disp(cat(2,int2str(k),' ',DRNS{FF(k)}));
44         end
45         answer=input('please pinpoint the right file - ');
46         F=FF(answer);
47         drns=DRNS{F};
48         drnf=DRNF{F};
49         ddt=DDT(F);
50         dt=(ddt-sdt)*24*60;
51         disp(['Matched "' cell2mat(srn) '" to "' drns "' . Timediff was ' int2str(dt) ' minutes']); disp(' '); disp(' '); disp(' '); % pause
52     else
53         disp(['Matched "' cell2mat(srn), '" to "', drns "' . Timediff was ' int2str(dt) ' minutes'])
54     end
55     MATCHEDFILENAMESSHORT(sid,1) = {drns};
56     MATCHEDFILENAMEFULL(sid,1) = {drnf};
57
58 end
59
60 clear SRN SDT DRNS DRNF DDT F SID nos j sid srn sdt timediff F srns srnf ddt dt k FF answer
```

A.8 vindta222_setbaseline.m

```
1 a=[1 2 3 3 4 5 6 6 6 7 8 9]% Let user specify the blank level (to use in calculating DIC later on)
2
3 % Initialize figure
4 figure('Position',[1 200 1400 700],'Color','w','PaperOrientation','Landscape','ToolBar','none','Menubar','none'); clf;
5
6 % Determine the coulometric cells' start sampledattimes from file
7 drdt=[0;diff(rundatetime)];
8 F=drdt>.25; F(1)=true;
9 celldatetime=rundatetime(F);
10 celldatetime=[celldatetime;max(rundatetime)];
11 useretblank = nan(length(at),1); % Preallocate a vector for user-set blank values
12 cdt=celldatetime;
13
14 FA=ctgood==1; % all samples
15 for i = 1:length(rundatetime)-1;
16     start = cdt(i);
17     stop = cdt(i+1);
18     FT=rundatetime>(start-1) & rundatetime<=(stop+1); % Index for all runs in period + 1 days around
19
20     % *****
21     % TOP PANEL
22     % *****
23     subplot(2,1,1,'align'); cla;
24
25     % Draw all blank values during this cruise for this machine
26     for i = 1:length(rundatetime)
27         plot([rundatetime(i) rundatetime(i)],[perrunblank(i)-perrunblankstd(i) perrunblank(i)+perrunblankstd(i)],'-','color',[.5 0 0]); hold on
28     end
29     plot(rundatetime,perrunblank,'ro'); hold on
30
31     % Draw corrections from previous periods, too
32     plot(rundatetime,useretblank,'b.');
```

21

```
33
34     % Draw period-markers
35     ylim=get(gca,'Ylim');
36     plot([start start],[ylim(1) ylim(2)],'b-','linewidth',2);
37     plot([stop stop],[ylim(1) ylim(2)],'b-','linewidth',2);
38     title('CT during cruise');
39     datetick('x',19);
40     set(gca,'xlim',[min(rundatetime)-1 max(rundatetime)+1]);
41     set(gca,'ylim',[0 250]);
42
43     % *****
44     % BOTTOM PANEL
45     % *****
46     subplot(2,1,2,'align'); cla;
47
48     % Draw corrections from previous periods
49     ylim=[0 250]; F=FT;
50     plot(rundatetime(F),useretblank(F),'bo','linewidth',1,'markersize',4); hold on
51
52     % Draw times of measurement as gray lines
53     x=[rundatetime(F) rundatetime(F)];
54     y=[ones(sum(F),1).*ylim(1) ones(sum(F),1).*ylim(2)];
55     plot(x,'y','-','color',[.9 .9 .9]); hold on
56
57     % Draw blank
58     rdt=rundatetime(F); blk=perrunblank(F); blkstd=perrunblankstd(F);
59     for j = 1:length(rundatetime(F))
60         plot([rdt(j) rdt(j)],[blk(j)-blkstd(j) blk(j)+blkstd(j)],'-','color',[.5 0 0]); hold on
61     end
62     plot(rdt,blk,'r.-');
63
64     % Draw period-markers
65     plot([start start],[ylim(1) ylim(2)],'b-','linewidth',2);
66     plot([stop stop],[ylim(1) ylim(2)],'b-','linewidth',2);
67     title('Per-run coulometer blank. One coulometric cell period.');
```

70

```
68     set(gca,'ylim',ylim); datetick('x',19); set(gca,'xlim',[start-2 stop+2])
69
70     % *****
71     % DONE WITH BASE PLOT
```

```

72 % so now, because only runs in the period are to be regarded, redefine FT
73 FT=rundatetime>start & rundatetime<=stop; % Index for all runs in period
74 RDT=rundatetime(FT);
75
76 % Ask user to draw correctionline
77 disp('Please draw correction line in lower panel. Press SPACEBAR or right mouse button at last point.')
78 done=0;
79 while done==0
80     y=0; x=0; j=0; but=0; xy=[]; next=0;
81     while ~(next==1 && j>1) % while it is not true that user is done AND more than 2 points were supplied...
82         [x,y,but] = ginput(1); % ... ask for another point
83
84         if isempty(but); but=0; continue; end
85
86         if but==1 || but==3 || but==32;
87             j=j+1;
88             plot(x,y,'bo')
89             xy(:,j)=[x;y];
90         end
91
92         if but==3 || but==32; next=1; end
93
94         if j>1; h=plot(xy(1,[j-1 j]),xy(2,[j-1 j]),'k-'); hold on; end
95
96     end
97
98     ints=[min([start;RDT]):0.1:max([stop;RDT])];
99     F=-any(diff(xy,1,2)); xy(:,F)=[]; % this line removes duplicate points
100     xys=interp1(xy(1,:),xy(2,:),ints,'linear');
101     h1=plot(ints,xys,'-','color',[.7 .7 1]); hold on
102     ints=RDT;
103     xys=interp1(xy(1,:),xy(2,:),ints,'linear');
104     h2=plot(ints,xys,'b.');
```

22

```

105
106     drawnow; figure(gcf)
107     answer=input('Satisfied? [Y/n] >> ','s'); figure(gcf)
108
109     if strcmp(upper(answer),'N')
110         delete(h1); delete(h2);
111     else
112         done=1;
113     end
114 end
115 usersetblank(FT)=xys;
116 end
117
118 clear done answer h2 xys ints h1 F but j h i xy next rdt x y ylim drdt FA cdt celldatetime F start stop FT
```

A.9 vindta222_recalculatedic.m

```
1 % Recalculate DIC!
2
3 F=samplotype==4 & crmbatch==53; po4(F) = 0.41; si(F) = 2.1 ; salinity(F) = 33.453; % CRMct=2012.03; at=2222.68
4 F=samplotype==4 & crmbatch==70; po4(F) = 0.36; si(F) = 1.77; salinity(F) = 33.016; % ct=1989.53; at=2160.46
5 F=samplotype==4 & crmbatch==71; po4(F) = 0.30; si(F) = 2.1 ; salinity(F) = 33.923; % ct=2032.84; at=2254.50
6 F=samplotype==4 & crmbatch==73; po4(F) = 0.35; si(F) = 1.1 ; salinity(F) = 34.523; % ct=2057.30; at=2253.50
7 F=samplotype==4 & crmbatch==74; po4(F) = 0.22; si(F) = 1.8 ; salinity(F) = 34.739; % ct=2085.53; at=2305.34
8 F=samplotype==4 & crmbatch==76; po4(F) = 0.38; si(F) = 2.23; salinity(F) = 34.835; % ct=2101.69; at=2314.49
9
10 densSW = sw_dens0(salinity , pitempct) ./ 1000; % Used the Seawater library of routines. Google it!
11 netcounts = rawcounts - (runlength.*useretblank);
12 sampmass = (pipvolct.*densSW) ./ 1000; % in kg
13 ct = (netcounts ./ 4824.45); % in microgram (per sample)
14 ct = ct ./ sampmass; % in microgram/kg
15 ct = ct .* coulocalfacs; % in microgram/kg
```

A.10 vindta222_recalculated.m

