DATA PRODUCT SPECIFICATION FOR FLUX OF CO_2 FROM THE OCEAN INTO THE ATMOSPHERE

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Document Control Sheet

Version	Date	Description	Author
0-01	2012-03-28	Initial Draft	M. Lankhorst
0-02	2012-04-18	Included feedback from one outside review. Minor edits for clarity. Corrected headers/footers.	M. Lankhorst
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1-03	2012-07-03	Corrected units on L1 PCO2 inputs and added conversion in processing flow.	M. Lankhorst

Signature Page

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

OOI Senior Systems Engineer: ______________________________

Date: 2012-05-22

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

OOI CI Signing Authority: ______________________________

Date: 2012-05-22

Table of Contents

1 Abstract

This document describes the computation of the flux of CO_2 (carbon dioxide) across the air-sea interface. It is computed from measurements of pCO_2 (partial pressure of carbon dioxide) in the air and in the water, and uses auxiliary data such as wind speed, sea surface temperature, and salinity. These measurements are made on surface buoys in the coastal and global arrays of the OOI.

2 Introduction

2.1 Author Contact Information

Please contact Matthias Lankhorst (mlankhorst@ucsd.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 Name for this product is

- CO2FLUX

The OOI Core Data Product Descriptive Name for this product is

- Flux of CO2 from the ocean into the atmosphere

2.2.2 Data Product Abstract (for Metadata)

The OOI Level 2 core data product "CO2FLUX" reports the flux of CO_2 from the ocean into the atmosphere. It is computed using data from the pCO_2 air-sea (PCO2A) and bulk meteorology (METBK) families of instruments.

2.2.3 Computation Name

N/A

2.2.4 Computation Abstract (for Metadata)

The OOI Level 2 core data product "CO2FLUX" reports the flux of CO_2 from the ocean into the atmosphere. It is computed using data from the pCO_2 air-sea (PCO2A) and bulk meteorology (METBK) families of instruments.

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

N/A

2.2.7 Similar Data Products

There are different methods to estimate the gas exchange between the ocean and the atmosphere. The method used here utilizes in-situ measurements of the partial pressure of carbon dioxide in both the surface ocean and the overlying air. The flux is then estimated as proportional to the difference of these partial pressures. The proportionality factor is parameterized using the wind speed. Sea surface temperature and salinity are used to further adjust this factor. See references for further details.

Other computational techniques include different estimates of the factor (Sweeney et al., 2007).

The flux as used herein is expressed in units of amount of substance per surface area and time, i.e. in SI units of $mol\ m^{-2}\ s^{-1}$. Other units, such as those of mass instead of amount of substance, are possible alternatives. Usage of days instead of seconds as the time unit is also common.

The sign of the resulting flux is arbitrarily chosen. Here, the convention is used that positive values indicate flux from the ocean into the atmosphere.

2.3 Instruments

For information on the instruments from which the CO2FLUX core data product inputs are obtained, see the PCO2A Processing Flow document (DCN 1342-00260) and the documents on instrument classes PCO2A and METBK (pCO_2 air-sea and bulk meteorology).

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

2.4 Literature and Reference Documents

Sweeney, C., E. Gloor, A. R. Jacobson, R. M. Key, G. McKinley, J. L. Sarmiento, R. Wanninkhof: “Constraining global air-sea gas exchange for CO_2 with recent bomb ^{14}C measurements”. Global Biogeochemical Cycles, vol. 21, GB2015, 2007.

Wanninkhof, R.: “Relationship Between Wind Speed and Gas Exchange Over the Ocean”. Journal of Geophysical Research, vol. 97, no. C5, pp. 7373-7382, 1992.

Weiss, R. F.: “Carbon dioxide in water and seawater: the solubility of a non-ideal gas”. Marine Chemistry, vol. 2, pp203-215, 1974.

2.5 Terminology

2.5.1 Definitions

N/A

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.

