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Data processing procedures for SNOMS project 2007 to 2012 Version-1: 28 August 2012

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ABSTRACT

The Swire NOC Monitoring System (SNOMS) has enabled the collection of a global set of surface hydrological and dissolved gas measurements from the MV *Pacific Celebes*. The data is being used to assess the rate of transfer of carbon dioxide between the atmosphere and the sea in different regions and to assess the forces that control this exchange. During the period from summer 2007 through to summer 2009 the ship crossed the North Atlantic, North Indian and Equatorial Pacific oceans with one voyage via the Cape of Good Hope. From 2009 until March 2012 repeat transects of the Pacific Ocean were made between Australia, New Zealand and North America. Its route has included areas of the World Ocean that are largely under sampled in terms of the carbonate system, the daily sampling of salinity, total alkalinity and dissolved inorganic carbon has provided valuable additional coverage to this data set. The system was a novel design developed to require a minimum of maintenance that was provided by the ship's crew. This report describes the bespoke processes that were developed in the SNOMS project to assemble and check the quality of the data being returned. The purpose of this report is to provide a complete description of the processing used to move from the raw data collected on the ship to the final archived data set. This document forms part of the meta-data set produced by the SNOMS project, and will be available with the main data set when it is provided to users by BODC and CDIAC.

KEYWORDS

Data acquisition and processing, SNOMS, GTD, Gas Exchange, Oxygen anomaly, DIC, TA, FerryBox, SWIRE, Monitoring, Time Series

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Note this is a "live" document allowing access to the files named in the text. Currently this only works for those with access to folders at server location \\Mira\SHARED1\OBEPRIV\ at NOC.

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1.0 Introduction

1.1 Basis of this report

The Swire NOCs Monitoring System (SNOMS) was designed for the collection of high quality, global surface hydrological and dissolved gas measurements from the MV Pacific Celebes (Hydes et al., 2007). The system was designed to be low maintenance so that the ship's crew could carry out all the work associated with it on the ship. The data from the SNOMS project is being archived at the British Oceanographic Data Centre (NOC; http://www.bodc.ac.uk) and the Carbon Dioxide Information and Advisory Center (CDIAC; Oak Ridge, USA; http://cdiac.ornl.gov/). The purpose of this report is to provide a complete description of the processing used to move from the raw data collected on the ship to the final archived data set. This document forms part of the meta-data set produced by the SNOMS project, and will be available with the main data set when it is provided to users by BODC or CDIAC. These long-term global data from many oceanic environments are an invaluable tool in the investigation of the interplay of the atmosphere and ocean, hydrology and biology. The repeat transects of 3 of the major oceanic basins provided a unique opportunity for insight into conditions and changes within these information visit the SNOMS Web environments. For further site at http://www.noc.soton.ac.uk/snoms/.

To monitor the operation of all the sensors in the system (listed in Table 1.1) a subset of the data (spot values at intervals of 5 minutes) were telemetered via an Iridium satellite link to the NOC and displayed in near real-time on a public web-page at http://www.noc.soton.ac.uk/snoms/. On board the ship the full data set from all the sensors was logged in binary format to two Compact Flash cards; one mounted above the bridge that collected data from the meteorological instruments, the other mounted in the engine room that collected data from the hydrographic instrumentation. This document deals with the data that were written to these flashcards.

Two methods were used to provide quality control (QC) of the data sets.

(1) In the case of the smaller less expensive sensors providing data on seawater tank temperature, conductivity and concentration of dissolved oxygen the measurements were replicated by using three of each type of sensor. The use of triplicate readings enabled the identification of less well functioning sensors when this occurred and generation of a single output measurement based on the choice of the best functioning instruments. In addition a fourth temperature measurement was provided by a hull mounted temperature

sensor and these data were also used to provide further quality control (see also Hartman et al., In Prep; Beggs et al., 2012).

(2) Water samples (that are able to be stored without deteriorating for extended periods) were also collected, these provided quality control of the measurements of conductivity and the measurements of pCO2 (by calculation of pCO2 from measurements of Total Alkalinity -TA and Total Dissolved Inorganic Carbon - DIC made on the water sample). The seawater samples were collected on a daily basis by the ship's crew while the ship was underway. These consisted of a 200 ml salinity sample and a 250 ml sample for TA/DIC. The samples were shipped back to NOC from the break point ports in the operation, listed in Table 1.2, for analysis in the laboratories there.

Table 1.1 Sensor list					
Manufacturer	Measurement	Model	Method	Serial numbers	
Aanderaa	Sea water Temperature	4050	thermistor	11 13 15 25 34 55 90	
Aanderaa	Sea water O₂concentration by Optode	3835	Fluorescence Quenching	338 339 340 641 34 1008 1009 1014 1357	
Aanderaa	Sea water Conductivity	3919	Inductive	136 138 139 674 952 1061	
Pro-Oceanus	Sea water CO ₂ concentration	CO2-Pro	Infra Red absorption	47 48 94	
Pro-Oceanus	Sea water dissolved gas fugacity	GTD-Pro	gas tension	49 98	
Sea-Bird	Ship's Hull Temperature (in situ water)	SBE-48	Contact Thermistor	23 25	
Vaisala	Atmospheric CO ₂	GMP343	Infra Red absorption	B2840006 D4150004	
Vaisala	Atmospheric pressure, temperature and humidity.	PTU-200	Press & Humidity – capacitive, temperature - PRT		
Vaisala	Atmospheric pressure, temperature and humidity.	PTU-300	Press & Humidity – capacitive, temperature - PRT		
Vector Instruments	Wind Direction	W200G	Vane	2118	
Vector Instruments	Wind speed	A100R3	Cup anemometer	1894	

In the following document we describe the steps taken to achieve a "best" data set on a 5-minute time base, which are then adjusted if necessary on the basis of the water sample data. All, if any, adjustments to the data are recorded in the meta-data set.

A pictorial overview of the processing procedure is given in Figures 3.0a through 3.0d, these can be used in conjunction with the written descriptions in the following sections to derive an understanding of the procedures involved - the linked originating documents themselves provide http links to the folders and programs that were used.

Table 1.2 Break point ports for division of the data sets all equipment on board (ON) and indication of how well the main CO2 sensor was working (OK).							
Voyage	Start Port	End Port	Start date	On	CO2 OK		
1	Singapore	Livorno	2/6/07	Y	No		
2	Livorno	Livorno	12/9/07	Y	?		
3	Livorno	Livorno	29/1/08	Y	??		
4	Livorno	St John	13/6/08	N	Ν		
5	St John	St John	25/10/08	Y	Y		
6	St John	Livorno	21/3/09	Y	Y		
7	Livorno	Vancouver	18/8/09	Y	Y		
8	Vancouver	Vancouver	27/11/09	Y	Y		
9	Vancouver	Vancouver	21/3/10	Y	Y		
10	Vancouver	Vancouver	23/6/10	Y	Y		
11	Vancouver	Vancouver	28/9/10	Y	Y		
12	Vancouver	Vancouver	14/1/11	N	Ν		
13	Vancouver	Vancouver	29/4/11	Y	Y		
14	Vancouver	Vancouver	26/7/11	Y	Y		
15	Vancouver	Vancouver	29/10/11	Y	Y		
16	Vancouver	Melbourne	5/2/12	Y	Y		

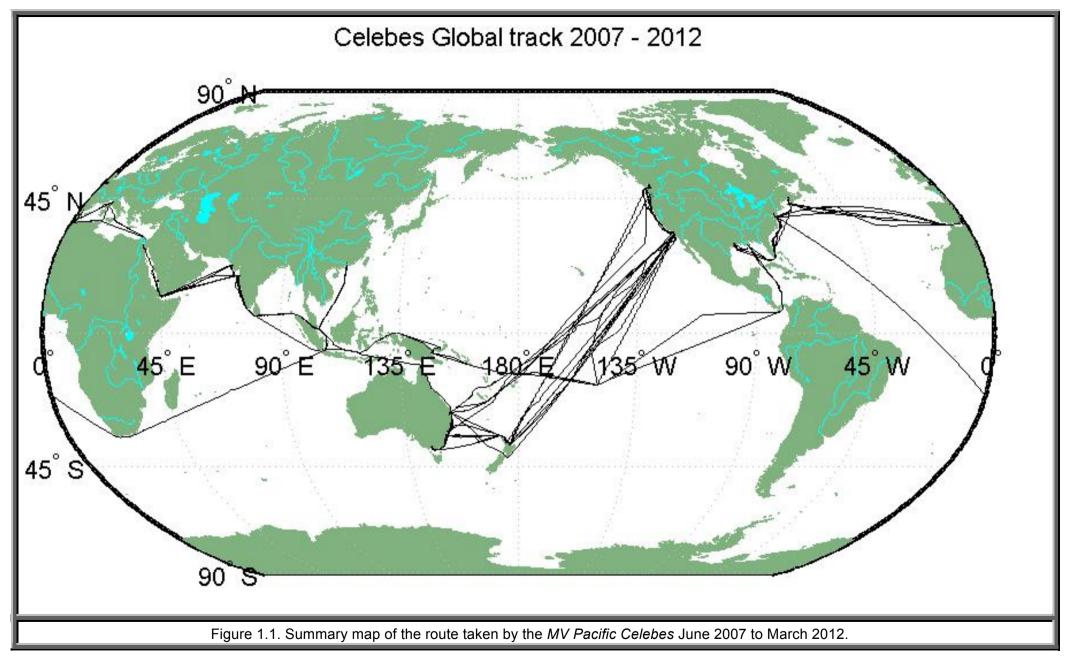
The basic steps described in detail later are:-

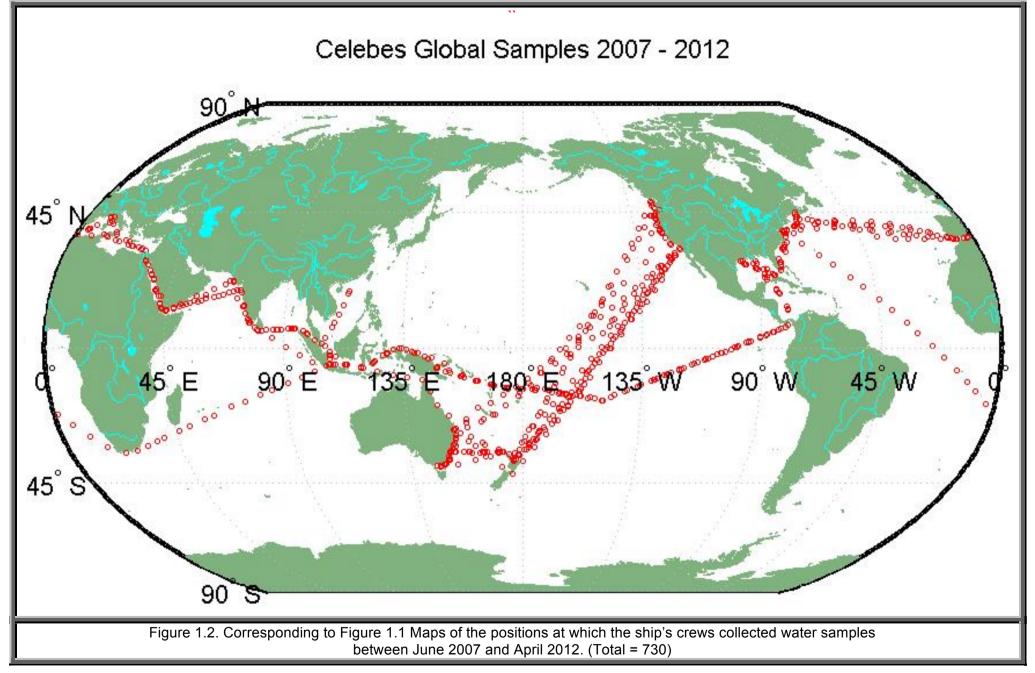
(1) After the data were transferred from the flashcards they were processed using bespoke NOC software coded in C developed in LabWindows CVI. This software concatenates, averages and merges the parameters from all of the instruments and converts the binary files into ASCII files for further processing.