```
1 % Fetch raw tit data associated files and calculate TALK
2
3 basedir='/Users/Steven/Documents/-WORK/CarboOcean/CarboOcean Cruises/ARK22-2 - Arctic Ocean/vindta222/RECALCOUTPUT/';
4 mkdir(basedir)
5
6 % Select subset of runs to recal (enter '>0' for all runs)
7 F=samplotype>0; %(samplotype==3 | samplotype==2);
8 SID=find(F); % Sample ID's
9 TITVOLS=cell(length(samplotype),1);
10 TITEMFS=cell(length(samplotype),1);
11 TITTMPs=cell(length(samplotype),1);
12
13 % Preallocate
14 at = nan(length(at),1);
15 atDIC = nan(length(at),1);
16 atRMS = nan(length(at),1);
17 atE0 = nan(length(at),1);
18 atK1 = nan(length(at),1);
19 accidens = nan(length(at),1); accidens(:)=1.022;
20
21 CC=2;
22 showiterations=0;
23 showfigure=0;
24 savefigure=0;
25 counter=0;
26
27 % for each of the samples, try to find a matching .dat-file
28 diary(cat(2,basedir,'-titraties.txt'));
29 output=nan(length(SID),5);
30 z=0;
31 E0=600;
32 for j = SID'
33     z=z+1;
34     counter=counter+1;
35     filename = MATCHEDFILENAMEFULL{j};
36     filenameshort = MATCHEDFILENAMESSHORT{j};
37     fid = fopen(filename);
38     data = textscan(fid, '%n%n%n', 'headerlines', 2); % Load only the titration data
39     fclose(fid);
40
41 % Get titration results
42 titvols = data{1};
43 titemfs = data{2};
44 tittmps = data{3}; tittmps(:)=25;
45
46 % Store titration results
47 TITVOLS(j) = {titvols}; % Volumes of acid added (ml)
48 TITEMFS(j) = {titemfs}; % EMF readings electrode (mV)S
49 TITTMPs(j) = {tittmps}; % Temperatures (oC)
50
51 machinename='VINDTA C (#14)';
52
53 if isempty(titvols)
54     disp(cat(2,'*** Run ',filenameshort,' skipped due to empty datafile ***'));
55     continue
56 end
57
58 tittmpc=tittmps(1);
59 figurefilename=cat(2,basedir,datestr(rundatetime(j),'yyyymmddHHMM'),' - ',filenameshort(1:end-4),'.pdf');
60 runname=cat(2,'ARK222 - ',int2str(station(j)),'-',int2str(cast(j)),'-',int2str(niskin(j)),'-',int2str(depth(j)),'m');
61 runtime=datestr(rundatetime(j));
62
63 if ismember(counter,[0:10:length(SID)]);
64     disp(cat(2,'Now processing ',runname,'.',int2str(counter), '/',int2str(length(SID))));
65 end
66
67 [OutputGran OutputX2 SystemDetails] = ...
68 VINDTA_CALCALK(titvols, titemfs, tittmpc, salinity(j), po4(j), si(j), pipvolat(j), acidconc(j), accidens(j), ...
69 E0, showiterations, showfigure, savefigure, figurefilename, runname, runtime, machinename);
70
71 output(z,:)=OutputX2';
```



```
72
73     at(j) = OutputX2(1);
74     atDIC(j) = OutputX2(2);
75     atRMS(j) = OutputX2(3);
76     atE0(j) = OutputX2(4);
77     atK1(j) = OutputX2(5);
78
79     end
80     nums=[1:size(output,1)]';
81     output=[nums output];
82     csvwrite(cat(2,basedir, '-output.txt'),output);
83     diary off
84     clear output OutputGran OutputX2 SystemDetails tittempc tittmps titemfs titvols filename figurefilename
85     clear runname runtime machinename TITVOLS TITEMFS TITMPS datacounter z j SID showfigure savefigure basedir
```

A.11 vindta222 flagbadcrms.m

```
1 clear mean*
2 close('all')
3
4 machinename=['A';'B']; % Names of machines used
5 colors={1 0 0],[0 0 1],[1 .5 .5],[.5 .5 1]};
6 nos = length(ct);
7 ec = nan(nos,1); % empty column
8 userhappy=0;
9
10 disp('The following batch of CRM were used:')
11 disp(unique(crmbatch(sampletype==4)))
12
13 % Ask user whether or not to reuse Excel's quality flags
14 reset=input('Reset CRM quality flags? [y/N] --- ','s');
15 if lower(reset)=='y'
16     disp('resetting');
17     ctgood(1:end)=1;
18     atgood(1:end)=1;
19 end
20
21 % Automatically marks the really outlandish values in the dataset
22 ctgood(ct<1800 | ct>2400)=0;
23 atgood(at<2000 | at>2600)=0;
24
25 disp('PLEASE FLAG THE OBVIOUSLY BAD CRMS!!!')
26
27 % Preload the figure
28 crmstdfig = figure('Position',[1 750 1280 800],'Color','w','PaperOrientation','Landscape','ToolBar','none','Menubar','none'); clf;
29
30 % *****
31 % Calculate, plot and filter CRM and STD data.
32 % *****
33 while userhappy==0;
34
35     % Calculate deviation from avg for CRMs, scale as percentages
36     atcrmdev=(at./crmAT-1).*100;
37     ctcrmdev=(ct./crmCT-1).*100;
38
39     % Plot CRM absolute values.
40     figure(crmstdfig); clf
41     subplot(2,2,1);
42     F=sampletype==4 & atgood==1;
43     plot(rundatetime(F),at(F),'ro');
44     title('AT-values of CRMs')
45     set(gca,'UserData',{1 'at' F});
46     subplot(2,2,2);
47     F=sampletype==4 & ctgood==1;
48     plot(rundatetime(F),ct(F),'ro');
49     title('CT-values of CRMs')
50     set(gca,'UserData',{2 'ct' F});
51
52     % Plot CRMs deviations
53     subplot(2,2,3);
54     F=sampletype==4 & atgood==1;
55     plot(rundatetime(F),atcrmdev(F),'ro'); hold on;
56     plot(rundatetime(F),atcrmdev(F),'r-');
57     title('Deviation (in %) from average CRM value for AT');
58     set(gca,'UserData',{3 'at' F});
59     subplot(2,2,4);
60     F=sampletype==4 & ctgood==1;
61     plot(rundatetime(F),ctcrmdev(F),'ro'); hold on;
62     plot(rundatetime(F),ctcrmdev(F),'r-');
63     title('Deviation (in %) from average CRM value for CT');
64     set(gca,'UserData',{4 'ct' F});
65
66     answer=input('Data acceptable? [Y/n] --- ','s');
67     if lower(answer)~='y'
68         userhappy=0; % stays 0
69         disp('Please mark samples for deletion. Click right mouse button or press [enter] when done. ');
70         but=1; n=1; clear squares
71     end
72 end
```

```

72 % Record user-input coordinates
73 while but == 1
74     [x1,y1,but] = ginput(1);
75     Userdata=get(gca,'Userdata');
76     o1=Userdata{1};
77     hold on; plot(x1,y1,'g-');
78     if but==1
79         [x2,y2,but] = ginput(1);
80         Userdata=get(gca,'Userdata');
81         o2=Userdata{1};
82         plot(x1,y1,'g-');
83         if o1==o2 & but==1;
84             xmin=min([x1 x2]); xmax=max([x1 x2]);
85             ymin=min([y1 y2]); ymax=max([y1 y2]);
86             ypar=Userdata{2};
87             F=Userdata{3};
88             squares(n,:){xmin xmax ymin ymax ypar F};
89             n=n+1;
90             plot([xmin xmin],[ymin ymax],'g-',[xmax xmax],[ymin ymax],'g-',[xmin xmax],[ymin ymin],'g-',[xmin xmax],[ymax ymax],'g-');
91         end
92     end
93 end
94
95 % Filter out the user-marked measurements:
96 for i = 1:size(squares,1)
97     F=squares{i,6};
98     F=eval(cat(2,'F & rundatetime > ',int2str(squares{i,1}),' & rundatetime < ',int2str(squares{i,2}),' & ',...
99             squares{i,5},' > ',int2str(squares{i,3}),' & ',...
100            squares{i,5},' < ',int2str(squares{i,4})));
101     eval(cat(2,squares{i,5},'good(F)=0;'));
102 end
103 else
104     userhappy=1;
105     disp('Done.')
```

A.12 vindta222_correctcrmsdic.m

