DATA PRODUCT SPECIFICATION FOR PARTIAL PRESSURE OF CO_2 IN AIR AND SURFACE SEAWATER

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Document Control Sheet

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0-01	2012-05-09	Initial Draft	M. Vardaro
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Signature Page

This document has been reviewed and approved for release to Configuration Management.

OOI Senior Systems Engineer: 

Date:2012-07-03

This document has been reviewed and meets the needs of the OOI Cyberinfrastructure for the purpose of coding and implementation.

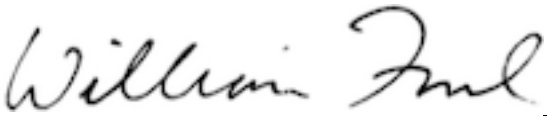
OOI CI Signing Authority: 

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Table of Contents

1 Abstract

This document describes the procedure used to obtain the OOI Level 1 Partial Pressure of CO_2 in Air and Surface Seawater core data products, which are calculated using the output from the Pro-Oceanus PSI CO2-Pro™. This document is intended to be used by OOI programmers to construct appropriate processes to create the L1 data products.

2 Introduction

2.1 Author Contact Information

Please contact Michael Vardaro (mvardaro@coas.oregonstate.edu) or the Data Product Specification lead (DPS@lists.oceanobservatories.org) for more information concerning the computation and other items in this document.

2.2 Metadata Information

2.2.1 Data Product Name

The OOI Core Data Product Names for these products is:

- PCO2ATM
- PCO2SSW

The OOI Core Data Product Descriptive Names for these products are:

- Atmospheric Partial Pressure of CO_2
- Partial Pressure of CO_2 In Surface Seawater

2.2.2 Data Product Abstract (for Metadata)

The PCO2ATM data product is the partial pressure of CO_2 (pCO_2) in air, which is the pressure that would be exerted by CO_2 if all other gases were removed. pCO_2 in the air is determined optically by measuring the infrared absorbance level of CO_2.

The PCO2SSW data product is the partial pressure of CO_2 (pCO_2) in surface seawater, which is the pressure that would be exerted by CO_2 if all other gases were removed. Partial pressure of a gas dissolved in water is understood as the partial pressure in air that the gas would exert in a hypothetical air volume in equilibrium with that water. pCO_2 in surface seawater is determined optically by measuring the infrared absorbance level of CO_2

2.2.3 Computation Name

Not required for data products.

2.2.4 Computation Abstract (for Metadata)

The OOI Level 1 Partial Pressure of CO_2 in Air and Surface Seawater core data products PCO2ATM and PCO2SSW are created by converting the Level 0 XCO2ATM or XCO2SSW CO2 Mole Fractions (xCO_2, in ppm), into µatm units by using an equation that incorporates the L0 Gas Stream Pressure PRESAIR (in mbar). The instrument computes the xCO2 value internally by measuring the infrared absorbance level of CO_2 and compensating for the measured pressure, temperature, and humidity.

2.2.5 Instrument-Specific Metadata

See Section 4.4 for instrument-specific metadata fields that must be part of the output data.

2.2.6 Data Product Synonyms

Synonyms for this data product are

- pCO_2 (this is a generic term and may also refer to the similar data products listed below)

2.2.7 Similar Data Products

A similar product that this data product may be confused with is PCO2WAT, the Partial Pressure of CO_2 in Seawater, which is calculated using a different instrument (the Sunburst $SAMI^2$-CO_2) from samples taken at depth rather than in surface seawater.

2.3 Instruments

For information on the instruments from which the L1 Partial Pressure of CO_2 in Air and Surface Seawater core data product inputs are obtained, see the PCO2A flow document (1342-00260). This document contains information on the instrument class and make/model; it also describes the flow of data from the PSI CO2-Pro through all of the relevant QC, calibration, and data product computations and procedures.

Please see the Instrument Application in the SAF for specifics of instrument locations and platforms.