(2) Further processing of the data was performed (with procedures that were coded using MathWorks Inc's Matlab software) to inspect, quality control, adjust and write the archiveable data files.

1.2 Synopsis of ship activity

From summer 2007 through to early 2009 the ship worked a route which was a global circumnavigation from Canada across the North Atlantic, Mediterranean, around India to Indonesia, across the Equatorial Pacific, through the Panama Canal into the Gulf of Mexico and then up to Canada. In 2009 the *Celebes* worked one triangular route from Indonesia to North America via the Cape of Good Hope. Then from 2009 until March 2012 she worked repeat transects of the Pacific Ocean between Australia, New Zealand and North America. These routes included areas of the ocean that are largely under sampled in terms of the carbonate system, the daily sampling of salinity, total alkalinity and dissolved inorganic carbon have added valuable additional information in their own right to the data set. The breakdown of the work into sections is listed in Table 1.2; corresponding maps of the routes are shown in Figure 1.1 and discrete DIC samples obtained in Figure 1.2.





2.0 Data collection and processing

To support "readability" of this document the following convention is used; the location of a file on the NOC server computer "Mira" is represented as a path that is split into two parts, the root remains the same and is represented by the mapping $R:\ = \Mira\SHARED1\OBEPRIV\Ferrybox$. The sub-folder can vary and consists of the path relative to the root R:\. Processing is performed in Matlab workspace and the pertinent m-files that are kept in the directory R:\ARCHIVE_MCH\m-files\Celebes\. M-files have the extension .m and data files have the extension .mat.

2.1 Instrument overview

The instruments (listed in Table 1.1) reporting data to the flash cards in the two data loggers are described below; further detail is available in NOC report 10 (Hydes et al 2007).

The ship's position was determined by a GPS system that provided the master time reference, latitude and longitude. These were combined with the atmospheric and hydrographic instrument data which are termed dependent parameters.

The atmospheric instrumentation was mounted in a Stevenson-screen directly over the bridge at an estimated height of 34 m above sea level, the sensors included: a Vaisala instruments GMP 343 measuring atmospheric carbon dioxide concentration in parts per million and a PTU-200 (02-Jun-07 to 17-Aug-09, 28-Apr-11 onwards) and a PTU-300 (19-Aug-09 to 25-Apr-11) for pressure, humidity and temperature. On the 30th Jan 2008, a Vector Instruments A100R3, measuring wind speed and a Vector Instruments W200G measuring wind direction were mounted on a pole situated on the railings on the port side forward of the Stevenson screen and elevated 2.5 metres above the deck at a height of 35 m above sea level.

The hydrographic sensors were mounted in a specially designed flow-through pressure tank that was installed in the engine room. Additionally a Seabird 48 hull mounted sensor provided the in situ seawater temperature. Measurements made in the tank were temperature and conductivity (from which salinity was derived), total dissolved gas pressure, oxygen concentration and carbon dioxide concentration. More information on the instrumentation can be found on the website at the following address http://www.noc.soton.ac.uk/snoms/instrumentation and instrument descriptions can be found in R:\Celebes\Sensor database\Calibrations.

From instrument to combined ASCII files 2.2

The initial stages of the Celebes data processing converted the binary files that were written to flash card into an ASCII format which are maintained on the server called Mira at the following address; R:\Celebes\Merged averaged flash card data. The data from the ship have been divided into the sections that are tabulated in Table 2.2 which shows the relevant ASCII files together with their start and stop times; date, day of year and the Matlab serial date number - the number of days elapsed since 1st January 0000. The file name is representative of the start time of the file as follows. Cel_merge_YYYY_DDD_HHMM.txt where YYYY is the year, DDD is the day number, HH hours and MM minutes. Note that for two periods all the sensors apart from the hull temperature and Vaisala PTU were removed for recalibration. These periods were from 12th June to 27th October 2008 and from 14th January to 25th April 2011. No water samples were collected during these times. Furthermore, no samples were available in 2011 until August.

Table 2.2 Table of names and durations of 5 minute merged files.						
		Start				
File	Day	Date	Matday	Day	Date	Matday
Cel_merge_2007_161_0000	161.00	10.06.2007	733203.00	254.9340	11.09.2007	733296.93
Cel_merge_2007_255_0000	255.00	12.09.2007	733297.00	027.4965	27.01.2008	733434.50
Cel_merge_2008_029_0000	029.00	29.01.2008	733436.00	164.5694	12.06.2008	733571.57
Cel_merge_2008_164_1300	164.58	12.06.2008	733571.58	299.7292	25.10.2008	733706.73
Cel_merge_2008_301_1400	301.62	27.10.2008	733708.62	077.5903	18.03.2009	733850.59
Cel_merge_2009_079_1700	079.73	20.03.2009	733852.73	230.6042	18.08.2009	734003.60
Cel_merge_2009_230_1400	230.61	18.08.2009	734003.61	330.0590	26.11.2009	734103.06
Cel_merge_2009_330_0100	330.07	26.11.2009	734103.07	079.8403	20.03.2010	734217.84
Cel_merge_2010_079_2000	079.85	20.03.2010	734217.85	173.8020	22.06.2010	734311.80
Cel_merge_2010_173_1900	173.81	22.06.2010	734311.81	270.7326	27.09.2010	734408.73
Cel_merge_2010_270_1700	270.74	27.09.2010	734408.74	013.6771	13.01.2011	734516.68
Cel_merge_2011_013_1900	013.81	13.01.2011	734516.81	116.6563	26.04.2011	734619.66
Cel_merge_2011_116_1500	116.66	26.04.2011	734619.66	206.7500	25.07.2011	734709.75
Cel_merge_2011_206_1800	206.76	25.07.2011	734709.76	301.8368	28.10.2011	734804.84
Cel_merge_2011_301_2000	301.84	28.10.2011	734804.84	035.7917	04.02.2012	734903.79
Cel_merge_2012_035_1900	035.80	04.02.2012	734903.80	084.8889	24.03.2012	734952.89

2.3 From ASCII files to pCO₂ measurements

Data from a 30-minute period following every automatic zero calibration made by the Pro-Oceanus CO_2 sensor were ignored; this is the time required for the sensor to reequilibrate with the seawater after a reference check. The partial pressure of p CO_2 was calculated from the CO_2 dry mole fraction, xCO2 and the total pressure of the gas stream, a temperature correction is also applied. The m-files are stored at R:\Ferrybox\Celebes\ZP_processing\mfiles.

The three m-files that relate to the pCO2 processing are Z1 Get5minMatData SNOMS 2011.m, Z2 GetCO2MatData SNOMS 2011.m and Z3 CO2AZPC SNOMS 2011.m. The 5-minute pCO2 data can be found in R:\Ferrybox\Celebes\ZP processing\data. The 20-column matrixes (see the document R:\Ferrybox\Celebes\ZP processing\README ZP Processing for an explanation of each column) are saved in 'Cel xxx PCO2 5minAZPC.mat' as variables 'CO2 AZPC 5min'. They have been matched with the time stamp of ASCII 5-minute merged data. The processing of the SNOMS underway pCO2 data starts from the 30 seconds averaged output recorded by the engine room data logger. These 30-s frequency data can be found in the shared drive at R:\Ferrybox\Celebes\Flash card. They were named as 'all PCO2.txt' in each flash card record. All the txt data were renamed as 'Cel xxx pCO2.txt' (where xxx is the string yyyy jday hhmm such as 2012 035 1900 which matched the time of the 5-minute averaged and merged data) and then copied to: R:\Ferrybox\Celebes\Merged averaged flash card data\All ProCO2 data. These data were processed by Matlab and the m-files for processing reside in: R:\Ferrybox\Celebes\ZP processing/mfiles. The processed data were then saved in: R:\Ferrybox\Celebes\ZP processing\data. The plots were saved in: R:\Ferrybox\Celebes\ZP processing\plots

2.3.1 Copy and convert the 5-minute averaged and merged data using

The 5 min merged ASCII SWIRES files are copied to the data directory by Z1_GetMatData_SNOMS_2011.m. It then converts the ASCII files to Matlab file as 'Cel_merge_xxx.mat', where 'xxx' is used to represent the string 'yyyy_jday_hhmm' such as 2012_035_1900. The 30th column 'LON360', (longitude ranges from 0-360), is an additional column, not included in the original text file. 'META' (30 column data) is the Meta data as one matrix, 'META_header' (30 column cell) is the header of 'META'. The 30 columns in 'META' are shown in table 2.3.1.

Tabl	e 2.3.1				
1	Matday	Matlab format day fraction for sample time			
2	YR	Year			
3	Jd	Day fraction for sample time			
4	LAT	Latitude			
5	LON	Longitude			
6	SPEED	Ships speed in knots			
7	TEMP1	Aanderaa Temperature sensor 1			
8	TEMP2	Aanderaa Temperature sensor 2			
9	TEMP3	Aanderaa Temperature sensor 3			
10	COND1	Aanderaa Conductivity sensor 1 (conductivity only)			
11	COND2	Aanderaa Conductivity sensor 2			
12	COND3	Aanderaa Conductivity sensor 3			
13	OXY1	Aanderaa Oxygen sensor 1 (concentration only)			
14	OXY2	Aanderaa Oxygen sensor 2			
15	OXY3	Aanderaa Oxygen sensor 3			
16	CO2	Pro CO2 - CO2 concentration in umol/mol			
17	CO2_AZPC	Pro CO2 - CO2 concentration in umol/mol with AZPC blanking			
18	CO2T_CELL	Pro CO2 - optical cell temperature/°C			
19	CO2V_PRESS	Pro CO2 - humidity sensor water vapour pressure/mbar			
20	CO2T_HUMID	Pro CO2 - humidity sensor temperature/°C			
21	CO2PRESS	Pro CO2 - gas stream pressure/mbar			
22	GTD_PRESS	Pro GTD total dissolved gas pressure/mbar			
23	THULL	Hull temperature/ºC			
24	FLOW	Flow in litres/min			
25	V_CO2	Vaisala atmospheric CO2 concentration/ppm			
26	V_CO2CORR	Corrected Vaisala atmospheric CO2 concentration/ppm			
27	V_PRESS	Vaisala atmospheric pressure/mbar (height corrected34m)			
28	V_TEMP	Vaisala atmospheric temperature/°C			
29	V_HUMID	Vaisala atmospheric relative humidity			
30	LON360	Longitude format in 360			

2.3.2 Convert the data to Matlab to get a uniform format for processing

The Matlab program Z2_Get5minCO2MatData_SNOMS_2011.m converts the 30 second ASCII flashcard CO₂ data to Matlab formatted data, 'Cel_xxx_PCO2.mat' (which matches the timestamp of the 5-minute averaged and merged data), with variables saved as 'RAWCO2' (12-column data) and 'RAWCO2_header' (headers for 'RAWCO2'). The 12 columns in 'RAWCO2' are shown in table 2.3.2.