```
1 % Close all figures
2 close('all')
3
4 % Preallocate the vector that will hold the user-specified correction factors
5 ctfactors = nan(length(ct),1);
6
7 % Initialize figure
8 figure('Position',[1 200 1400 700],'Color','w','PaperOrientation','Landscape','Toolbar','none','Menubar','none'); clf;
9
10 % Determine the coulometric cells' start sampledattimes from file
11 drdt=[0;diff(rundatetime)];
12 F=drdt>.25; F(1)=true;
13 celldatetime=rundatetime(F);
14 celldatetime=[celldatetime;max(rundatetime)];
15
16 % FS=samplotype==2 & ctgood==1 & ct>1800 & ct<2400; % FC indexes all good ct STD runs on machine k
17
18 cdt=celldatetime;
19
20 FA=ctgood==1; % all good samples
21 FC=ctgood==1 & samplotype==4; % all good CRMs
22
23 for i = 4:length(cdt)-1;
24     dct=crmCT./ct;
25     start = cdt(i);
26     stop = cdt(i+1);
27     FT=rundatetime>(start-1) & rundatetime<=(stop+1); % Index for all runs in period + 1 days around
28
29     % *****
30     % TOP PANEL
31     % *****
32     subplot(2,1,1,'align'); cla;
33
34     % Draw all dct's during this cruise for this machine
35     F=FC; plot(rundatetime(F),dct(F),'ro'); hold on
36     F=FA; plot(rundatetime(F),ctfactors(F),'b.');
```

28

```
37
38     % Draw period-markers
39     ylim=get(gca,'Ylim');
40     plot([start start],[ylim(1) ylim(2)],'b-','linewidth',2);
41     plot([stop stop],[ylim(1) ylim(2)],'b-','linewidth',2);
42     title('CT during cruise');
43     datetick('x',19);
44     set(gca,'xlim',[min(rundatetime)-1 max(rundatetime)+1]);
45     % set(gca,'ylim',[0 500]);
46
47     % *****
48     % BOTTOM PANEL
49     % *****
50     subplot(2,1,2,'align'); cla;
51
52     % Draw times of measurement as gray lines
53     F=FT&FA;
54     x=[rundatetime(F) rundatetime(F)];
55     y=[ones(sum(F),1).*ylim(1) ones(sum(F),1).*ylim(2)];
56     plot(x,'y','-','color',[.6 .6 .6]); hold on
57
58     % Draw period-markers
59     plot([start start],[ylim(1) ylim(2)],'b-','linewidth',2);
60     plot([stop stop],[ylim(1) ylim(2)],'b-','linewidth',2);
61
62     % Draw the CRM measurements
63     F=FT&FC;
64     plot(rundatetime(F),dct(F),'b-o','linewidth',1,'markersize',4); hold on
65
66     % Write titles
67     title('Per-run coulometer blank. One coulometric cell period.');
```

70

```
71     set(gca,'ylim',ylim);
72     datetick('x',19);
73     set(gca,'xlim',[start-2 stop+2])
74 end
```

```

72
73 % *****
74 % DONE WITH BASE PLOT
75 % *****
76
77 % Now, because only runs in the period are to be regarded, redefine FT
78 FT=rundatetime>start & rundatetime≤stop; % Index for all runs in period
79 RDT=rundatetime(FT);
80
81 % Ask user to draw correctionline
82 disp('Please draw correction line in lower panel. Press SPACEBAR or right mouse button at last point.')
83 done=0;
84 while done==0
85     y=0; x=0; j=0; but=0; xy=[]; next=0;
86     while ~(next==1 && j>1) % while it is not true that user is done AND more than 2 points where supplied...
87         [x,y,but] = ginput(1); % ... ask for another point
88
89         if isempty(but); but=0; continue; end
90
91         if but==1 || but==3 || but==32;
92             j=j+1;
93             plot(x,y,'bo')
94             xy(:,j)=[x;y];
95         end
96
97         if but==3 || but==32; next=1; end
98
99         if j > 1; h=plot(xy(1,[j-1 j]),xy(2,[j-1 j]),'k-'); hold on; end
100
101     end
102
103     ints=[min([start;RDT]):0.1:max([stop;RDT])];
104     F=-any(diff(xy,1,2)); xy(:,F)=[]; % this line removes duplicate points
105     xys=interp1(xy(1,:),xy(2,:),ints,'linear');
106     h1=plot(ints,xys,'-', 'color',[.7 .7 1]); hold on
107     ints=RDT;
108     xys=interp1(xy(1,:),xy(2,:),ints,'linear');
109     h2=plot(ints,xys,'b.');
```

29

```

110
111     drawnow
112     figure(gcf)
113     answer=input('Satisfied? [Y/n] >> ','s');
114     figure(gcf)
115
116     if strcmp(upper(answer),'N')
117         delete(h1); delete(h2);
118     else
119         done=1;
120     end
121
122 end
123 ctfactors(FT)=xys;
124 end
125
126 % Correct for dilution effect of addition of 50 L HgCl (adds -0.4 mol/kg)
127 F=samplotype==3;
128 ct(F)=ct(F).*(250.05./250);
129
130
131 % Correct values for VINDTA response
132 ctcorrected=ct.*ctfactors;
```

A.13 vindta222_correctcrmstalk.m

```
1 % Close all figures
2 close('all')
3
4 % Preallocate the vector that will hold the user-specified correction factors
5 atfactors = nan(length(ct),1);
6
7 % Initialize figure
8 figure('Position',[1 200 1400 700],'Color','w','PaperOrientation','Landscape','Toolbar','none','Menubar','none'); clf;
9
10 % determine the days on which measurements were taken
11 cdt=unique(floor(rundatetime));
12
13 cdt=[floor(min(rundatetime)):4:ceil(max(rundatetime))+4];
14
15 FA=atgood==1; % all good samples
16 FC=atgood==1 & samplotype==4; % all good CRMs
17
18 for i = 1:length(cdt)-1;
19     dat=crmAT./at;
20     start = cdt(i);
21     stop = cdt(i+1);
22     FT=rundatetime>(start-1) & rundatetime<=(stop+1); % Index for all runs in period + 1 days around
23
24     % *****
25     % TOP PANEL
26     % *****
27     subplot(2,1,1,'align'); cla;
28
29     % Draw all det's during this cruise for this machine
30     F=FC; plot(rundatetime(F),dat(F),'ro'); hold on
31     F=FA; plot(rundatetime(F),atfactors(F),'b.');
```

30

```
32
33     % Draw period-markers
34     ylim=get(gca,'Ylim');
35     plot([start start],[ylim(1) ylim(2)],'b-','linewidth',2);
36     plot([stop stop],[ylim(1) ylim(2)],'b-','linewidth',2);
37     title('CT during cruise');
38     datetick('x',19);
39     set(gca,'xlim',[min(rundatetime)-1 max(rundatetime)+1]);
40     % set(gca,'ylim',[0 500]);
41
42     % *****
43     % BOTTOM PANEL
44     % *****
45     subplot(2,1,2,'align'); cla;
46
47     % Draw times of measurement as gray lines
48     F=FT&FA;
49     x=[rundatetime(F) rundatetime(F)];
50     y=[ones(sum(F),1).*ylim(1) ones(sum(F),1).*ylim(2)];
51     plot(x,'y','-','color',[.6 .6 .6]); hold on
52
53     % Draw period-markers
54     plot([start start],[ylim(1) ylim(2)],'b-','linewidth',2);
55     plot([stop stop],[ylim(1) ylim(2)],'b-','linewidth',2);
56
57     % Draw the CRM measurements
58     F=FT&FC;
59     plot(rundatetime(F),dat(F),'b-o','linewidth',1,'markersize',4); hold on
60
61     % Write titles
62     title('Per-run coulometer blank. One coulometric cell period.');
```

66