2.5.3 Variables and Symbols

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

F	Air-sea flux of carbon dioxide [mol m^{-2} s^{-1}], positive indicating flow from sea into air
k	Gas transfer velocity (see Wanninkhof, 1992)
K_0	Gas solubility (see Weiss, 1974)
pCO_2	Partial pressure of carbon dioxide [µatm]
pCO_{2W}	Partial pressure of carbon dioxide in sea water [µatm]
pCO_{2A}	Partial pressure of carbon dioxide in air [µatm]
S	Salinity of sea water
Sc	Schmidt number (see Wanninkhof, 1992)
t,T	Temperature of sea water in ºC (t) or K (T)
u_{10}	Wind speed at 10m height [m s^{-1}]

3 Theory

3.1 Description

The flux of CO_2 across the air-sea interface is computed from in-situ measurements of the partial pressures of carbon dioxide in both the surface ocean and the overlying air. The flux is then estimated as proportional to the difference of these partial pressures. The proportionality factor is parameterized using the wind speed. Sea surface temperature and salinity are used to further adjust this factor. See references for computational details.

3.2 Mathematical Theory

Known inputs are:

t, S, pCO_{2W}, pCO_{2A}, u_{10}

Convert pCO_2 units from µatm to atm by dividing by 1000000.

Compute Schmidt number as follows (Wanninkhof, 1992, table A1):

$$Sc = 2073.1 - 125.62t + 3.6276t^2 - 0.043219\mathrm{t}^3$$

Compute gas transfer velocity (in m s^{-1}) as follows (Sweeney et al., 2007, figure 3 and table 1):

$$k = \left[0.27\mathrm{u_{10}}^2\left(\frac{660}{\mathrm{Sc}}\right)^{\frac{1}{2}}\right]/360000$$

Compute absolute temperature as follows:

$$T = t + 273.15$$

Compute solubility (in mol atm^{-1} m^{-3}) as follows (Weiss, 1974, equation 12 and table I):

$$K_0 = 1000 * \exp\left(-58.0931 + 90.5069\left(\frac{100}{T}\right) + 22.2940\, ln\left(\frac{T}{100}\right) + S\left[0.027766 - 0.025888\left(\frac{T}{100}\right) + 0.0050578\left(\frac{T}{100}\right)^2\right]\right)$$

Compute CO_2 flux as follows (Wanninkhof, 1992, equation A2):

$$F = k\, K_0(pCO_{2W} - pCO_{2A})$$

F is the desired output, the CO_2 flux in SI units of mol m^{-2} s^{-1}.

3.3 Known Theoretical Limitations

There are multiple different methods to compute a gas flux across the air-sea interface. The choice of parameterization type, and the particular implementation thereof, each have an inherent uncertainty. The equations and coefficients used herein are only meaningful for input parameters typically encountered in the ocean, and are an estimate rather than a deterministic result. In particular, there are different approaches to parameterize the effect of the wind speed (note the differences between Sweeney et al., 2007, and Wanninkhof, 1992).

The scales for the input parameters temperature and salinity have undergone changes over the years (temperature: IPTS-68 vs. ITS-90; salinity: PSS-1978 vs. TEOS-10), in particular between the times when the different references used herein were published. The effect of these changes in reference scales are expected to be small compared to the inherent uncertainty of the estimation.

3.4 Revision History

No revisions to date.

4 Implementation

4.1 Overview

The implementation is a step-by-step computation that exactly follows the equations of the mathematical theory.

4.2 Inputs

pCO_{2W}	L1 PCO2SSW: partial pressure of carbon dioxide in sea water [µatm]
pCO_{2A}	L1 PCO2ATM: partial pressure of carbon dioxide in air [µatm]
S	L2 SALSURF: sea surface salinity from METBK
t	L1 TEMPSRF: Sea surface temperature from METBK [ºC]
u_{10}	L2 WIND10M: normalized wind speed at 10m height from METBK [m s^{-1}]

The pCO_2 variables are obtained from the PCO2A instrument class.
All others are obtained from the METBK instrument class.