Table	Table 2.3.2					
1	MATDAY	MATDAY Matlab format day fraction (since 1st Jan 0000)				
2	YEAR	Year				
3	JDAY	Day number fraction (JDAY1.5 = 1st Jan 12:00)				
4	XCO2	The mole fraction of the CO2 in µmol mol-1				
5	XCO2_AZPC	The mole fraction of the CO2 in µmol mol-1 with the auto AZPC blanking applied. The Pro-Oceanus sensor comes with the function of Automatic Zero Point Calibration (AZPC) to maintain its accuracy. The frequency of the AZPC is set as 3 hour (00:00, 03:00, 06:00) during Jun. 2007 to Jan. 2008, and then changed to 6 hour (00:00, 06:00, 12:00, 18:00). After each AZPC, the sensor requires 30-45 minute to re-equilibrate with the seawater. The measurement results during this recovery period after AZPC should be discarded. These data were removed according to the time (30 minute after AZPC time).				
6	TCELL	The optical cell temperature in °C				
7	HUMIDITY	The humidity of the equilibrated gas in mbar				
8	THUMIDITY	The temperature of the equilibrated gas in °C				
9	PRESSURE	The gas stream pressure of the equilibrated gas in mbar				
10	ZERO16bit	The 'raw' 16-bit auto zero value (NDIR signal as counts) which remains constant until the next AZPC				
11	SIGNAL16bit	The 'raw' 16-bit CO2 measured value				
12	TIMEelapsed	The time since the previous record (after averaging) in seconds				

Note: only the CO₂ files after 26 April 2011 contain the 16 bit records (column 10 & 11).

2.3.3 Calibration and quality control, match with other underway data

Z3_CO2AZPC_SNOMS_2011.m applies calibration and quality control to the 30 second CO2 data. 7 columns were appended to the 'RAWCO2' and 'RAWCO2_header' and then saved as 'CO2_AZPC' and 'CO2_AZPC_header'. The Quality Controlled CO2 data (20-columns) were then averaged and matched to the time stamp of the merged 5 minute data. The 5 minute CO2 data matching other underway data were saved as 'CO2_AZPC_5min', its header is the same as 'RAWCO2_header'. The 7 columns appended are shown in table 2.3.3.

Table	Table 2.3.3					
13	PCO2	All uncorrected p CO2, p CO2=XCO2* PRESSURE/1013.25.				
14	PCO2_AZPC	Uncorrected pCO2 with AZPC blanking, PCO2_AZPC =XCO2_AZPC * PRESSURE/1013.25.				
15	PCO2_CORR	All temperature-corrected pCO2. In the early versions of ProOceanus sensors without a temperature control module, the temperature of the detector cell was not well stabilized. Lab test shows that the temperature difference between the calibration and the measurement can import bias in the CO2 result. A temperature correction coefficient of 15ppm/degree was found in the lab calibration. The Matlab program finds the temperature during the corresponding AZPC. The pCO2 was corrected using the temperature coefficient and the temperature difference.				
16	PCO2_AZPC_CORR	temperature-corrected pCO2 with AZPC blanking				
17	Ind_AZPC	1=valid CO2 measurement which are fully re-equilibrated with seawater after the zero calibration. Apart from the scheduled AZPC, AZPC will be triggered every time when the sensor is being turned on (when cleaning was carried out or when the system was turned on when leaving a port). Therefore, these time slots after AZPC should also be removed from the dataset. These are indicated by the changes in the column TIMEelapsed, when the sensor was running continuously, the seconds since the previous record should be ~30. When the number is higher, it indicates that the sensor was turned on after being shut down for a certain time.				
18	Ind_Pressure	1=valid pressure measurements within the plus/minus 5% of 1013.25mb				
19	Ind_Diff	1= continuous measurements did not show significant drift, the difference between two consecutive measurements was lower than certain value (10uatm as default).				
20	Ind_auto	Combined QC indicator				

Plots were created for each file.

2.4 Triplicate measurement optimisation

The following method employs three sensors to measure a single parameter. Thus for each 5 minute data point there are nominally 3 examples of each measurement. These 3 examples are formed from the arithmetic mean of all the samples that fall within the 5 minute interval. In the case of conductivity, temperature and oxygen, individual measurements are made every 15 to 30 seconds (9 > N > 21).

The SNOMS instruments are calibrated prior to installation. In the following scenario it is assumed that there has been no systematic drift in any of the sensors between the time

of the calibration and the time of the measurement. The true value of the measurand is obviously an unknown and the three independent measurements are insufficient to produce a statistical estimate of the measurand. Consequently each 5 minute measurement is considered to be an independent estimate of the measurand and should have an equal chance of accurately representing the true value; it also has the same chance of either being higher or lower than the true value. Thus with three independent examples it is more likely that the median example will be adjacent to the true value than all three examples being either higher or lower. However experience can be used to set the limit of acceptability (see Table 2.6.1) which at times excludes data from a sensor and likewise at times individual sensors failed (ceased to out put data). In these cases the median value is taken to be the mean of the output from the two remaining units for the same rationale as for three examples. The term "optimum" has been adopted as representing the median value that has been used.

In addition where one of the 3 sensors is subject to drift or some other change in its apparent calibration its output will only be considered when its value lies between those of the other two sensors. Note in the rarer scenario where there is only one sensor reporting accurately, for example one sensor has died completely and the other is drifting, it is not possible to know which sensor is drifting. Our method can only provide a value that is also drifting albeit at half the rate of the drifting sensor.

2.5 Calculation of salinity and oxygen concentrations

An overview of the procedures that allowed the salinity and oxygen concentrations in the seawater to be determined follows. The Underway Data processing flowchart in Figure 3.0b shows diagrammatically the programs that were used in the data processing routine. Salinity is calculated from the temperature and a nominal pressure value after the best values from the triplicate temperature and conductivity sensors have been determined. This derived salinity value is then corrected by comparison with measurements of the water samples that were collected on the ship and returned to shore to be analysed under stable laboratory conditions.

The optimum oxygen concentration is obtained from triplicate oxygen optode measurements (which assume the water has zero salinity) which are adjusted for the actually salinity when the measurement was made. The oxygen saturation concentration

is calculated from the salinity and the in situ (hull) temperature. The oxygen anomaly is then derived by calculating the difference between the measured oxygen concentration and the calculated oxygen saturation concentration (Hydes et al. 2009) at the same temperature and salinity.

2.6 Calculation of salinity and oxygen: Description

2.6.1 Structures and flags, quality control, match with other underway data

A duplicate set of ASCII files are created in a separate directory; processing is applied to the most recently created files by checking the difference in the directory contents listings in <u>Get_SW_data2010.m</u>. The SNOMS data are then converted from ASCII (.xng) to Matlab (.mat) files using <u>convert_SW_data2010.m</u> according to the format specified in the document R:\Celebes\Flash_card\Pacific Celebes Flash Card processing.doc.

Matlab uses a construct called a "structure" as a way of storing data of differing types under a common name. A structure called "meta_var" that contains metadata for each of the parameters is created; this includes the date of execution, process name, input and output paths, descriptions of the parameters being processed and the method applied. Subsequent programs then append to this structure and in so doing generate a process history.

The temperature, conductivity and oxygen concentration values for each of the input files were plotted out with <u>SW_CTOchk.m</u> which also plotted the differences between the triplicate sensors for conductivity, temperature and oxygen. The plots have been assembled in file <u>R:\Celebes\CTOS plots.pdf</u>. Similarity between channels was initially taken as a criterion for reliability; however this approach has now been superseded by a routine in <u>channel_quality.m</u>. This program creates a structure called FLAG which holds quality flags for each of the measured parameters in fields denoted FLAG.[A].VAR where [A] is a capital letter and VAR is the name of the parameter. Subsequent additional flags can be added to fields with names that increment the capital letter through the alphabet. Flag values are set to true (or 1) for good data and false (or 0) for data that were deemed suspect. FLAG.A.VAR is initialised true for all VAR where VAR is one of the 29 parameters shown in table 2.6.1.

Table fall)	Table 2.6.1 Table of coarse limits of data acceptability (range in which data may be expected to fall)						
	Parameter	Min	max		Parameter	min	max
1	matday	732678	735234	16	CO2	200	1000
2	YR	2006	2012	17	CO2_AZPC	200	1000
3	jd	0	366	18	CO2T_CELL	0	100
4	LAT	-90	90	19	CO2V_PRESS	0	1000
5	LON	-180	180	20	CO2T_HUMID	-10	70
6	SPEED	0	20	21	CO2PRESS	500	1500
7	TEMP1	-5	50	22	GTD_PRESS	500	1500
8	TEMP2	-5	50	23	THULL	-10	50
9	TEMP3	-5	50	24	FLOW	25	35
10	COND1	10	100	25	V_CO2	200	1000
11	COND2	10	100	26	V_CO2CORR	200	1000
12	COND3	10	100	27	V_PRESS	900	1500
13	OXY1	100	500	28	V_TEMP	-10	70
14	OXY2	100	500	29	V_HUMID	5	100
15	OXY3	100	500				

FLAG.B.VAR is then set False for any of the parameters that fall outside the ranges given in the table of coarse limits of data acceptability (Table 2.6.1).

2.6.2 Temperature, Oxygen & Conductivity triplicates

Separate structures were created to manage the triplicate Oxygen, Conductivity and Temperature channels and were named O, C & T, where T.ONE, T.TWO & T.THREE hold the temperature data for instance. A duplicate of these structures was made and these were called fO, fC & fT. These are copies of O, C & T with the exception that those data lying outside the coarse limits in Table 2.6.1 have been set to the absent data value `NaN`, (Not a Number).

The median value (using nanmedian.m) of each of the 3 sets of Oxygen, Conductivity and Temperature values (fO, fC & fT) were derived to determine the optimum value for each parameter. The files that are output from this process have the character `a` appended so an input file with the name Cel_merge_2012_035_1900.mat becomes Cel_merge_2012_035_1900a.mat. Salinity is then calculated within the program celebes_cal_2010.m. It calculates the SNOMS system derived Salinity parameter called SAL from the temperature, conductivity and pressure vectors (TEMP, COND & PRES) which it then adds to the originating file e.g. Cel_merge_2012_035_1900a.mat. It creates the salinity variable by calling two functions $\underline{sw_c3515.m}$ and $\underline{sw_salt.m}$. $\underline{sw_c3515.m}$ returns a conductivity value for S=35, T=15 C [ITPS 68] and P=0 db of 42.914 mmho.cm⁻¹. $\underline{sw_salt.m}$ then applies the UNESCO 1983 polynomial to generate salinity from conductivity. The system pressure, P is deemed constant at 40 db.

2.6.3 Salinity Matchup

In order to constrain the underway salinity measurements bottle samples, which are collected daily and returned ashore in batches, are analysed in laboratory conditions using a Guildline autosalinometer. The resulting salinity data are compared with the underway data from the nearest 5 minute mean in calc_meanSWsal.m. This generates 5 minute mean values of the three salinity channels for comparison with the bottle samples. lt sources the sample times from the Excel file R:\ARCHIVE MCH\calibration\Celebes\SNOMSsamples120616.xls which in turn was assembled from sample times reported by the Chief Engineer of the Pacific Celebes via e-mail attachment at the end of each month (these can be found in R:\Celebes\120528 djh SNOMS lists\sample lists\SNOMS raw monthly lists). The file also recorded the year the sample was collected. A Matlab serial date number is allocated to each entry and the means were calculated based on these.