```
67
68     % *****
69     % DONE WITH BASE PLOT
70     % *****
71
```

```

72 % Now, because only runs in the period are to be regarded, redefine FT
73 FT=rundatetime>start & rundatetime<=stop; % Index for all runs in period
74 RDT=rundatetime(FT);
75
76 % Ask user to draw correctionline
77 disp('Please draw correction line in lower panel. Press SPACEBAR or right mouse button at last point.')
78 done=0;
79 while done==0
80     y=0; x=0; j=0; but=0; xy=[]; next=0;
81     while ~(next==1 && j>1) % while it is not true that user is done AND more than 2 points were supplied...
82         [x,y,but] = ginput(1); % ... ask for another point
83
84         if isempty(but); but=0; continue; end
85
86         if but==1 || but==3 || but==32;
87             j=j+1;
88             plot(x,y,'bo')
89             xy(:,j)=[x;y];
90         end
91
92         if but==3 || but==32; next=1; end
93
94         if j>1; h=plot(xy(1,[j-1 j]),xy(2,[j-1 j]),'k-'); hold on; end
95
96     end
97
98     ints=[min([start;RDT]):0.1:max([stop;RDT])];
99     F=-any(diff(xy,1,2)); xy(:,F)=[]; % this line removes duplicate points
100     xys=interp1(xy(1,:),xy(2,:),ints,'linear');
101     h1=plot(ints,xys,'-','color',[.7 .7 1]); hold on
102     ints=RDT;
103     xys=interp1(xy(1,:),xy(2,:),ints,'linear');
104     h2=plot(ints,xys,'b.');
```

31

```

105
106     drawnow
107     figure(gcf)
108     answer=input('Satisfied? [Y/n] >> ','s');
109     figure(gcf)
110
111     if strcmp(upper(answer),'N')
112         delete(h1); delete(h2);
113     else
114         done=1;
115     end
116 end
117 atfactors(FT)=xys;
118 end
119 atcorrected=at.*atfactors;
```

A.14 vindta222 flagbadsamples.m

```
1 % *****
2 % Calculate, plot and filter sample data.
3 % *****
4
5 close('all')
6
7 reset=input('Reset sample quality flags? [y/N] --- ','s');
8 if upper(reset)=='y'
9     F=samplotype==3;
10    ctgood(F)=1;
11    atgood(F)=1;
12 end
13
14 profilefig = figure('Position',[1 302 1280 1000],'Color','w','PaperOrientation','Landscape','Toolbar','none','Menubar','none'); clf;
15
16 userhappy=0;
17 while userhappy==0;
18     % draw AT- and CT-plots
19     get(gcf,'Children');
20     figure(profilefig); clf
21     ustats=unique(station(station > 200));
22     handles=nan(length(ustats),5);
23
24     for i=1:length(ustats) % Plot all profiles of cruise a in light color
25         subplot(2,1,1,'align');
26         F = station==ustats(i) & samplotype==3 & atgood==1;
27         X=atcorrected(F); Y=depth(F); [Y,I]=sort(Y); X=X(I);
28         markhandleAAT=plot(X,Y,'ro','markersize',4); hold on;
29         linehandleAAT=plot(X,Y,'-', 'color',[1 .4 .4]);
30
31         subplot(2,1,2,'align')
32         F = station==ustats(i) & samplotype==3 & ctgood==1;
33         X=ctcorrected(F); Y=depth(F); [Y,I]=sort(Y); X=X(I);
34         markhandleACT=plot(X,Y,'ro','markersize',4); hold on;
35         linehandleACT=plot(X,Y,'-', 'color',[1 .4 .4]);
36
37         % Generate info for per-station highlighting, later on.
38         if isempty(markhandleAAT); markhandleAAT=NaN; end
39         if isempty(linehandleAAT); linehandleAAT=NaN; end
40         if isempty(markhandleACT); markhandleACT=NaN; end
41         if isempty(linehandleACT); linehandleACT=NaN; end
42         handles(i,[1:5])=[ustats(i) markhandleAAT linehandleAAT markhandleACT linehandleACT];
43     end
44
45     % Set axis limits.
46     subplotIDs=get(gcf,'Children');
47     subplotIDs=subplotIDs(length(subplotIDs):-1:1); % reverse this vector
48     y=get(subplotIDs([1 2]),'Ylim');
49
50     % set(subplotIDs([1 2]),'grid','on');
51     set(subplotIDs([1 2]),'ydir','rev');
52
53     % Filter out unwanted data. See 'vindtacrm' for a more advanced
54     % method, involving 'Userdata'.
55     answer=input('Is the bottle data acceptable? [Y/n] --- ','s');
56     if lower(answer)~= 'y'
57         userhappy=0; % stays 0
58         disp('Please mark samples for deletion. Click right mouse button or press [enter] when done. ');
59         but=1;
60         n=1;
61         squares=[];
62         while but == 1
63
64             hold on
65             [x1,y1,but] = ginput(1); o1=gco;
66             hold on; plot(x1,y1,'g. ');
67             if but==1
68                 [x2,y2,but] = ginput(1); o2=gco;
69                 hold on; plot(x1,y1,'g. ');
70
71                 if o1==o2 & but==1;
```



```

72         xmin=min([x1 x2]);
73         xmax=max([x1 x2]);
74         ymin=min([y1 y2]);
75         ymax=max([y1 y2]);
76         squares(n,:)= [o1 xmin xmax ymin ymax];
77         plot([xmin xmin],[ymin ymax], 'g-', [xmax xmax],[ymin ymax], 'g-', [xmin xmax],[ymin ymin], 'g-', [xmin xmax],[ymax ymax], 'g-');
78         n=n+1;
79     end
80 end
81 end
82
83 % Filter out the user-marked CRM AT values:
84 F=find(squares(:,1)==subplotIDs(1));
85 if ~isempty(F)
86     for i=1:length(F)
87         FF = atcorrected>squares(F(i),2) & atcorrected<squares(F(i),3) & depth>squares(F(i),4) & depth<squares(F(i),5) & samplotype==3;
88         atgood(FF)=0;
89     end
90 end
91
92 % Filter out the user-marked CRM CT values:
93 F=find(squares(:,1)==subplotIDs(2));
94 if ~isempty(F)
95     for i=1:length(F)
96         FF = ctcorrected>squares(F(i),2) & ctcorrected<squares(F(i),3) & depth>squares(F(i),4) & depth<squares(F(i),5) & samplotype==3;
97         ctgood(FF)=0;
98     end
99 end
100
101 else
102     userhappy=1;
103     disp('Done. ');
104 end
105 end

```

A.15 vindta222_updatebottlefile.m