4.3 Processing Flow

The only step to obtain the CO2FLUX output from the input parameters is execution of code like the exemplar given in the appendix (conversion from µatm to atm for the pCO_2 inputs has been added after initial release of this code). Prior to that, the input parameters need to become available (lower-level data products). After the CO2FLUX output is computed, QC algorithms need to be called to subsequently produce QC flags for the CO2FLUX values.

4.4 Outputs

The output of the computation is:
F: L2 flux of CO_2 from the ocean into the atmosphere [mol m^{-2} s^{-1}]

The metadata that must be included with the output are

- the version of the algorithm
- linkages to the input data that were used to compute the output
- the version of the Matlab execution engine, if used.

4.5 Computational and Numerical Considerations

4.5.1 Numerical Programming Considerations

n/a

4.5.2 Computational Requirements

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 output. 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 output.

pCO2W	pCO2A	U10	t	S	F
360	390	5	0	34	-2.063e-08

360	390	5	0	35	-2.052e-08
360	390	5	10	34	-1.942e-08
360	390	5	10	35	-1.932e-08
360	390	5	20	34	-1.869e-08
360	390	5	20	35	-1.860e-08
360	390	10	0	34	-8.250e-08
360	390	10	0	35	-8.207e-08
360	390	10	10	34	-7.767e-08
360	390	10	10	35	-7.728e-08
360	390	10	20	34	-7.475e-08
360	390	10	20	35	-7.440e-08
360	390	20	0	34	-3.300e-07
360	390	20	0	35	-3.283e-07
360	390	20	10	34	-3.107e-07
360	390	20	10	35	-3.091e-07
360	390	20	20	34	-2.990e-07
360	390	20	20	35	-2.976e-07
400	390	5	0	34	6.875e-09
400	390	5	0	35	6.839e-09
400	390	5	10	34	6.472e-09
400	390	5	10	35	6.440e-09
400	390	5	20	34	6.229e-09
400	390	5	20	35	6.200e-09
400	390	10	0	34	2.750e-08
400	390	10	0	35	2.736e-08
400	390	10	10	34	2.589e-08
400	390	10	10	35	2.576e-08
400	390	10	20	34	2.492e-08
400	390	10	20	35	2.480e-08
400	390	20	0	34	1.100e-07
400	390	20	0	35	1.094e-07
400	390	20	10	34	1.036e-07
400	390	20	10	35	1.030e-07
400	390	20	20	34	9.966e-08
400	390	20	20	35	9.920e-08
440	390	5	0	34	3.438e-08
440	390	5	0	35	3.420e-08
440	390	5	10	34	3.236e-08
440	390	5	10	35	3.220e-08
440	390	5	20	34	3.114e-08
440	390	5	20	35	3.100e-08
440	390	10	0	34	1.375e-07
440	390	10	0	35	1.368e-07
440	390	10	10	34	1.294e-07
440	390	10	10	35	1.288e-07
440	390	10	20	34	1.246e-07
440	390	10	20	35	1.240e-07
440	390	20	0	34	5.500e-07
440	390	20	0	35	5.471e-07
440	390	20	10	34	5.178e-07
440	390	20	10	35	5.152e-07
440	390	20	20	34	4.983e-07
440	390	20	20	35	4.960e-07