2.6.4 Salinity Calibration

Conductivity, temperature and pressure were combined to generate values of salinity, S_{CTD} using the UNESCO 1983 polynomial. S_{CTD} = function (conductivity, temperature, pressure) units: dimensionless. However a correction needs to be applied to these calculated salinity values as the conductivity measured by the sensors (in fact the inductive field around the head of the sensor) is affected to a small extent by the position of the sensor in the lid of the SNOMS tank. To correct for this and any drift in the sensors, the data from salinity samples collected by the ship's crew are used. Calibration of the SWIRE system derived Salinity is performed in the program calSWsal 2010.m. The SNOMS Salinity vector (SAL) is constrained using bottle sample data that are collected daily during the period of the file (see Table 2.2 for a list of file durations). The results from the laboratory analysed daily bottle samples (which have been stored in the structure 'salcal' and we refer to here as 'S_{BOT}') and the contemporaneous SNOMS salinity (which have been stored in the structure 'ev' and we refer to here as 'S_{CTD}') are read by calSWsal_2010.m. Here, two linear regressions are performed. Regression (1) is independent of time; all the samples taken during the extent of the file are regressed against their corresponding underway measurements; S_{BOT} is taken as the abscissa and S_{CTD} the ordinate. Regression (2) is time dependent; the ratio of the salinities (S_{BOT} / S_{CTD}) obtained at each sample time is calculated, these ratios are then linearly regressed against time. The preferred method is to use the time dependent method of calibrating the salinity as it can compensate for drift that the sensors may undergo during the measurement period. The ability to use this method is dependent on there a) being sufficient samples collected and b) the samples are evenly distribution across the whole period of sampling.

The correction factor applied to the salinity vector, 'SAL' to derive the time dependent bottle sample corrected salinity 'BESTSAL' is achieved through applying a linear least squares regression called robustfit.m; this uses an iteratively reweighted method with a bi-square weighting function with a default tuning constant of 4.685 which reduces the influence of outliers on the regression results. The robustfit.m function estimates the variance-covariance matrix of the coefficient estimates producing Standard Errors and correlations derived from this estimate. The corrected salinity, BESTSAL is obtained using the following equation: BESTSAL = SAL*[(matday*Correction slope) + (Correction intercept)] where the corrections are the time dependent values. The time independent correction values are also included. If this method were used then the corrections are the time independent values.

Plots of the regressions are generated; the names of the output files take the form 'salregCel_merge_YYYY_DDD_HHMMa' and can be found in the following directory <u>R:\ARCHIVE_MCH\SWIRES\data_download\all_5min\plots</u>. These have been compiled into the document <u>R:\\Celebes\ SNOMS salinity regressions.pdf</u> these plots show from top to bottom:

- 1. The regression of the S_{BOT} against S_{CTD} and the time independent correction equation.
- 2. The time dependent ratio of (S_{BOT} / S_{CTD}) plotted against time. The time dependent correction ratio is also shown.
- 3. The relationship between S_{BOT} , S_{CTD} and BESTSAL with time.

An example of such a file is shown in figure 2.6.4. A full set of the salinity calibration coefficients used to correct the salinity is given in table 2.6.4.

For the duration of the file Cel_merge_2011_116_1500a no salinity samples were available. If there were no change in the sensors between consecutive files before and

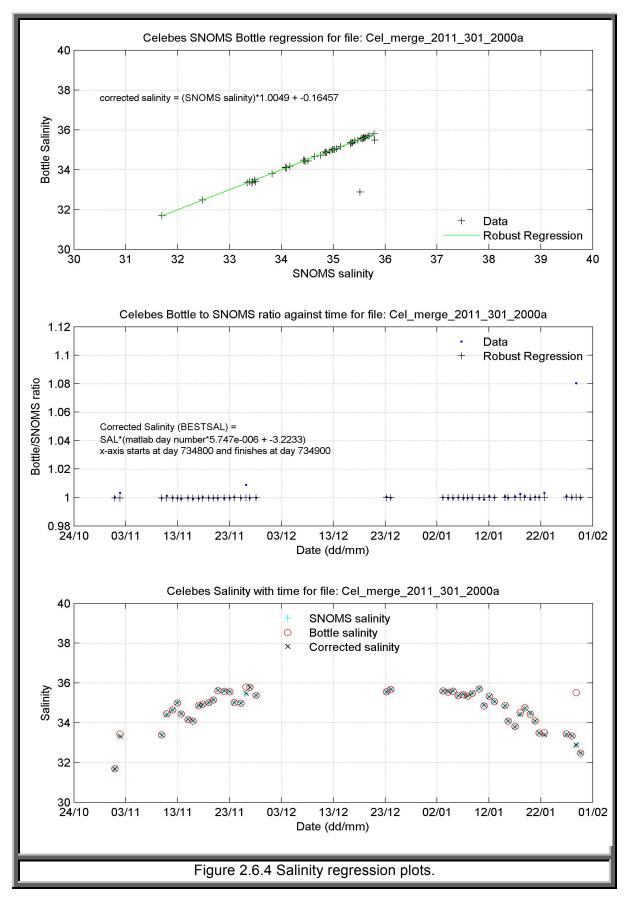
after then it may have been possible to apply offsets based on these, however this was not the case. All the sensors were changed in Vancouver prior to sailing. The file ended in Crofton. Of the 3 conductivity cells, #1008 was drifting and then stopped and so was replaced by #338, #1357 died shortly after the port call on day 219 leaving #1014 only. Although the channel 2 conductivity showed some erratic behaviour during this file, the remaining 2 channels agreed to within 0.08 mmho.cm⁻¹ which is equivalent to a salinity change of 0.08; twice the estimated precision of the measurements. The accuracy however can only be estimated from a) the historical accuracy of the system. b) the accuracy of the subsequent file, 2011_206_1800, for which one of the conductivity sensors, #1014 remained. The historical accuracy over the two year period 2009- 2010 suggests (DS), the calibrated salinity, reads lower than the un-calibrated (optimum) salinity by between 0.02 and 0.08 psu. The subsequent file's corrected salinity is less reliable with only 7 data points indicating DS = 0.03. The extent of the variation between any 2 of the sensors is 0.05. Taking the previous points into consideration the best estimate for the salinity correction is $DS = 0.04 \pm 0.06$. For consistency in Table 2.6.4 this is shown as a slope of 0.9989.

In the subsequent file, 2011_206_1800, salinity samples were only available from 15^{th} to the 22nd September, one week; a little after half way through the file. A time dependent correction based on such a short period results in extrapolation that can produce errors in the resulting salinity – in this case at both ends of the file from +0.5 to -0.23 psu. Reference to the relative differences between any pair of conductivities (R:\Celebes\CTOS plots.pdf) shows that they vary by less than 0.05mmhocm⁻¹ throughout the file, similarly relative temperatures vary by less than 0.005 °C. The maximum range of the error in the salinity attributable to these independent errors in this case is 0.055 at lower temperatures and salinities (t = 10 °C, s = 31.9) rising to 0.059 in equatorial waters (t = 29 °C, s = 36.8).

For the majority of the files in Table 2.6.4 the corrected salinity has been obtained from the time dependent correction: Corrected Salinity (BESTSAL) = (slope * matday) + intercept. Those that have been marked with an asterisk have had the time independent correction applied instead:

Corrected Salinity (BESTSAL) = (slope * (SNOMS salinity)) + intercept.

Table 2.6.4				
File	File start	File end	slope	intercept
Cel_merge_2007_161_0000	733203.00	733296.93	-3.9872e-5	30.2304
Cel_merge_2007_255_0000	733297.00	733434.50	-2.5806e-5	19.9158
Cel_merge_2008_029_0000	733436.00	733571.57	-2.0208e-5	15.8112
Cel_merge_2008_164_1300	733571.58	733706.73	No salinit	y data
Cel_merge_2008_301_1400	733708.62	733850.59	+6.5738e-7	0.5169
Cel_merge_2009_079_1700	733852.73	734003.60	-2.9101e-6	3.1346
Cel_merge_2009_230_1400	734003.61	734103.06	-4.4795e-7	1.3281
Cel_merge_2009_330_0100	734103.07	734217.84	-7.0786e-6	6.1956
Cel_merge_2010_079_2000	734217.85	734311.80	+1.0294e-5	-6.5598
Cel_merge_2010_173_1900	734311.81	734408.73	+7.1147e-7	0.47554
Cel_merge_2010_270_1700	734408.74	734516.68	-3.9779e-6	3.9194
Cel_merge_2011_013_1900	734516.81	734619.66	No salini	ty data
Cel_merge_2011_116_1500	734619.66	734709.75	+0.9989	0
Cel_merge_2011_206_1800*	734709.76	734804.84	+1.0081	-0.31375
Cel_merge_2011_301_2000	734804.84	734903.79	+5.747e-6	-3.2233
Cel_merge_2012_035_1900	734903.80	734952.89	-2.9798e-5	22.899



2.6.5 Oxygen Calculation

The SNOMS oxygen vector (OXY) is derived from measurements that are made from Aanderaa oxygen optodes and as such need to be corrected for the effects of salinity and temperature; this is done using the function optode_corrSW2010.m which is run as part of calSWOXY_2010.m . The calibration of optodes after October 2008 (matday 733708.6) is made prior to deployment by using an aerated water bath and a sodium sulphite solution (10 grams per litre) to give 100% and 0% saturation. Prior to this the optode channel calibrations were derived from spring 2007 when the SWIRE-SNOMS system was mounted on the Pride of Bilbao and the sensor output was calibrated against Winkler titrated bottle samples. The calibration factors from the 2007 Pride of Bilbao Winkler titration calibrations are shown in table 2.6.4a.

Table 2.6.4a						
Channel	slope	Intercept				
1	1	0				
2	1.094	1.28				
3	1.1186	-2.836				

The variable (ch) holds details of which channel combinations have been used for which files. Table 2.6.4b lists the coefficients that have been applied to OXY_CORR to derive the calibrated oxygen concentration values that are stored in OXY_CAL, these are measured in micromoles per litre (μ mol.I⁻¹). The following equation was used: OXY_CAL = slope*OXY_CORR + intercept;

Table 2.6.4b						
File name	slope	intercept	Channel number			
Cel_merge_2007_161_0000a	1.094	1.28	2			
Cel_merge_2007_255_0000a	1.094	1.28	2			
Cel_merge_2008_029_0000a	1.1186	-2.836	3			
Cel_merge_2008_164_1300a	1.1186	-2.836	3			
subsequent files	1	0	optimum			

The variables written to file by calSWOXY_2010.m are;

- 1. OXY_CORR: Aanderaa optode output (µmol.l⁻¹) corrected for salinity and temperature.
- O2_SAT: The saturation oxygen concentration, [O2]* (µmol.l⁻¹), at the temperature and salinity of the sample water. This is calculated using the June 2004 operating

manual Oxygen Optode 3830 Aanderaa reference Garcia and Gordon (Limnology and Oceanography, 1992).

 OXY_CAL: the salinity and temperature corrected optode output that has had calibration factors applied. For files after Cel_merge_2008_164_1300a, OXY_CAL = OXY_CORR.