```
1 co2file='co2correctedFINAL.csv';
2
3 data=nan(1000,8);
4 unqstats=unique(station(sampletype==3));
5 m=0;
6
7 % Find those samples that are currently still listed as good, but show dodgy blank characteristics
8 F = ctgood==1 & (perrunblank-perrunblankstd>usersetblank | perrunblank+perrunblankstd<usersetblank | perrunblankstd>80 | usersetblank>120 | usersetblank<5); ctgood(F)=4; % Map those
9
10 % Remap QF of 0 to 8 (ODV standard for BAD)
11 ctgood(ctgood==0)=8;
12 atgood(atgood==0)=8;
13
14 disp(cat(2,int2str(sum(ctgood==1))),' DIC-samples are rated as good!')
15 disp(cat(2,int2str(sum(ctgood==4)),' DIC-samples are considered questionable...')
16 disp(cat(2,int2str(sum(ctgood==8)),' DIC-samples are considered bad.')
17
18 for i = unqstats '
19
20     F=sampletype==3 & station==i;
21     unqcasts=unique(cast(F));
22
23     for j=unqcasts '
24
25         F=sampletype==3 & station==i & cast==j;
26         unqbots=unique(niskin(F));
27
28         for k=unqbots '
29
30             m=m+1; bat=nan; bct=nan; batqf=1; bctqf=1; atfound=0; ctfound=0;
31
32             if atfound==0
33                 F=sampletype==3 & station==i & cast==j & niskin==k & atgood==1; % Find any good AT values
34                 if sum(F)>0 % If something is found...
35                     bat = nanmean(atcorrected(F)); % store value and
36                     batqf=1; % ... set QF to good.
37                     atfound=1;
38                 end
39             end
40             if atfound==0
41                 F=sampletype==3 & station==i & cast==j & niskin==k & atgood==4; % Find questionable AT values
42                 if sum(F)>0 % If something is found...
43                     bat = nanmean(atcorrected(F)); % store value
44                     batqf=4; % ... set QF to ques.
45                     atfound=1;
46                 end
47             end
48             if atfound==0
49                 F=sampletype==3 & station==i & cast==j & niskin==k & atgood==8; % Find BAD AT values
50                 if sum(F)>0 % If something is found...
51                     bat = nanmean(atcorrected(F)); % store value
52                     batqf=8; % ... set QF to bad.
53                     atfound=1;
54                 end
55             end
56         end
57     end
58     if ctfound==0
59         F=sampletype==3 & station==i & cast==j & niskin==k & ctgood==1; % Find any good CT values
60         if sum(F)>0 % If something is found...
61             bct = nanmean(ctcorrected(F)); % store value
62             bctqf=1; % ... set QF to good.
63             ctfound=1;
64         end
65     end
66     if ctfound==0
67         F=sampletype==3 & station==i & cast==j & niskin==k & ctgood==4; % Find questionable CT values
68         if sum(F)>0 % If something is found...
69             bct = nanmean(ctcorrected(F)); % store value
70             bctqf=4; % ... set QF to ques.
71             ctfound=1;
72         end
73     end
74 end
```

```

72         end
73         if ctfound==0
74             F=sampletype==3 & station==i & cast==j & niskin==k & ctgood==8; % Find BAD CT values
75             if sum(F)>0 % If something is found...
76                 bct = nanmean(ctcorrected(F)); % store value
77                 bctqf=8; % ... set QF to bad.
78                 ctfound=1;
79             end
80         end
81
82         data(m,[1:8])=[m i j k bat batqf bct bctqf];
83
84     end
85 end
86 end
87
88 data=data(~isnan(data(:,1)),:); % remove trailing empty rows
89 data(data==0)=8; % Map QF's of zero to 8 (odv standard). Zero's only appear in qf columns.
90
91 % csvwrite(co2file ,data)
92
93 bottlefile='bottlefilegood.csv';
94 fid=fopen(bottlefile);
95 A=textscan(fid, '%f%f%f%f%f%f%f%f%f%f%f%f%f%f%f%f%f%f%f%f%f%f', 'delimiter', ',', 'headerlines', 1);
96 A=cell2mat(A);
97 sa=size(A);
98 A=[A nan(sa(1),4)];
99 ns=data(:,2);
100 nc=data(:,3);
101 nb=data(:,4);
102 nd=data(:,5:8);
103
104 for i = 1:sa(1)
105     F = ns==A(i,1) & nc==A(i,2) & nb==A(i,18);
106     if sum(F)==1;
107         A(i,sa(2)+[1:4])=nd(F,:);
108     elseif sum(F)>1;
109         keyboard
110     elseif sum(F)==0
111         disp(cat(2,'No vindtasample found for ',int2str(A(i,1)), '-',int2str(A(i,2)), '-',int2str(A(i,18)), '.'));
112     end
113 end
114 A(isnan(A))=-9999;
115 csvwrite(co2file ,A)
116
117 fclose(fid);

```

A.16 vindta222_makefigs.m

```
1 close('all')
2
3 F=[false;diff(sampletype)]==0 & sampletype==4;
4 F=find(F);
5 ctduplos=nan(size(F));
6 atduplos=nan(size(F));
7 for i = 1:length(F)
8     f1=F(i)-1;
9     f2=F(i);
10    if ctgood(f1)==1 & ctgood(f2)==1;
11        ctduplos(i)=ct(f1)-ct(f2);
12    end
13    if atgood(f1)==1 & atgood(f2)==1;
14        atduplos(i)=at(f1)-at(f2);
15    end
16 end
17
18 end
19
20
21 % plot CT CRM histogram figure
22 figure(1); clf
23 set(gcf,'PaperSize',flip1r(get(gcf,'PaperSize'))); % Trick to get @
```

A.17 vindta222_tableforlatex.m

```

1  runnumber=[1:length(station)]';
2  F1=samplotype==1; F3=samplotype==3; F4=samplotype==4;
3  sts=cell(size(samplotype));
4  sts(F1)={'JNK'}; sts(F3)={'SMP'}; sts(F4)={'CRM'};
5
6  perrunblank(perrunblank>999)=nan;
7  perrunblankstd(perrunblankstd>999)=nan;
8  atRMSx=atRMS;
9  atRMSx(atRMSx>99)=nan;
10 atcorrectedx=atcorrected;
11 atcorrectedx(atcorrectedx>9999)=nan;
12
13 a01 = runnumber;          a01=num2cell(a01);
14 a02 = sts;
15 a03 = station;          a03(-F3)=nan; a03=num2cell(a03);
16 a04 = round(depth);    a04(-F3)=nan; a04=num2cell(a04);
17 a05 = round(perrunblank); a05=num2cell(a05);
18 a06 = round(perrunblankstd); a06=num2cell(a06);
19 a07 = round(userblank); a07=num2cell(a07);
20 a08 = round(ct.*10)/10; a08=num2cell(a08);
21 a09 = 1./(ctcrmddev./100+1); a09(F1)=nan; a09=num2cell(a09);
22 a10 = ctfact;          a10(F1)=nan; a10=num2cell(a10);
23 a11 = round(ctcorrected*10)/10; a11(F1)=nan; a11=num2cell(a11);
24 a12 = ctgood;          a12(F1)=nan; a12=num2cell(a12);
25 a13 = round(at*10)/10; a13(F1)=nan; a13=num2cell(a13);
26 a14 = atRMS;           a14(F1)=nan; a14=num2cell(a14);
27 a15 = 1./(atcrmddev./100+1); a15(F1)=nan; a15=num2cell(a15);
28 a16 = atfact;          a16(F1)=nan; a16=num2cell(a16);
29 a17 = round(atcorrected*10)/10; a17(F1)=nan; a17=num2cell(a17);
30 a18 = atgood;          a18(F1)=nan; a18=num2cell(a18);
31 a19 = crmbatch;        a19(-F4)=nan; a19=num2cell(a19);
32 a20 = rundatetimestr;
33
34 headers={'\# ' 'T' 'STN' 'DPT' 'BK' '±' 'SBK' 'DIC' 'CRMfac' 'DICfac' 'DICcor'...
35           'QF' 'TAIk' 'RMS' 'CRMfac' 'TAIkfac' 'TAIkcor' 'QF' 'Batch' 'Date \& time'};
36 data=[a01 a02 a03 a04 a05 a06 a07 a08 a09 a10 a11 a12 a13 a14 a15 a16 a17 a18 a19 a20];
37
38 datab=cell(size(data)); a=size(data);
39 for i = 1:a(1)*a(2);
40     if isnan(data{i});
41         data(i)={' '};
42     end
43 end
44
45 data(1:20,:);
46 keyboard
47
48 matrix2latexsvh243(data, '../Datareport/datatableforreport.tex', 'columnLabels', headers);
49
50
51
52 return
53
54
55
56
57
58
59
60
61
62 runnumber=[1:length(station)]';
63 F1=samplotype==1; F3=samplotype==3; F4=samplotype==4;
64 sts=cell(size(samplotype));
65 sts(F1)={'JNK'}; sts(F3)={'SMP'}; sts(F4)={'CRM'};
66
67 perrunblank(perrunblank>999)=nan;
68 perrunblankstd(perrunblankstd>999)=nan;
69
70 a01 = runnumber;          a01=num2cell(a01);
71 a02 = sts;

```