2.4 Literature and Reference Documents

PSI CO2-Pro Setup, Deployment and Trouble Shooting Manual, Version 9.3; September 13, 2011.
(*see REFERENCE >> DPS Artifacts >> 1341-00260_PCO2ATM_PCO2SSW >> PSI CO2-Pro User Manual*)

In-Situ Dissolved Gas Sensor Systems, Oceanus Logger Integration Guide, Version 1.1.6 (2012) Pro-Oceanus Systems, Inc.
(*see REFERENCE >> DPS Artifacts >> 1341-00260_PCO2ATM_PCO2SSW >> CO2 Pro ATM Oceanus Logger Integration Guide 300412.pdf*)

2.5 Terminology

2.5.1 Definitions

Definitions of general OOI terminology are contained in the Level 2 Reference Module in the OOI requirements database (DOORS).

2.5.2 Acronyms, Abbreviations and Notations

General OOI acronyms, abbreviations and notations are contained in the Level 2 Reference Module in the OOI requirements database (DOORS). The following acronyms and abbreviations are defined here for use throughout this document.

IRGA = Infrared Gas Analyser
AZPC = Automatic Zero Point Calibration

2.5.3 Variables and Symbols

The following variables and symbols are defined here for use throughout this document.

xCO_2 = CO_2 Mole Fraction in Air or Surface Seawater aka “Measured CO_2”, in ppm
pCO_2 = partial pressure of CO_2, in µatm
p = pressure, in mbar
STD = standard atmospheric pressure = 1013.25 mbar/atm

3 Theory

3.1 Description

The OOI Level 1 Partial Pressure of CO_2 in Air core data product PCO2ATM and the OOI Level 1 Partial Pressure of CO_2 in Surface Seawater core data product PCO2SSW are created by converting the L0 XCO2ATM CO2 Mole Fraction in Air or L0 XCO2SSW CO2 Mole Fraction in Surface Seawater (both referred to as xCO_2, in ppm), into µatm units by using an equation that also incorporates the L0 Gas Stream Pressure PRESAIR (in mbar). The instrument computes the xCO2 value internally by measuring the infrared absorbance level of CO_2 and compensating for the measured pressure, temperature, and humidity.

3.2 Mathematical Theory

From the PSI CO2-Pro Manual and Craig McNeil (personal communication):

The L0 CO2 Mole Fraction XCO2AIR or XCO2SSW (xCO_2) and the L0 Gas Stream Pressure (PRESAIR, p) of the instrument's internal gas volume are among the data output by the CO2-Pro. These data may be used to compute the CO_2 partial pressure of the internal gas volume (PCO2ATM or PCO2SSW), which has equilibrated with the water being flushed through the instrument's gas exchange interface. A sample calculation for converting xCO_2 to pCO_2 is shown below:

$pCO_2 = xCO_2 \bullet p / STD$

where:
pCO_2 = partial pressure of CO_2 (µatm)
xCO_2 = CO_2 mole fraction (ppm)
p = internal barometric pressure (mbar)
STD = standard atmospheric pressure = 1013.25 mbar/atm

Because xCO_2 is represented as a ppm value (10^{-6}), without further manipulation the result is given in units of µatm.

Given a measured values of xCO_2 = 390.41 ppm, and p = 1011 mbar:

pCO_2 = 390.41 ppm • 1011mbar / 1013.25 mbar/atm = 399.93 µatm

3.3 Known Theoretical Limitations

Instrument results are only valid between 0 – 35 °C

3.4 Revision History

No revisions to date.

4 Implementation

4.1 Overview

The output from the instrument is in RS-232 serial output format and all temperature, humidity, and pressure compensation is done by onboard firmware. An automatic zero point calibration (AZPC) must be done every 8 hours (minimum once per day) by cycling the power. The measured CO_2 output and pressure output values are used to calculate the L1 pCO_2 data product. Gas stream pressure (p), all temperature values (humidity sensor, IRGA detector, and IRGA source), and humidity values should be included as metadata along with the pCO_2 measurement.