2.6.6 Oxygen Quality Control

Manufacturers specifications for the accuracy of the optodes that were used on board the *Pacific Celebes* are given as 8 µmol/l or 5% whichever is the greater (Aanderaa, 2005) – however based on the experience gained from using optodes on the Pride of Bilbao during 2005 and 2006, optode measurements were found to be within 2% of contemporaneously sampled Winkler titration values, furthermore the optodes maintained good stability with no evidence of instrumental drift during the course of a year. For coarse oxygen Quality Control the percentage saturation should fall within 10% of full saturation 90% to 110%. Data outside this range are flagged as suspect. In addition to the coarse QC the optimum oxygen value is compared to its nearest neighbour; if the two measurements lie within double the individual measurement tolerance of 2% of each other the oxygen data are considered to be good, if the closest measurement falls outside this range then the oxygen data are considered suspect. This quality control is performed in the file <u>calSW_qc2010.m</u>. The percentage data return over each file using this approach is provided in the variable, PCNTOXY. The procedure is further summarised as a table in Section 4.1.

2.7 Current and Further work

This document provides coverage of the bespoke data processing stages that have been and are being developed to obtain seawater measurements along the track of the *MV Pacific Celebes*. These include but are not limited to measurements of temperature, salinity and the concentrations of oxygen and carbon dioxide that are both discretely and continuously sampled. Whilst a subset of these measurements namely; temperature (CTDTMP), salinity (SALNTY), oxygen concentration (OXYGEN), total carbon (TCARBN) and alkalinity (ALKALI) have been archived at CDIAC, (Hydes et al., 2010) together with their associated metadata. These are point samples both associated with and derived from the discrete bottle samples and range from the start date: 2007/06/11 to the end date: 2010/06/07. SNOMS operations aboard the *Celebes* continued until spring 2012 requiring that the samples collected between 2010/06/08 and 2012/03/24 to be analysed. During this period there have been improvements in the approaches that will be used to quality control the underway measurements. These improvements will necessarily be implemented prior to the underway data set being archived at BODC and will promote a methodology consistent with the wider community. They will also promote a drive towards a more automated processing approach that will ultimately reduce the level of effort that is applied. The following assessments are required before this can be achieved.

- 1. Assessment of current best practice used for the quality control of autonomous sensor suites.
- 2. Measurements that are made with the hull thermometer, T_{HULL} are the closest to the in-situ water temperature. This measurement was provided by a Sea-Bird SBE 48 Hull temperature sensor, with specifications that include an initial accuracy of 0.002 °C, a typical stability per month of 0.0002 °C and a resolution of 0.0001 °C. Details of the method of temperature quality control are to be added in Version 2 of this document which should evaluate the accuracy of the Hull temperature measurement against independent sources such as the triplicate temperature measurements and satellite.
- Identification of the accuracy of the triplicate temperature, salinity and oxygen measurements reporting on the sensors' relative stabilities and relative drift after their initial calibration. In the case of salinity using the comparison against the laboratory measured samples
- 4. Assessment of all of the independent pressure measurements including those made by the GTD-Pro, and CO2-Pro sensors.
- 5. Further value could be added to the 'meta_var' method in section 2.6.1 if the individual sensor details were added to the initial merged ASCII file; as an example the sensor serial numbers and corresponding channel numbers would provide traceability to the sensor calibration information.

2.8 References

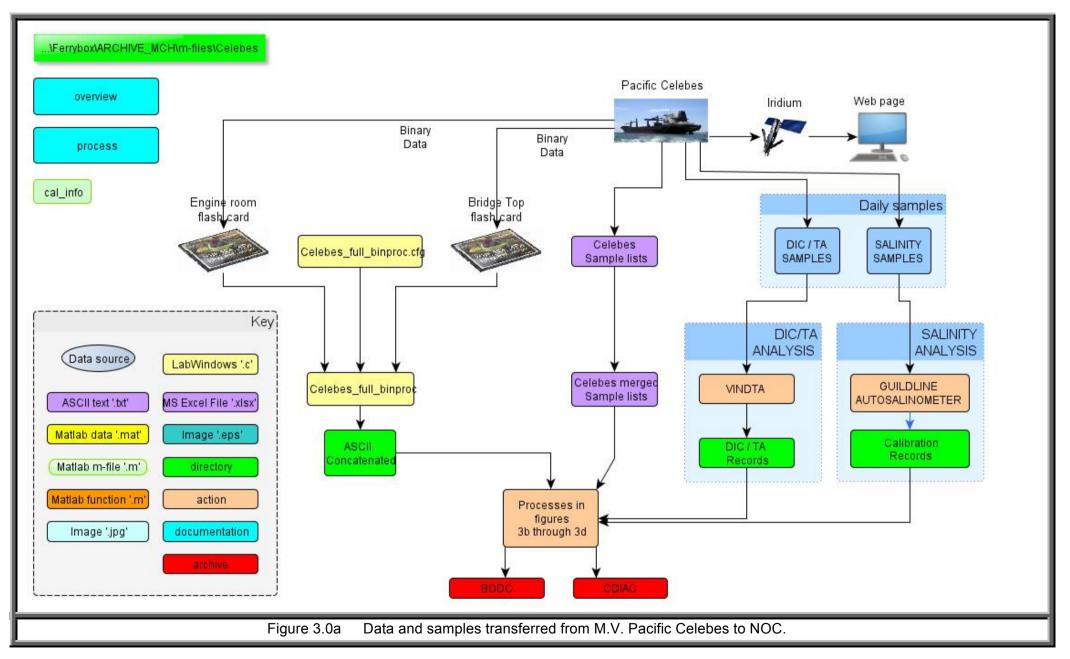
Aanderaa. (June 2004) Operating manual Oxygen Optode 3830.

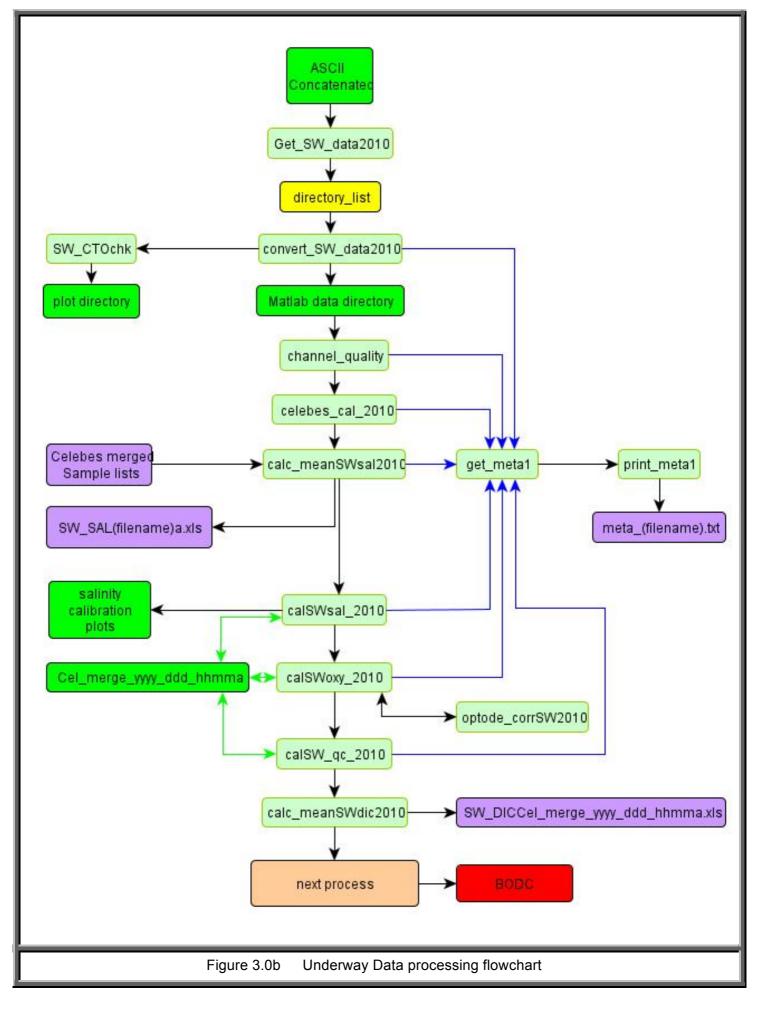
Aanderaa. (2005) Aanderaa OptodeDataSheet

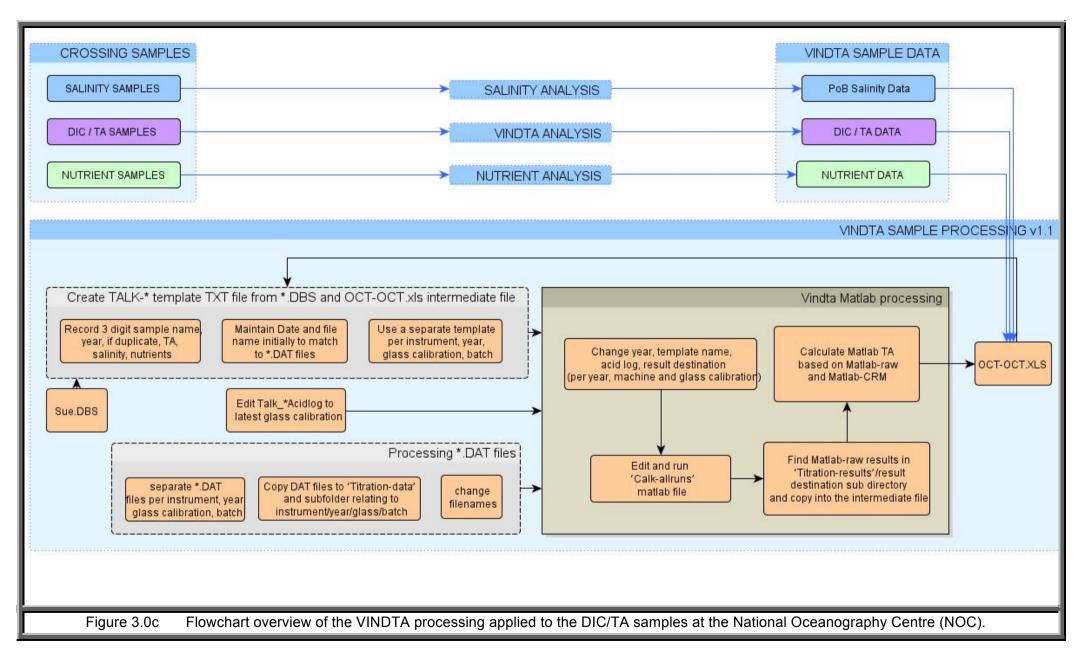
Oxygen_Optode_3830_3930_3975_D33.pdf 4pp www.aanderaa.com/AanderaaBergen (2005)