```

72 a03 = station;                a03(-F3)=nan; a03=num2cell(a03);
73 a04 = round(depth);          a04(-F3)=nan; a04=num2cell(a04);
74 a05 = round(perrunblank);    a05=num2cell(a05);
75 a06 = round(perrunblankstd); a06=num2cell(a06);
76 a07 = round(useretblank);    a07=num2cell(a07);
77 a08 = round(ct.*10)/10;      a08=num2cell(a08);
78 a09 = 1./(ctcrmdev./100+1);  a09(-F4)=nan; a09=num2cell(a09);
79 a10 = ct factors;            a10( F1)=nan; a10=num2cell(a10);
80 a11 = round(ctcorrected*10)/10; a11( F1)=nan; a11=num2cell(a11);
81 a12 = ctgood;                a12( F1)=nan; a12=num2cell(a12);
82 a13 = round(at*10)/10;      a13( F1)=nan; a13=num2cell(a13);
83 a14 = atRMS;                 a14( F1)=nan; a14=num2cell(a14);
84 a15 = 1./(atcrmdev./100+1);  a15(-F4)=nan; a15=num2cell(a15);
85 a16 = at factors;            a16( F1)=nan; a16=num2cell(a16);
86 a17 = round(atcorrected*10)/10; a17( F1)=nan; a17=num2cell(a17);
87 a18 = atgood;                a18( F1)=nan; a18=num2cell(a18);
88 a19 = crmbatch;              a19(-F4)=nan; a19=num2cell(a19);
89 a20 = rundatetimestr;
90
91 headers={'\##' 'T' 'STN' 'DPT' 'BK' '±' 'SBK' 'DIC' 'CRMfac' 'DICfac' 'DICcor'...
92          'QF' 'TAlk' 'RMS' 'CRMfac' 'TAlkfac' 'TAlkcor' 'QF' 'CRM#' 'Date \& time'};
93 data=[a01 a02 a03 a04 a05 a06 a07 a08 a09 a10 a11 a12 a13 a14 a15 a16 a17 a18 a19 a20];
94
95 datab=cell(size(data)); a=size(data);
96 for i = 1:a(1)*a(2);
97     if isnan(data{i});
98         data(i)={' '};
99     end
100 end
101 matrix2latexsvh222(data, '../Datareport/datatableforreport.tex', 'columnLabels', headers);

```

B Appendix: Data

T Sample type designator. Valid values:

SMP – Regular oceanographic sample

JNK – Junk sample

CRM – Certified Reference Material

STN Station number (only for oceanographic samples)

DPT Depth (only for oceanographic samples)

BK Coulometer blank during this run (as determined from titration tail) [counts/min]

± Standard deviation of coulometer blank [counts/min]

SBK Blank as determined by the user (user for calculating DIC) [counts/min]

DIC Uncorrected DIC value of this run [$\mu\text{mol}/\text{kg}$]

CRMfac Deviation of CRM DIC from certified value (DIC/certified value)

DICfac Correction factor applied to DIC values of samples

DICcor Corrected and FINAL DIC value [$\mu\text{mol}/\text{kg}$]

QF Quality flag for DIC measurement (1=good, 4=questionable, 8=bad)

TAlk Uncorrected TAlk value of this run [$\mu\text{mol}/\text{kg}$]

RMS RMS of residuals of TAlk calculation from raw titration results [$\mu\text{mol}/\text{kg}$]

CRMfac Deviation of CRM TAlk from certified value (TAlk/certified value)

TAlkfac Correction factor applied to TAlk values of samples

TAlkcor Corrected and FINAL TAlk value [$\mu\text{mol}/\text{kg}$]

QF Quality flag for TAlk measurement (1=good, 4=questionable, 8=bad)

Batch The batch number of CRMs

Date & time Date and time the run was performed

Table starts here...

#	T	STN	DPT	BK	±	SBK	DIC	CRMfac	DICfac	DICcor	QF	TAlk	RMS	CRMfac	TAlkfac	TAlkcor	QF	Batch	Date & time	
1	JNK																			2007-08-05-22-46
2	JNK					150	0.0													2007-08-06-08-54
3	JNK					150	0.0													2007-08-06-13-56
4	JNK					150	0.0													2007-08-06-21-53
5	JNK				225	150	2261.0													2007-08-09-16-36
6	JNK				124	150	1185.9													2007-08-09-18-11
7	JNK				98	150	1153.3													2007-08-09-18-36
8	JNK				106	150	1121.7													2007-08-09-19-05
9	JNK			790	86	150	1036.8													2007-08-09-19-36
10	JNK			463	54	150	568.1													2007-08-09-20-01
11	JNK			406	88	150	2086.9													2007-08-09-20-31
12	JNK			96	145	150	2040.2													2007-08-10-10-55
13	JNK			325	30	150	2084.7													2007-08-10-12-27
14	JNK			324	54	150	2077.9													2007-08-10-12-54
15	JNK			330	51	150	2082.1													2007-08-10-13-19
16	JNK					150	0.0													2007-08-10-16-21
17	JNK			452	77	150	2103.0													2007-08-10-17-02
18	JNK			401	82	150	2090.0													2007-08-10-17-36
19	JNK			235	92	150	2073.9													2007-08-10-18-29
20	JNK			277	69	150	2069.4													2007-08-10-18-55
21	JNK			259	100	150	2069.1													2007-08-10-20-16
22	JNK			225	93	150	2068.5													2007-08-10-20-44
23	JNK			126	49	150	2031.7													2007-08-12-11-02
24	JNK			224	68	157	2053.5													2007-08-12-11-35
25	JNK			146	39	157	2029.7													2007-08-12-12-07
26	JNK			96	33	157	2025.1													2007-08-12-12-30
27	JNK			140	69	157	2023.2													2007-08-12-13-11
28	JNK			142	26	157	2030.8													2007-08-12-13-44
29	JNK			154	40	156	2032.4													2007-08-12-14-33
30	CRM			174	42	156	2095.6	1.002899	1.002494	2100.8	4	2304.5	3.3	1.004339	1.003067	2311.6	1	76	2007-08-12-15-01	
31	CRM			146	43	149	2097.3	1.002073	1.002552	2102.7	4	2307.3	3.5	1.003136	1.003067	2314.3	1	76	2007-08-12-15-36	
32	SMP	261	3700	184	53	138	2148.5		1.002846	2154.7	4	2292.8	1.9		1.003156	2300.0	1		2007-08-12-16-14	
33	SMP	261	3300	121	23	131	2147.8		1.003040	2154.3	4	2291.3	1.7		1.003219	2298.6	1		2007-08-12-16-39	
34	SMP	261	3501	121	50	122	2149.2		1.003265	2156.3	4	2293.2	1.9		1.003291	2300.8	1		2007-08-12-17-08	
35	SMP	261	3199	104	28	115	2147.0		1.003451	2154.4	1	2290.4	2.2		1.003351	2298.0	1		2007-08-12-17-32	