4.2 Inputs

- Measured CO_2 (xCO_2), XCO2ATM or XCO2SSW [ppm], as a 6 character floating point number, %.3f
- Gas stream pressure (p), PRESAIR [ppm], as a 4 character floating point number, %.0f

Inputs are derived from the CO2-Pro serial output, which includes the following variables, as per the PSI CO2-Pro Manual and Oceanus Logger Integration Guide:

Instrument Measurement format (RS232 Serial Output):
YYYY/MM/DD HH:MM:SS M aaaaa bbbbb **ccc.ccc** dd.d ee.eeee ff.ffff **gggg** hh.h ii.i **A**
or
YYYY/MM/DD HH:MM:SS M aaaaa bbbbb **ccc.ccc** dd.d ee.eeee ff.ffff **gggg** hh.h ii.i **W**

Where:
YYYY/MM/DD HH:MM:SS = Timestamp (year/month/day hour:minute:second)
M = Begin Measurement
aaaaa = Zero A/D [counts] from most recent autozero sequence
bbbbb = Current A/D [counts]
ccc.ccc = Measured CO_2 (xCO_2), XCO2ATM or XCO2SSW [ppm]
dd.d = Average IRGA temperature [°C]
ee.eeee = Humidity [mbar]
ff.ffff = Humidity sensor temperature [°C]
gggg = Gas stream pressure (p), PRESAIR [ppm]
hh.h = IRGA detector temperature [°C]
ii.i = IRGA source temperature [°C]
A = Air sample (indicating XCO2ATM L0 data product)
W = Water sample (indicating XCO2SSW L0 data product)

4.3 Processing Flow

The specific steps necessary to create all calibrated and quality controlled data products for each OOI core instrument are described in the instrument-specific Processing Flow documents (DCN 1342-00260). These processing flow documents contain flow diagrams detailing all of the specific procedures (data product and QC) necessary to compute all levels of data products from the instrument.

The processing flow for the pCO2 data product computation is as follows:

Step 1: Download and parse the serial output data (already temperature, humidity, and pressure compensated) from the CO2-Pro.

Step 2: Use the L0 Measured CO_2 (XCO2ATM or XCO2SSW) and L0 Gas stream pressure (PRESAIR) to calculate pCO_2 using the equation provided [$pCO_2 = xCO_2 \bullet p / STD$]

Step 3: Report the L1a pCO2 (PCO2ATM or PCO2SSW, depending on L0 input) and associated metadata (see section 4.4)

Step 4: Publish empty or dummy value upon computational error. See Processing Flow document (DCN 1342-00260) for additional post-processing steps.

4.4 Outputs

The outputs of the Measured pCO2 computation are

- L1a Partial pressure of CO_2 (PCO2ATM or PCO2SSW, pCO_2) in µatm, as a 6 character floating point number, %.3f

The metadata that must be included with the output are

- Xxxxx.xxxxx = Timestamp as a 10 character floating point number, %.5f
- dd.d = Average IRGA temperature [°C] as a 3 character floating point number, %.1f
- ee.eeee = Humidity [mbar] as a 6 character floating point number, %.4f
- ff.ffff = Humidity sensor temperature [°C] as a 6 character floating point number, %.4f
- hh.h = IRGA detector temperature [°C] as a 3 character floating point number, %.1f
- ii.i = IRGA source temperature [°C] as a 3 character floating point number, %.1f

See Appendix B for a discussion of the accuracy of the output.

4.5 Computational and Numerical Considerations

N/A

4.6 Code Verification and Test Data Set

The code will be verified using the test data set provided, which contains inputs and their associated correct outputs. CI will verify that the code is correct by checking that the output, generated using the test data inputs, is identical to the test data density output. This test data set contains L0 XCO2ATM (indicated by the “A” at the end of each string) but is applicable to XCO2SSW as well.