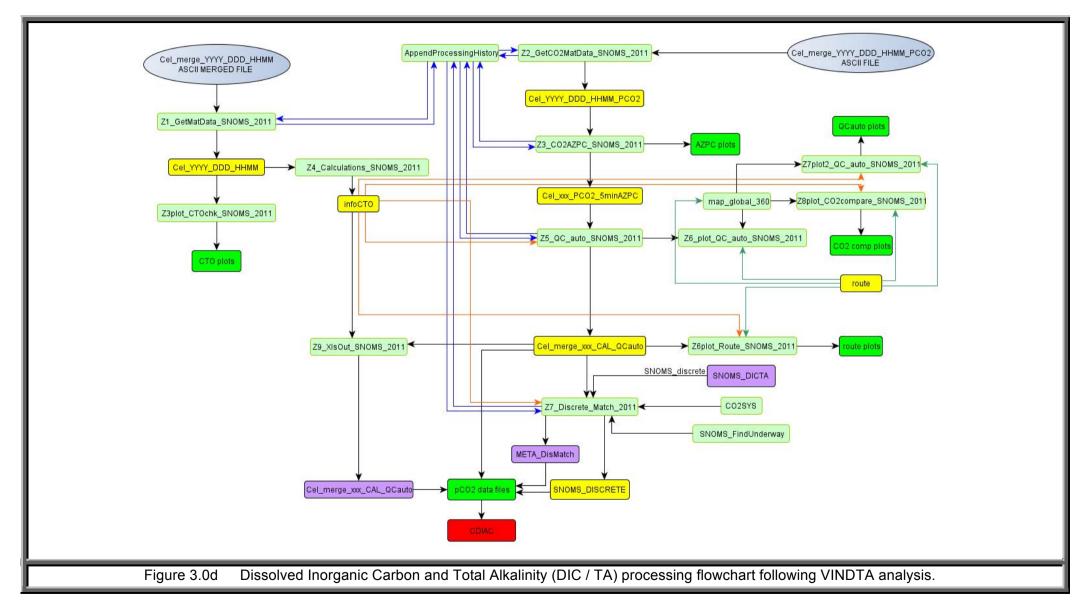
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 http://cdiac.ornl.gov/ftp/oceans/VOS_Pacific_Celebes_line/. Carbon Dioxide Information Analysis Center, Oak Ridge National Laboratory, US Department of Energy, Oak Ridge, Tennessee. (doi: 10.3334/CDIAC/otg.VOS_PC_2007-2010)

3.0 Flowcharts









4.0 Supplementary Information

- 4.1 Glossary
- BODC British Oceanographic Data Centre
- CDIAC the Carbon Dioxide Information and Advisory Center
- Matlab a matrix based programming environment.
- m-file a program or script written in Matlab.
- Optode a submersible sensor that measures the concentration of dissolved gas in a liquid. Here they are used to measure oxygen concentration.

Terms below that have been written in uppercase refer to variables that have been created in the Matlab environment.

- BESTSAL salinity data that has been derived from the optimum temperature and optimum conductivity and has been compared to calibrated bottle samples to produce the best estimate of salinity. This is a ratio and so has no units, although practical salinity units (psu) are sometimes quoted.
- GTD_PRESS Total Dissolved gas pressure or fugacity.
- OXY Aanderaa optode output (µmol.l⁻¹)
- OXY_CORR Aanderaa optode output (μ mol.I⁻¹) corrected for salinity and temperature.
- O2_SAT The saturation oxygen concentration, [O2]* (µmol.l⁻¹) calculated from in-situ temperature and salinity
- PCNT_OXY The percentage oxygen saturation

4.2 Oxygen Process Overview

ID	Output	Input	Process	Description
1	S _{CTD}	C, T, D	sw_salt.m	Conductivity, temperature and pressure are combined to generate salinity from conductivity ratio, based on UNESCO 1983 polynomial
2	S _{cal}	S _{CTD}	Salinity calibration	Salinity is calibrated against bottle samples measured with an Autosalinometer.
3	O _{sat}	T _{in_situ} , S _{cal}	Garcia & Gordon 1992	<i>In situ</i> temperature and salinity combine to give oxygen equilibrium saturation concentration equivalent.
4	O _{conc}	O _{opt} , T _{optode} , S _{cal}	Optode manual June 2004 p30	The Optode temperature and the salinity are used to correct the Optode Oxygen concentration for the effects of salinity.
6	O _{anom}	O_{conc}, O_{sat}	O _{anom} = O _{corr} - O _{sat} .	The difference between the measured concentration and the saturation concentration at equivalent temperature and salinity gives the oxygen anomaly.

4.3 Pacific Celebes Flash Card Processing File Formats

The Lab Windows program Celebes_full_binproc.c processes the binary files recorded on CompactFlash cards in the engine room and on the bridge top. The program assumes that the contents of the flash cards have been copied into ROOT\EngineRm and ROOT\Met_GPS directories, where ROOT is defined in the configuration file Celebes_full_binproc.cfg. The configuration file also defines start and end times for the merged file, the sample averaging interval and the AZPC blanking time for the ProOceanus CO2 sensor.

```
;************************ Celebes full binproc.cfg *********************** 30 May 12 **
; parameter 1 = drive:path\ for root dir of binary files to process
D:\Projects\Celebes\SNOMS Halifax\30 May12\
; parameter 2 = Produce merged, averaged file? (Y or N)
YES
; parameter 3 = Use start/end times below? (Y or N) (if NO, process all data)
YES
; parameter 4 = Sample averaging time for merged file in seconds
300.0
; parameter 5 = AZPC blanking time in minutes
30.0
; parameter 6 = start year (only used if param3 = YES)
2012
; parameter 7 = start dayfrac
136.8
; parameter 8 = end year
2013
; parameter 9 = end dayfrac
100.0
```

The program first produces concatenated text files for each sensor, e.g. all_CO2.txt. All of these concatenated files begin with 3 fields defining the sampling instant for that data record:

- 1. Matlab format day fraction (since 1 Jan 0000)
- 2. Year
- 3. Day fraction (since start of year, such that 12:00 on 1st January is 1.5000)

These files contain all the data present on the flash cards regardless of the start and end times specified in the configuration file. These concatenated files are then truncated (if necessary), averaged and merged according to the parameters defined in Celebes_full_binproc.cfg. The averaging is performed by setting a sample time at the nearest exact hour and defining a window centred on this time and having the width of the sample interval. Any sensor records that fall within this window are averaged. If no sensor records fall within this window, the field is set to NaN. The sample time is then incremented by the sample interval and new average values are computed. All sensor data and the ship's speed are averaged over the sample intervals. The latitude and longitude are not averaged. The time stamp at the beginning of each merged record is the sample time (the centre of the averaging window), and the latitude and longitude are the closest position fix to that sample time. The merged files have 29 fields as follows:

- 1. Matlab format day fraction for sample time
- 2. Year
- 3. Day fraction for sample time
- 4. Latitude
- 5. Longitude
- 6. Ship's speed in knots
- 7. Aanderaa Temperature sensor 1 in °C
- 8. Aanderaa Temperature sensor 2
- 9. Aanderaa Temperature sensor 3
- 10. Aanderaa Conductivity sensor 1 (conductivity only) in mS/cm
- 11. Aanderaa Conductivity sensor 2
- 12. Aanderaa Conductivity sensor 3
- 13. Aanderaa Oxygen sensor 1 (concentration only) in µM
- 14. Aanderaa Oxygen sensor 2
- 15. Aanderaa Oxygen sensor 3
- 16. Pro CO2 The CO2 concentration in mol mol⁻¹
- 17. Pro CO2 The CO2 concentration in mol mol⁻¹ with AZPC blanking
- 18. Pro CO2 The optical cell temperature in °C
- 19. Pro CO2 The humidity sensor water vapour pressure in mbar
- 20. Pro CO2 The humidity sensor temperature in °C
- 21. Pro CO2 The gas stream pressure in mbar
- 22. Pro GTD total dissolved gas pressure in mbar
- 23. Hull temperature in °C
- 24. Flow in litres/min
- 25. Vaisala atmospheric CO2 concentration in ppm
- 26. Corrected Vaisala atmospheric CO2 concentration in ppm
- 27. Vaisala atmospheric pressure in mbar (corrected for bridge height of 34m)
- 28. Vaisala atmospheric temperature in °C
- 29. Vaisala atmospheric relative humidity

4.4 Salinity and CO2 water sample times

When the vessel is at sea the engineers collect two seawater samples every day. The exact times of these samples are recorded in a simple log sheet such as the one below.

Date	Salinity Time	CO2 Time	COMMENTS
01/01/2010	365.9234	365.9247	UNIT ON (DEPT BRISBANE) 22:06:15
			UNIT OFF(F.W.G. OFF) 03:55:05 UNIT ON 04:24:25
02/01/2010	1.8816	1.8831	
03/01/2010	2.9215	2.923	UNIT OFF ARR MELBOURNE10:27 03/01/2010
04/01/2010	OFF	OFF	
05/01/2010	OFF	OFF	
06/01/2010	OFF	OFF	
07/01/2010	OFF	OFF	
08/01/2010	OFF	OFF	
09/01/2010	9.0927	9.0944	UNIT ON DEP MELBOURNE 18:39:37; 08/01/2010
10/01/2010	9.8905	9.8924	UNIT OFF ARR KEMBLA 09:25:03
11/01/2010	OFF	OFF	
12/01/2010	OFF	OFF	
23/01/2010	OFF	OFF	
24/01/2010			UNIT ON 23 JAN 2010, 21:08:07, DEP PORT KEMBLA
24/01/2010	OFF	OFF	UNIT OFF 22:09:35
25/01/2010	24.3216	24.3232	UNIT ON 07:29:10
25/01/2010	24.8772	24.8792	UNIT OFF 21:09:40, 25/01/10; UNIT ON 06:32:35, 26/01/10
26/01/2010	26.1905	26.1921	
27/01/2010	27.0488	27.0506	
28/01/2010	28.1236	28.1253	UNIT OFF10:09:00; 28/01/2010 ARRIVAL TAURANGA

M.V. PACIFIC CELEBES SAMPLE LOG SHEET

Every 3-4 months a batch of water samples is shipped back to NOCS to be analysed. When the salinity measurements have been made a modified spreadsheet is created with the measured salinity values added in a fourth column as shown below.