36	SMP	261	3000	119	30	109	2151.8		1.003715	2159.7	1	2290.4	2.1		1.003436	2298.3	1		2007-08-12-18-06	
37	SMP	261	2750	104	54	109	2146.7		1.003917	2155.1	1	2290.7	2.2		1.003501	2298.7	1		2007-08-12-18-32	
38	SMP	261	2500	143	55	109	2151.1		1.004126	2160.0	1	2290.0	1.6		1.003568	2298.2	1		2007-08-12-18-59	
39	SMP	261	2301	109	30	109	2152.6		1.004320	2161.9	1	2290.9	2.0		1.003631	2299.2	1		2007-08-12-19-24	
40	SMP	261	2301	128	50	109	2148.9		1.004514	2158.6	1	2291.2	2.1		1.003693	2299.6	1		2007-08-12-19-49	
41	SMP	261	1751	107	55	109	2151.2		1.004700	2161.3	1	2288.6	2.5		1.003753	2297.2	1		2007-08-12-20-13	
42	SMP	261	1501	77	72	109	2149.5		1.004886	2160.0	1	2287.8	2.7		1.003813	2296.5	1		2007-08-12-20-37	
43	SMP	261	1002	103	36	109	2153.7		1.005072	2164.6	1	2290.3	2.3		1.003873	2299.2	1		2007-08-12-21-01	
44	SMP	261	702	63	54	109	2149.4		1.005235	2160.7	1	2286.1	3.0		1.003926	2295.1	1		2007-08-12-21-22	
45	SMP	261	502	124	37	109	2150.1		1.005444	2161.8	1	2289.9	2.5		1.003993	2299.0	1		2007-08-12-21-49	
46	SMP	261	352	85	45	109	2144.3		1.005615	2156.3	1	2288.2	1.9		1.004048	2297.4	1		2007-08-12-22-11	
47	SMP	261	201	147	45	109	2139.5		1.005793	2151.9	1	2286.9	2.1		1.004105	2296.3	1		2007-08-12-22-34	
48	SMP	261	125	89	71	109	2133.4		1.005964	2146.1	1	2270.2	2.0		1.004160	2279.6	1		2007-08-12-22-56	
49	SMP	261	101	31	47	109	2121.0		1.006134	2134.0	4	2260.8	2.2		1.004215	2270.3	1		2007-08-12-23-18	
50	CRM			23	45	109	2089.7	1.005716	1.006367	2103.0	4	2304.5	3.5	1.004338	1.004290	2314.4	1	76	2007-08-12-23-48	
51	CRM			4	12	109	2086.9	1.007085	1.006410	2100.3	4	2303.2	3.2	1.004906	1.004531	2313.6	1	76	2007-08-13-00-10	
52	JNK			272	69															2007-08-14-12-00
53	JNK			167	64	128	2000.0													2007-08-14-12-35
54	JNK			111	35	128	2023.3													2007-08-14-13-01
55	JNK			89	30	128	2021.4													2007-08-14-13-24
56	JNK			73	21	128	2024.9													2007-08-14-13-47
57	JNK			61	50	128	2020.8													2007-08-14-14-10
58	CRM			141	41	129	2092.4	1.004430	1.004700	2102.3	4	2305.0	3.3	1.004124	1.004427	2315.2	1	76	2007-08-14-14-56	
59	CRM			114	59	129	2091.3	1.004966	1.004681	2101.1	4	2303.8	3.3	1.004649	1.004429	2314.0	1	76	2007-08-14-15-26	
60	SMP	266	2950	139	63	129	2150.7		1.004627	2160.7	4	2291.5	2.3		1.004432	2301.7	1		2007-08-14-16-01	

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#	T	STN	DPT	BK	±	SBK	DIC	CRMfac	DICfac	DICcor	QF	Talk	RMS	CRMfac	Talkfac	Talkcor	QF	Batch	Date & time
121	SMP	268	201	60	31	77	2144.4		1.001038	2146.6	1	2288.0	1.9		1.004862	2299.1	1		2007-08-16-19-34
122	SMP	268	201	57	43	77	2143.6		1.001038	2145.8	1	2285.0	2.4		1.004864	2296.1	1		2007-08-16-19-55
123	SMP	268	150	70	43	76	2144.1		1.001038	2146.3	1	2285.3	2.3		1.004865	2296.4	1		2007-08-16-20-17
124	SMP	268	125	74	58	76	2147.6		1.001038	2149.8	1	2286.2	2.2		1.004867	2297.4	1		2007-08-16-20-40
125	CRM			76	74	76	2099.5	1.001035	1.001038	2101.7	1	2303.8	4.6	1.004632	1.004869	2315.0	1	76	2007-08-16-21-12
126	CRM			38	52	76	2091.9	1.004676	1.001038	2094.1	1	2301.5	4.2	1.005643	1.004871	2312.7	1	76	2007-08-16-21-34
127	JNK			89	30														2007-08-17-13-09
128	JNK			97	24	106	2021.8												2007-08-17-14-14
129	JNK			193	53	106	2031.8												2007-08-17-14-38
130	JNK			115	35	106	2022.6												2007-08-17-15-46
131	JNK					106	2041.3												2007-08-17-16-19
132	JNK			182	43														2007-08-18-08-24
133	JNK			0	0	90	-13.1												2007-08-18-08-46
134	JNK			62	41	90	1969.3												2007-08-18-09-37
135	JNK			95	22	90	1969.1												2007-08-18-09-58
136	CRM			147	67	90	2103.4	0.999207	0.999230	2101.7	1	2304.2	3.1	1.004448	1.004766	2315.2	1	76	2007-08-18-10-23
137	CRM			95	69	90	2101.9	0.999879	0.999230	2100.3	1	2303.1	3.3	1.004962	1.004766	2314.0	1	76	2007-08-18-10-53
138	SMP	268	100			90	2324.7		0.999230	2322.9	8	2287.7	1.9		1.004766	2298.6	1		2007-08-18-11-19
139	SMP	268	100	900		90	2421.0		0.999230	2419.8	8	2283.9	2.2		1.004766	2294.7	1		2007-08-18-11-41
140	SMP	268	75	0	0	90	2166.5		0.999230	2164.8	4	2282.9	2.1		1.004766	2293.8	1		2007-08-18-12-05
141	SMP	268	75	658		90	2190.7		0.999230	2189.0	4	2283.1	2.5		1.004766	2294.0	1		2007-08-18-12-41
142	SMP	268	75	131	219	90	2136.2		0.999230	2134.5	4	2271.6	2.8		1.004766	2282.4	1		2007-08-18-13-06
143	JNK			70	48	75	1969.3												2007-08-18-18-28
144	JNK			71	38	75	2085.6												2007-08-18-18-49
145	JNK			147	65														2007-08-19-09-34
146	JNK			114	84	100	1976.2												2007-08-19-10-03
147	JNK			57	37	100	1980.6												2007-08-19-11-21
148	JNK					100	2209.8												2007-08-19-13-27
149	JNK			134	96	100	1969.3												2007-08-19-13-50
150	JNK			78	68	100	1966.9												2007-08-19-14-12
151	JNK			82	60	100	1965.0												2007-08-19-14-35
152	CRM			68	51	100	2094.6	1.003370	1.003353	2101.7	1	2302.8	4.3	1.005075	1.005000	2314.3	1	76	2007-08-19-14-58
153	CRM					100	2512.8	0.836409	1.003391	2521.3	8	2303.1	3.5	1.004951	1.005000	2314.6	1	76	2007-08-19-15-24
154	SMP	276	302	81	73	100	2174.3		1.003436	2181.8	1	2290.1	1.9		1.005000	2301.5	1		2007-08-19-15-54
155	JNK			139	68	100	1973.9												2007-08-19-16-25
156	SMP	276	501	97	58	100	2157.3		1.003519	2164.8	1	2286.5	2.8		1.005000	2297.9	1		2007-08-19-16-50