Appendix A Example Code

The following code runs under MatLab:

```
% CO2FLUX   Flux of CO2 across the air-sea interface
%
% Time-stamp: <2012-03-28 11:53:24 mlankhorst>
%
% Compute flux of carbon dioxide between air and sea from partial
% pressures of CO2 in air and sea, sea water temperature and
% salinity, and wind speed via Bulk formula.
%
% USAGE:  f=co2flux(pco2w,pco2a,u10,t,s);
%
%   f:     CO2 flux, positive from sea to air [mol m-2 s-1]
%   pco2w: Partial pressure of CO2 in sea water [microatm]
%   pco2a: Partial pressure of CO2 in air [microatm]
%   u10:   Instantaneous wind speed at 10m above sea level
%          [m s-1]
%   t:     Sea surface temperature [deg C] (note: difference
%          between temperature scales of 1968 and 1990 is
%          negligible for this algorithm)
%   s:     Sea surface salinity [g/kg] (note: difference between
%          absolute/practical salinity is negligible for this
%          algorithm)
%
% References:
%
%   R.F. Weiss (1974): "Carbon Dioxide in Water and Seawater: The
%   Solubility of a Non-Ideal Gas". Marine Chemistry, vol. 2,
%   pp. 203-215.
%
%   R. Wanninkhof (1992): "Relationship Between Wind Speed and Gas
%   Exchange Over the Ocean". Journal of Geophysical Research,
%   vol. 97, no. C5, pp. 7373-7382.
%
%   C. Sweeney, E. Gloor, A. R. Jacobson, R. M. Key, G. McKinley,
%   J. L. Sarmiento, R. Wanninkhof (2007): "Constraining global
%   air-sea gas exchange for CO2 with recent bomb 14C
%   measurements". Global Biogeochemical Cycles, vol. 21,
%   no. GB2015.
%

function f=co2flux(pco2w,pco2a,u10,t,s);

  % convert micro-atm to atm:

  pco2a=pco2a./1e6;
  pco2w=pco2w./1e6


  % Compute Schmidt number (after Wanninkhof, 1992, Table A1):

  Sc=2073.1-(125.62.*t)+(3.6276.*(t.^2))-(0.043219.*(t.^3));



  % Compute gas transfer velocity
  % (after Sweeney et al., 2007, Fig. 3 and Table 1):

  k=0.27.*(u10.^2).*sqrt(660./Sc);
```

```
% convert cm h-1 to m s-1

k=k./(100*3600);



% Compute absolute temperature:

T=t+273.15;

% Compute solubility (after Weiss, 1974, Eqn. 12 and Table I).
% Note that there are two versions, one for units per volume and
% one per mass. Here, the volume version is used.

% mol atm-1 m-3
K0=1000.*exp(-58.0931+(90.5069.*(100./T))+(22.2940.*log(T./100))+ ...
            s.*(0.027766-(0.025888.*(T./100))+ ...
               (0.0050578.*((T./100).^2))));

% mol atm-1 kg-1
% K0=exp(-60.2409+(93.4517.*(100./T))+(23.3585.*log(T./100))+ ...
%     s.*(0.023517-(0.023656.*(T./100))+ ...
%         (0.0047036.*((T./100).^2))));



% Compute flux (after Wanninkhof, 1992, eqn. A2):

f=k.*K0.*(pco2w-pco2a);
```

Appendix B Output Accuracy

The accuracy of the output is discussed by Sweeney et al. (2007) and Wanninkhof (1992) to some extent, but neither reference puts a definite value on it. This has several reasons: all underlying computations of Sc, k, and K_0 use curve-fitting to some experimental data, not all of which are fully documented with an error budget. Further, the concept of deriving a flux from bulk measurements is inherently uncertain in that it is at best an estimate of the flux, but not a direct measurement of a flux, and there is no established estimate of the inherent uncertainty. Wanninkhof (pers. comm., 2012) suggests that the uncertainty of the flux estimate is on the order of 10%. Wanninkhof (1992) reports that the equations used are estimated for intermediate-strength wind situations, thereby suggesting that the parameterizations might be less accurate in wind speeds below 3 or above 20 m/s. Sweeney et al. (2007) discuss different previous parameterizations of k using wind speed (their figure 3), results of which differ among themselves by a factor of 2 for wind speeds of 10 m/s. In conclusion, there is no definite estimate of the output accuracy, but an assessment that the overall consensus of existing references converges to within approximately 10% of the measured value.