01/01/2008	1.658	1.6592	36.1934943
02/01/2008	2.5478	2.5501	32.9686931
08/01/2008	8.5968	8.5979	32.8989077
09/01/2008	9.5592	9.5685	32.4542217
10/01/2008	10.5049	10.5072	32.6137658
14/01/2008	14.5698	14.5714	32.5760092
15/01/2008	15.4651	15.4662	32.1735594
16/01/2008	16.4682		36.3942272
17/01/2008	17.4653		34.6574397
18/01/2008	18.4628		36.487727
19/01/2008	19.4245		36.3265041
20/01/2008	20.4255		36.4401798
21/01/2008	21.3806		36.4322563

This spreadsheet is then saved as a .csv file, so that the above data is stored as follows:-

1/1/08,1.658,1.6592,36.19349426 2/1/08,2.5478,2.5501,32.96869306 8/1/08,8.5968,8.5979,32.89890774 9/1/08,9.5592,9.5685,32.45422167 10/1/08,10.5049,10.5072,32.61376577 14/1/2008,14.5698,14.5714,32.57600917 15/1/2008,15.4651,15.4662,32.17355936 16/1/08,16.4682,,36.39422719 17/1/2008,17.4653,,34.65743965 18/1/2008,18.4628,,36.487727 19/1/2008,19.4245,,36.32650405 20/1/2008,20.4255,,36.4401798 21/1/2008,21.3806,,36.43225626 A LabWindows program called Celebes_samp_times.c can then be used to find data values for each sensor corresponding to the times that water samples were taken by the ship's engineers. The program reads the csv file and compares the sample times with those in the merged, averaged files to find the closest match. Two output files are produced, one for the salinity samples and one for the CO2 samples. Both these files contain the same 29 fields as the merged, averaged files, but these 29 are preceded by 5 new fields as follows:-

- 1. Matlab format day fraction of water sample time
- 2. Year of water sample time
- 3. Day number fraction of water sample time
- 4. Salinity measurement of the water sample
- 5. Time difference in seconds between the water sample time and the sensor data record

4.5 Individual sensor Flash Card concatenated file formats

4.5.7 GPS files

4.5.8 e.g. all_GPS.txt. These contain 9, space-delimited fields:-

- 1) Matlab format day fraction (since 1 Jan 0000)
- 2) Year
- 3) Day number fraction (since start of year)
- 4) The latitude for this position fix
- 5) The longitude for this position fix
- 6) The ship's speed over the ground in knots
- 7) The number of satellites used to calculate the fix
- 8) The estimated precision of the fix
- 9) The time in seconds since the previous record

e.g.734410.786458 2010 272.786458 47.945927 -125.257538 13.8 9 0.92 5.00

4.5.9 CO2 files after 26 April 2011

e.g. all_PCO2.txt. These contain 12, space-delimited fields:-

- 1) Matlab format day fraction (since 1 Jan 0000)
- 2) Year
- 3) Day number fraction (since start of year)
- 4) The CO2 concentration in mol mol⁻¹
- 5) The CO2 concentration in mol mol⁻¹ with AZPC blanking applied
- 6) The optical cell temperature in °C
- 7) The humidity sensor reading in mb(?)
- 8) The humidity sensor temperature in °C
- 9) The gas stream pressure in mbar
- 10) The 'raw' 16-bit auto zero value which remains constant until the next AZPC
- 11) The 'raw' 16-bit CO2 value

12) The time in seconds since the previous record (after averaging)

e.g. (showing start of AZPC)

734620.259924 2011 117.259924 488.89 488.89 55.0 21.3 34.9 1012 51678 47832 30.43

734620.260277 2011 117.260277 485.85 485.85 55.0 21.3 34.9 1012 51678 47851 30.48

734620.260685 2011 117.260685 290.26 NaN 55.0 22.3 34.9 1019 51947 49408 35.26 734620.261037 2011 117.261037 380.59 NaN 55.0 22.1 34.9 1018 51947 48760 30.43

4.5.10 GTD files

e.g. all_GTD.txt. These contain 5, space-delimited fields:-

- 1) Matlab format day fraction (since 1 Jan 0000)
- 2) Year
- 3) Day number fraction (since start of year)
- 4) The total dissolved gas pressure in mbar
- 5) The time in seconds since the previous record (after averaging)

e.g. 734620.649551 2011 117.649551 1017.8653 29.99

4.5.11 AT1, AT2 and AT3 files from Aanderaa 4050 temperature sensors

e.g. all_AT2.txt. These contain 6, space-delimited fields:-

- 1) Matlab format day fraction (since 1 Jan 0000)
- 2) Year
- 3) Day number fraction (since start of year)
- 4) The water temperature in °C
- 5) The binary (raw) temperature value
- 6) The time in seconds since the previous record

e.g. 734620.650988 2011 117.650988 20.2659 9214794 15.00

4.5.12 AC1, AC2 and AC3 files from Aanderaa 3919 conductivity sensors

e.g. all_AC1.txt. These contain 14, space-delimited fields:-

- 1) Matlab format day fraction (since 1 Jan 0000)
- 2) Year
- 3) Day number fraction (since start of year)
- 4) The conductivity in mS/cm
- 5) The water temperature in °C
- 6) The calculated salinity in PSU
- 7) The calculated density in Kg/m^3
- 8) The calculated sound speed in m/s
- 9) The raw "Cond" value
- 10) The raw "CompVal" value
- 11) The raw "CompAD" value
- 12) The raw "ZAmp" value
- 13) The raw "RawTemp" value
- 14) The time in seconds since the previous record

e.g. 734417.905927 2010 279.905927 44.555 18.419 33.513 1024.031 1515.32 9.6578

36007 36281 3239.57 1793.86 30.04

- 4.5.13 AO1, AO2 and AO3 files from Aanderaa 3835 oxygen sensors
 - e.g. all_AO1.txt. These contain 14, space-delimited fields:-
 - 1) Matlab format day fraction (since 1 Jan 0000)
 - 2) Year
 - 3) Day number fraction (since start of year)
 - 4) The oxygen concentration in μM
 - 5) The water temperature in °C
 - 6) The oxygen saturation as a percentage
 - 7) The raw "DPhase" value
 - 8) The raw "BPhase" value
 - 9) The raw "RPhase" value
 - 10) The raw "BAmp" value
 - 11) The raw "BPot" value
 - 12) The raw "RAmp" value
 - 13) The raw "RawTemp" value
 - 14) The time in seconds since the previous record

e.g. 734415.158477 2010 277.158477 328.99 16.52 108.03 33.56 30.13 0.00 241.69 6.00

0.00 339.31 30.05

4.5.14 HUL files from Seabird SBE48 hull temperature sensor

e.g. all_HULL.txt. These contain 5, space-delimited fields:-

- 1) Matlab format day fraction (since 1 Jan 0000)
- 2) Year
- 3) Day number fraction (since start of year)
- 4) The hull temperature in °C
- 5) The time in seconds since the previous record
- e.g. 734514.153999 2011 11.153999 8.0266 30.05

4.5.15 FLOW files from ABB flow meter sensor

- e.g. all_flow.txt. These contain 5, space-delimited fields:-
- 1) Matlab format day fraction (since 1 Jan 0000)
- 2) Year
- 3) Day number fraction (since start of year)
- 4) The flow through the tank in litres/min
- 5) The time in seconds since the previous record
- e.g. 734412.402604 2010 274.402604 27.39 59.98

4.5.16 PIC_temp files from PIC-controlled temperature sensors in engine room

electronics box or Met/GPS electronics box

e.g. all_PIC_temp.txt or all_Met_PIC_temp.txt. These contain 7, space-delimited fields:-

- 1) Matlab format day fraction (since 1 Jan 0000)
- 2) Year
- 3) Day number fraction (since start of year)
- 4) Box temperature sensor 1 in °C
- 5) Box temperature sensor 2 in °C
- 6) Box temperature sensor 3 in °C
- 7) The time in seconds since the previous record

e.g. 734408.747182 2010 270.747182 27.31 21.43 27.25 30.05

4.5.17 Wind files from PIC-controlled Vector wind sensors

e.g. all_Met_PIC_Wind.txt. These contain 6, space-delimited fields:-

- 1) Matlab format day fraction (since 1 Jan 0000)
- 2) Year
- 3) Day number fraction (since start of year)
- 4) The apparent wind speed in m/s
- 5) The apparent wind direction, where 000 is coming directly from the ship's bow.
- 6) The time in seconds since the previous record

e.g. 734411.523999 2010 273.523999 391.13 18.9 29.94

4.5.18 VCO2 files from Vaisala atmospheric CO2 sensor

e.g. all_VCO2.txt. These contain 6, space-delimited fields:-

- 1) Matlab format day fraction (since 1 Jan 0000)
- 2) Year
- 3) Day number fraction (since start of year)
- 4) The atmospheric CO2 concentration in ppm
- 5) The sensor temperature in °C
- 6) The time in seconds since the previous record
- e.g. 734411.523999 2010 273.523999 391.13 18.9 29.94

4.5.19 PTU files from Vaisala atmospheric pressure/temperature sensor

e.g. all_PTU.txt. These contain 7, space-delimited fields:-

- 1) Matlab format day fraction (since 1 Jan 0000)
- 2) Year
- 3) Day number fraction (since start of year)
- 4) The air pressure in mbar
- 5) The air temperature in °C
- 6) The air relative humidity as a percentage
- 7) The time in seconds since the previous record

e.g. 734413.230585 2010 275.230585 1012.94 14.31 86.76 29.98

4.6 Pacific Celebes Iridium Telemetry ASCII file types and formats

Binary data files were received via Iridium and processed into ASCII files by a UNIX program called Celebes_proc.c that produces concatenated files for each sensor, e.g. **\ascdata\Celebes\concat\Cel_concat_2011_119.gtd.** Each sensor has its own extension and these are list below. The date contained in the filename i.e. Day 119, 2011 in the above example, is the date the voyage (or circumnavigation) is deemed to have begun. File extensions for concatenated telemetry files:-

- .GP1 GPS data from the engine room box (not used at present)
- .GP2 GPS data from the Met/GPS PC
- .GP3 GPS data from the Iridium PC (not used at present)
- .CO2 Data from Pro-Oceanus CO2 sensor before 26 April 2011
- .CO3 Data from Pro-Oceanus CO2 sensor after 26 April 2011
- .GTD Data from Pro-Oceanus GTD sensor
- .AT1 Data from Aanderaa 4050 temperature sensor number 1
- .AT2 Data from Aanderaa 4050 temperature sensor number 2
- .AT3 Data from Aanderaa 4050 temperature sensor number 3
- .AC1 Data from Aanderaa 3919 conductivity sensor number 1
- .AC2 Data from Aanderaa 3919 conductivity sensor number 2
- .AC3 Data from Aanderaa 3919 conductivity sensor number 3
- .AO1 Data from Aanderaa 3835 oxygen optode sensor number 1
- .AO2 Data from Aanderaa 3835 oxygen optode sensor number 2
- .AO3 Data from Aanderaa 3835 oxygen optode sensor number 3
- .HUL Data from Seabird SBE48 hull temperature sensor
- .FL1 Data from ABB water flow meter sensor
- .PTU Data from Vaisala PTU air temperature/pressure/humidity sensor
- .VCO Data from Vaisala GMP343 atmospheric CO2 sensor
- .MWV Data from Vector wind speed and direction sensors
- .TM1 Data from temperature sensors in the engine room electronics box
- .TM2 Data from temperature sensors in the bridge top electronics box
- .ST1 Status information from the engine room computer
- .ST2 Status information from the Met/GPS computer
- .ST3 Status information from the Iridium telemetry computer
- .IRD Performance data from the Iridium modem before 26 April 2011
- .IR2 Performance data from the Iridium modem after 26 April 2011
- .SMS SMS message acknowledgement

4.7 Detailed formats

4.7.20 GPS files e.g. Cel_concat_2011_119.gp2

These can come from any one of the three PCs in the system, though normally PC2 is the only one programmed to send them (gp2). These contain 6, space-delimited fields:-

- 1) The year
- 2) The day number time stamp for this fix
- 3) The latitude for this position fix
- 4) The longitude for this position fix
- 5) The ship's speed over the ground in knots
- 6) The time in seconds since the previous record
- e.g. 2011 124.248148 34.058922 -120.984528 14.0 300.0
- 4.7.21 ProOceanus CO2 sensor files before 26 April 2011
- e.g. Cel_concat_2010_271.co2. These contain 8, space-delimited fields:-
 - 1) The year
 - 2) The day number time stamp for this sample
 - 3) The CO2 concentration in mol mol⁻¹
 - 4) The optical cell temperature in °C
 - 5) The humidity sensor reading in mb
 - 6) The humidity sensor temperature in °C
 - 7) The gas stream pressure in mbar
 - 8) The time in seconds since the previous record
- e.g. 2010 349.405950 385.61 53.4 13.0 27.2 1041 301.3
- 4.7.22 ProOceanus CO2 sensor files after 26 April 2011
- e.g. Cel_concat_2011_119.co3. These contain 10, space-delimited fields:-
 - 1) The year
 - 2) The day number time stamp for this sample
 - 3) The 'raw' 16-bit auto zero value which remains constant until the next AZPC
 - 4) The 'raw' 16-bit CO2 value
 - 5) The CO2 concentration in mol mol⁻¹
 - 6) The optical cell temperature in °C
 - 7) The humidity sensor reading in mb
 - 8) The humidity sensor temperature in °C
 - 9) The gas stream pressure in mbar
 - 10) The time in seconds since the previous record
- e.g. 2011 119.038584 52069 48440 453.04 55.0 21.7 34.4 1008 301.3