157	SMP	276	400	526	790	100	2239.7		1.003614	2247.7	8	2291.8	1.7		1.005000	2303.3	1		2007-08-19-17-54
158	SMP	276	302	390		100	2262.7		1.003663	2271.0	8	2291.1	2.0		1.005000	2302.5	1		2007-08-19-18-27
159	SMP	276	102	441		100	2195.7		1.003694	2203.8	4	2283.0	1.9		1.005000	2294.4	1		2007-08-19-18-48
160	SMP	276	50	57	40	100	2126.1		1.003727	2134.1	4	2261.6	1.9		1.005000	2272.9	1		2007-08-19-19-10
161	SMP	279	316	49	37	100	2166.5		1.003762	2174.6	4	2289.9	2.5		1.005000	2301.3	1		2007-08-19-19-34
162	SMP	279	250	60	28	100	2162.7		1.003796	2170.9	4	2287.9	2.6		1.005000	2299.4	1		2007-08-19-19-57
163	SMP	279	201	105	63	100	2166.0		1.003905	2174.4	1	2289.6	2.5		1.005000	2301.0	1		2007-08-19-21-10
164	SMP	279	150	132	37	100	2158.5		1.003945	2167.0	1	2287.0	2.6		1.005000	2298.4	1		2007-08-19-21-37
165	SMP	279	101	94	82	100	2150.9		1.003979	2159.5	4	2286.4	2.3		1.005000	2297.8	1		2007-08-19-22-00
166	SMP	279	49	101	23	100	2142.6		1.004015	2151.2	1	2271.6	2.5		1.005000	2283.0	1		2007-08-19-22-24
167	SMP	279	26	73	44	100	2103.2		1.004049	2111.7	1	2250.4	2.7		1.005000	2261.6	1		2007-08-19-22-47
168	CRM			86	52	100	2093.1	1.004112	1.004084	2101.6	1	2303.2	3.4	1.004909	1.005000	2314.7	1	76	2007-08-19-23-11
169	CRM			63	43	100	2093.0	1.004172	1.004100	2101.5	1	2302.4	3.0	1.005255	1.005000	2313.9	1	76	2007-08-19-23-33
170	JNK			61	63														2007-08-20-08-46
171	JNK			56	56	60	1970.4												2007-08-20-09-07
172	JNK			807		61	2066.8												2007-08-20-09-37
173	JNK			58	58	61	1972.6												2007-08-20-10-08
174	JNK			137	53														2007-08-21-10-04
175	JNK			85	46	94	1990.8												2007-08-21-10-36
176	JNK			77	72	94	1994.1												2007-08-21-11-01
177	JNK			156	79	94	2005.4												2007-08-21-11-39
178	JNK			101	63	94	1985.3												2007-08-21-13-07
179	JNK			177	98	94	2001.6												2007-08-21-16-53
180	JNK			95	68	94	1993.6												2007-08-21-17-20

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#	T	STN	DPT	BK	±	SBK	DIC	CRMfac	DICfac	DICcor	QF	TALK	RMS	CRMfac	TAlkfac	TAlkcor	QF	Batch	Date & time
781	SMP	257	3891	102	12	102	2148.7		1.001189	2151.2	1	2294.7	4.1		1.001036	2297.1	1		2007-09-28-17-37
782	SMP	257	3385	136	48	102	2152.0		1.001253	2154.6	1	2296.1	4.1		1.000980	2298.3	1		2007-09-28-18-19
783	SMP	257	3000	112	22	102	2153.2		1.001289	2156.0	1	2291.7	4.2		1.000949	2293.8	1		2007-09-28-18-43
784	SMP	257	2500	93	18	102	2147.4		1.001323	2150.3	1	2292.8	3.9		1.000920	2294.9	1		2007-09-28-19-05
785	CRM			90	33	102	2008.8	1.001622	1.001358	2011.5	1	2221.2	7.3	1.000667	1.000889	2223.2	1	53	2007-09-28-19-28
786	CRM			89	30	102	2008.0	1.002027	1.001395	2010.8	1	2221.5	7.0	1.000542	1.000856	2223.4	1	53	2007-09-28-19-53
787	JNK			174	52														2007-10-01-07-42
788	JNK			136	26	134	2120.0												2007-10-01-08-05
789	JNK			132	38	131	2118.3												2007-10-01-08-30
790	JNK			122	26	128	2113.7												2007-10-01-08-51
791	CRM			107	49	124	2008.7	1.001657	1.001841	2012.4	4	2223.2	5.4	0.999762	1.000500	2224.3	1	53	2007-10-01-09-20
792	CRM			116	41	121	2008.0	1.002030	1.001965	2011.9	4	2220.0	5.0	1.001187	1.000477	2221.1	1	53	2007-10-01-09-43
793	SMP	257	2000	123	43	117	2149.7		1.002146	2154.3	1	2293.2	2.4		1.000360	2294.0	1		2007-10-01-10-10
794	SMP	257	1500	109	67	114	2149.7		1.002307	2154.6	1	2294.9	2.4		1.000257	2295.5	1		2007-10-01-10-34
795	SMP	257	1000	123	31	111	2150.5		1.002468	2155.8	1	2292.6	2.2		1.000153	2292.9	1		2007-10-01-10-58
796	SMP	257	801	107	56	107	2150.2		1.002663	2155.9	1	2294.9	2.4		1.000028	2295.0	1		2007-10-01-11-27
797	SMP	257	701	99	39	103	2147.7		1.002817	2153.8	1	2294.6	2.2		0.999929	2294.4	1		2007-10-01-11-50
798	SMP	257	600	102	37	100	2146.7		1.003005	2153.2	1	2292.5	2.1		0.999808	2292.1	1		2007-10-01-12-18
799	SMP	257	500	94	16	96	2145.5		1.003159	2152.3	1	2294.8	2.9		0.999709	2294.2	1		2007-10-01-12-41
800	SMP	257	401	94	35	93	2144.0		1.003307	2151.1	1	2294.8	2.1		0.999614	2293.9	1		2007-10-01-13-03
801	SMP	257	300	96	25	90	2142.1		1.003475	2149.6	1	2298.9	3.0		0.999507	2297.8	1		2007-10-01-13-28
802	SMP	257	200	87	49	87	2140.5		1.003629	2148.3	1	2294.7	2.3		0.999408	2293.4	1		2007-10-01-13-51
803	SMP	257	150	83	38	86	2136.8		1.003763	2144.9	1	2295.3	3.6		0.999321	2293.8	1		2007-10-01-14-11
804	SMP	257	125	90	36	86	2134.6		1.003918	2142.9	1	2286.6	3.3		0.999222	2284.8	1		2007-10-01-14-34
805	SMP	257	99	84	38	86	2127.3		1.004058	2135.9	1	2273.7	2.3		0.999132	2271.8	1		2007-10-01-14-55
806	CRM			89	45	86	2003.8	1.004088	1.004199	2012.3	1	2225.5	5.0	0.998742	0.999041	2223.3	1	53	2007-10-01-15-16
807	CRM			82	18	86	2003.3	1.004359	1.004251	2011.8	1	2226.7	4.8	0.998176	0.999025	2224.6	1	53	2007-10-01-15-41
808	SMP	257	76	97	61	86	2084.6		1.004251	2093.5	1	2261.1	2.7		0.999025	2258.9	1		2007-10-01-16-18
809	SMP	257	50	97	25	86	2068.7		1.004251	2077.5	1	2246.1	3.0		0.999025	2243.9	1		2007-10-01-16-40
810	SMP	257	25	85	37	86	2069.6		1.004251	2078.4	1	2246.4	2.7		0.999025	2244.2	1		2007-10-01-17-03
811	SMP	257	10	86	29	86	2056.6		1.004251	2065.3	1	2232.3	2.6		0.999025	2230.1	1		2007-10-01-17-25
812	CRM			91	22	86	2003.9	1.004057	1.004251	2012.4	1	2224.4	4.7	0.999228	0.999025	2222.2	1	53	2007-10-01-17-48
813	CRM			81	44	86	2002.8	1.004589	1.004251	2011.4	1	2223.5	4.5	0.999614	0.999025	2221.4	1	53	2007-10-01-18-11