Data Samples
2011/08/16 16:46:15 - M 44634 40527 674 56.3 17.799 25.760 1000 55.8 56.8 A
2011/08/16 16:46:17 - M 44634 40779 619 56.3 18.465 25.760 1000 55.6 56.7 A
2011/08/16 16:46:18 - M 44634 39886 822 56.3 18.795 25.760 1000 55.7 56.8 A
2011/08/16 16:46:20 - M 44634 39285 973 56.3 18.841 25.800 1000 55.7 56.8 A
2011/08/16 16:46:21 - M 44634 39410 941 56.3 19.006 25.800 1000 55.7 56.8 A
2011/08/16 16:46:23 - M 44634 39720 863 56.3 19.170 25.800 1000 55.8 56.8 A
2011/08/16 16:46:25 - M 44634 39752 854 56.3 19.545 25.840 1000 55.8 56.9 A
2011/08/16 16:46:26 - M 44634 39841 833 56.3 19.708 25.840 1000 55.8 56.7 A
2011/08/16 16:46:28 - M 44634 39869 826 56.3 19.920 25.880 1000 55.7 56.8 A
2011/08/16 16:46:29 - M 44634 39916 814 56.3 20.245 25.880 1000 55.7 56.7 A
2011/08/16 16:46:31 - M 44634 39986 797 56.3 20.407 25.880 1000 55.7 56.8 A
2011/08/16 16:46:33 - M 44634 40049 782 56.3 20.568 25.880 1000 55.7 56.8 A
2011/08/16 16:46:34 - M 44634 40112 768 56.3 20.728 25.880 1000 55.7 56.9 A
2011/08/16 16:46:36 - M 44634 40172 754 56.3 20.728 25.880 1000 55.7 56.9 A
2011/08/16 16:46:37 - M 44634 40229 740 56.3 20.940 25.920 1000 55.7 56.8 A

Sample Data Output:

INPUT from raw data stream										OUTPUT
Date & Time	zero A/D [counts]	Current A/D [counts]	Measured CO2 (xCO2) in Air (XCO2ATM) [ppm]	Average IRGA temp [C]	Humidity [mbar]	Humidity sensor temp [C]	Gas stream pressure (p) [mbar]	IRGA detector temperature [C]	IRGA source temperature [C]	pCO2 in Air (PCO2ATM) [µatm]
2011/08/16 16:46:15	44634	40527	674	56.3	17.799	25.76	1000	55.8	56.8	665.19
2011/08/16 16:46:17	44634	40779	619	56.3	18.465	25.76	1000	55.6	56.7	610.91
2011/08/16 16:46:18	44634	39886	822	56.3	18.795	25.76	1000	55.7	56.8	811.25
2011/08/16 16:46:20	44634	39285	973	56.3	18.841	25.8	1000	55.7	56.8	960.28
2011/08/16 16:46:21	44634	39410	941	56.3	19.006	25.8	1000	55.7	56.8	928.69
2011/08/16 16:46:23	44634	39720	863	56.3	19.17	25.8	1000	55.8	56.8	851.71
2011/08/16 16:46:25	44634	39752	854	56.3	19.545	25.84	1000	55.8	56.9	842.83
2011/08/16 16:46:26	44634	39841	833	56.3	19.708	25.84	1000	55.8	56.7	822.11
2011/08/16 16:46:28	44634	39869	826	56.3	19.92	25.88	1000	55.7	56.8	815.20
2011/08/16 16:46:29	44634	39916	814	56.3	20.245	25.88	1000	55.7	56.7	803.36
2011/08/16 16:46:31	44634	39986	797	56.3	20.407	25.88	1000	55.7	56.8	786.58
2011/08/16 16:46:33	44634	40049	782	56.3	20.568	25.88	1000	55.7	56.8	771.77
2011/08/16 16:46:34	44634	40112	768	56.3	20.728	25.88	1000	55.7	56.9	757.96
2011/08/16 16:46:36	44634	40172	754	56.3	20.728	25.88	1000	55.7	56.9	744.14
2011/08/16 16:46:37	44634	40229	740	56.3	20.94	25.92	1000	55.7	56.8	730.32

Appendix A Example Code

N/A

Appendix B Output Accuracy

The Pro-Oceanus CO2-Pro instrument specifications indicate an accuracy of ±1 µatm, and a precision of ±0.01 µatm (at standard temperatures and pressures).

Listed below are the DOORS requirements for accuracy and precision:

PCO2-003 $p(CO_2)$ instruments shall have an accuracy of ±2 µatm in air and in water. [L4-CG-IP-RQ-198]

PCO2-004 $p(CO_2)$ instruments shall have a precision of 1 µatm in air and in water. [L4-CG-IP-RQ-199]

Appendix C Sensor Calibration Effects

N/A