ProOceanus GTD sensor files

- e.g. Cel_concat_2011_119.gtd. These contain 4, space-delimited fields:-
 - 1) The year
 - 2) The day number time stamp for this sample
 - 3) The total dissolved gas pressure in mbar
 - 4) The time in seconds since the previous record
- e.g. 2011 123.920725 1021.6898 300.0

4.7.23 Aanderaa 4050 temperature sensor files

e.g. Cel_concat_2011_119.at1. These contain 4, space-delimited fields:-

- 1) The year
- 2) The day number time stamp for this sample
- 3) The water temperature in °C
- 4) The time in seconds since the previous record
- e.g. 2011 118.264513 19.8315 300.0
- 4.7.24 Aanderaa 3919 conductivity sensor files e.g. Cel_concat_2010_271.ac2

These contain 3, space-delimited fields:-

- 1) The year
- 2) The day number time stamp for this sample
- 3) The conductivity in mS/cm
- 4) The time in seconds since the previous record
- e.g. 2010 279.926988 43.472 300.0

4.7.25 Aanderaa 3835 oxygen sensor files

- e.g. Cel_concat_2010_271.ao3. These contain 6, space-delimited fields:-
 - 1) The year
 - 2) The day number time stamp for this sample
 - 3) The oxygen concentration in μ M
 - 4) The water temperature in °C
 - 5) The oxygen saturation as a percentage
 - 6) The time in seconds since the previous record
- e.g. 2010 276.324905 306.72 14.32 96.06 300.0
- 4.7.26 Seabird SBE48 hull temperature sensor files
- e.g. Cel_concat_2011_119.hul. These contain 4, space-delimited fields:-
 - 1) The year
 - 2) The day number time stamp for this sample
 - 3) The hull temperature in °C
 - 4) The time in seconds since the previous record
- e.g. 2011 119.181241 9.4022 300.0

4.7.27 Water flow sensor files

- e.g. Cel_concat_2010_271.fl1. These contain 4, space-delimited fields:-
 - 1) The year
 - 2) The day number time stamp for this sample
 - 3) The flow through the tank in litres/min
 - 4) The time in seconds since the previous record
- e.g. 2010 280.605449 27.60 600.0

4.7.28 Vaisala PTU air pressure/temperature/humidity sensor files

e.g. Cel_concat_2011_119.ptu. These contain 6, space-delimited fields:-

- 1) The year
- 2) The day number time stamp for this sample
- 3) The air pressure in mbar
- 4) The air temperature in °C
- 5) The air humidity as a percentage
- 6) The time in seconds since the previous record
- e.g. 2011 124.187616 1012.98 11.97 89.20 300.0
- 4.7.29 Vaisala atmospheric CO2 sensor files
- e.g. Cel_concat_2011_119.vco. These contain 5, space-delimited fields:-
 - 1) The year
 - 2) The day number time stamp for this sample
 - 3) The atmospheric CO2 concentration in ppm
 - 4) The sensor temperature in °C
 - 5) The time in seconds since the previous record
- e.g. 2011 119.869432 396.98 19.0 298.8
- 4.7.30 Electronics box temperature files
- e.g. Cel_concat_2011_119.tm2. These contain 6, space-delimited fields:-
 - 1) The year
 - 2) The Day number time stamp for this sample
 - 3) Box temperature sensor 1 in °C
 - 4) Box temperature sensor 2 in °C
 - 5) Box temperature sensor 3 in °C
 - 6) The time in seconds since the previous record
- e.g. 2011 123.546518 13.2 12.9 11.0 3600.0

Note that tm1 files come from the engine room box, tm2 from the Iridium box on the bridge top.

4.7.31 Vector Instruments wind sensor files

e.g. Cel_concat_2011_119.mwv. These contain 5, space-delimited fields:-

- 1) The year
- 2) The Day number time stamp for this sample
- 3) The apparent wind speed in m/s
- 4) The apparent wind direction, where 000 is coming directly from the ship's bow.
- 5) The time difference in seconds since the last sample
- e.g. 2011 124.244500 6.59 29 300.0

4.8 PC status files

e.g. Cel_concat_2011_119.st3. The system contains 3 PCs, each of which produces status files in different formats.

4.8.32 Engine room PC – st1

These contain 21, space-delimited fields:-

- 1) The year
- 2) The day number time stamp for this status
- 3) The number of seconds since the last status record
- 4) The remaining space on the flash card in MB
- 5) The number of RMC GPS messages since last status record
- 6) The number of AC1 sensor messages since last status record
- 7) The number of AC2 sensor messages since last status record
- 8) The number of AC3 sensor messages since last status record
- 9) The number of AT1 sensor messages since last status record
- 10) The number of AT2 sensor messages since last status record
- 11) The number of AT3 sensor messages since last status record
- 12) The number of AO1 sensor messages since last status record
- 13) The number of AO2 sensor messages since last status record
- 14) The number of AO3 sensor messages since last status record
- 15) The number of PCO2 sensor messages since last status record
- 16) The number of GTD sensor messages since last status record
- 17) The number of HULL sensor messages since last status record
- 18) The number of PIC box temperature messages since last status record
- 19) The number of PIC flow messages since last status record
- 20) The number of SMS commands since last status record
- 21) The time difference in seconds since the status record
- 2011 123.250001 3600.0 1982.719 720 120 120 120 240 240 240 120 120 e.q.

120 2246 120 120 120 60 0 3600.0

4.8.33 *Met/GPS PC – st2*

These contain 18, space-delimited fields:-

- 1) The year
- 2) The day number time stamp for this status
- 3) The number of seconds since the last status record
- 4) The remaining space on the flash card in MB
- 5) The maximum pitch reading in degrees since last status record
- 6) The minimum pitch reading in degrees since last status record
- 7) The average pitch reading in degrees since last status record
- 8) The maximum roll reading in degrees since last status record
- 9) The minimum roll reading in degrees since last status record
- 10) The average roll reading in degrees since last status record
- 11) The number of inclinometer messages since last status record
- 12) The number of GPS1 messages since last status record
- 13) The number of GPS2 messages since last status record
- 14) The number of Vaisala CO2 sensor messages since last status record
- 15) The number of Vaisala PTU sensor messages since last status record
- 16) The number of PIC box temperature messages since last status record
- 17) The number of SMS commands since last status record
- 18) The time difference in seconds since the status record

2011 123.083333 3600.0 1913.438 -99.00 99.00 0.00 -99.00 99.00 0.00 0 720 e.q. 720 121 120 120 0 7200.0

4.8.34 Iridium PC – st3

These contain 9, space-delimited fields:-

- 1) The year
- 2) The day number time stamp for this status
- 3) The number of seconds since the last status record
- 4) The remaining space on the flash card in MB
- 5) The number of GPS messages since last status record
- 6) The number of messages from the engine room PC since last status record
- 7) The number of messages from the met/GPS PC since last status record
- 8) The number of SMS messages since last status record
- 9) The time difference in seconds since the status record
- e.g. 2011 124.010417 3600.0 972.734 696 15 8 0 3600.0

4.8.35 Iridium performance before 26 April 2011

- e.g. Cel_concat_2010_271.ird. These contain 8, space-delimited fields:-
 - 1) The year
 - 2) The day number time stamp for this dial up attempt
 - 3) The (chargeable) connection time in seconds
 - 4) The time between power on and registration in seconds
 - 5) The number of bytes sent
 - 6) The attempt number 1 is the first, then up to 3 re-tries
 - 7) The status byte 00 means no errors
 - 8) The time in seconds since the previous record
- e.g. 2010 277.013885 194.87 90 15429 1 00 21600.1
- 4.8.36 Iridium performance after 26 April 2011.
- e.g. Cel_concat_2011_119.ir2. These contain 8, space-delimited fields:-
 - 1) The year
 - 2) The day number time stamp for this dial up attempt
 - 3) The (chargeable) connection time in seconds
 - 4) The time between power on and registration in seconds
 - 5) The number of bytes sent
 - 6) The attempt number -1 is the first, then up to 3 re-tries
 - 7) The status byte 00 means no errors
 - 8) The time in seconds since the previous record
- e.g. 2011 123.263893 198.77 90 16008 1 00 21600.0
- 4.8.37 SMS message confirmation

e.g. Cel_concat_2010_271.sms. These contain 3, space-delimited fields:-

1) The year

2) The day number time stamp that the SMS message was processed by the iridium PC

3) The first 24 characters of the SMS message (padded with @ characters if necessary)

e.g. 2007 159.60765195 DF3,1,0@@@@@@@@@@@@@@@@@@

4.9 Pacific Celebes Iridium Telemetry Merged File Format

The, e.g. **\ascdata\Celebes\concat\Cel_concat_2011_119.gtd**, which were copied to a network drive.These concatenated files were then merged according to the GPS fix times by Unix program Celebes_merge.c. The merged files were named **\ascdata\Celebes\merged\Cel_merge_2009_230.txt** and have 33 fields as follows:

- 1. Year
- 2. Day fraction for GPS fix
- 3. Latitude
- 4. Longitude
- 5. Ship's speed over the ground in knots
- 6. Aanderaa Temperature sensor 1
- 7. Aanderaa Temperature sensor 2
- 8. Aanderaa Temperature sensor 3
- 9. Aanderaa Conductivity sensor 1 (conductivity only)
- 10. Aanderaa Conductivity sensor 2
- 11. Aanderaa Conductivity sensor 3
- 12. Aanderaa Oxygen sensor 1 (oxygen concentration only)
- 13. Aanderaa Oxygen sensor 2
- 14. Aanderaa Oxygen sensor 3
- 15. Pro CO2 The CO2 concentration in mol mol⁻¹
- 16. Pro CO2 The optical cell temperature in °C
- 17. Pro CO2 The humidity sensor water vapour pressure in mbar
- 18. Pro CO2 The humidity sensor temperature in °C
- 19. Pro CO2 The gas stream pressure in mbar
- 20. Pro GTD total dissolved gas pressure in mbar
- 21. Hull temperature in °C
- 22. Flow in litres/min
- 23. Vaisala atmospheric CO2 concentration
- 24. Corrected Vaisala atmospheric CO2 concentration
- 25. Vaisala atmospheric pressure (corrected for bridge height of 34m)
- 26. Vaisala atmospheric temperature in °C
- 27. Vaisala atmospheric relative humidity
- 28. Apparent wind speed in m/s
- 29. Apparent wind direction relative to ship's bow in degrees
- 30. Estimated true wind speed in m/s
- 31. Estimated true wind direction relative to true north in degrees (set to 999 when ship is stationary)
- 32. Estimated ship's course made good (CMG) in degrees

Flag set to 0 if atmospheric CO2 sensor is in the path of contaminated air from the ship's funnel, or 1 if it's in clean air.