An introduction to the Ocean Thematic Centre of the European RI ICOS

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Integrated Carbon Observation System (ICOS)

Scientific Mission:

• Increase fundamental understanding of carbon cycle, greenhouse gas budgets and perturbations, and underlying processes

• Increase ability to predict future changes

• Verify the effectiveness of policies aiming to reduce greenhouse gas emissions

• Foster technical and scientific innovation

• Contribute in education and capacity building
ICOS Stations

134 Measurement stations
12 Member countries

80 Ecosystem stations

33 Atmosphere stations

21 Ocean stations

including two stations in Greenland, one in French Guyana, La Reunion, Cape Verde (not visible here)
**ICOS Data Flow**

- **External metadata registry & catalogue services**
- **ICOS repository (data, metadata)**
- **High performance and throughput computing services**

**Sensor data**

**Finalized and elaborated data products**

- **External metadata registry & catalogue services**
- **ICOS repository (data, metadata)**
- **High performance and throughput computing services**

**Ecosystem Thematic Centre**

- **Data ingestion**
- **PID and DOI minting**
- **Metadata services**
- **Data discovery & access**
- **Usage tracking**

- **Calibration Labs**

**Oceanic Thematic Centre**

- **Standardized data processing**
- **Centralized quality control**
- **Scientific QC performed by the station PI**
- **Data provenance, curation and archiving**
- **Clear open data license**
- **Data citation**
- **FAIR services**
The Ocean Thematic Centre

Cargo to Greenland - Data to the World

ICOS OTC | https://otc.icos-cp.eu/
OTC tasks and mission

1. Leadership and management
2. Labelling and station liaison
3. Technical support
4. Technical innovation
5. Data unit
6. Network liaison and design
Labelling scheme for ocean stations

“ICOS shall provide harmonised and high-precision scientific data on carbon cycle and greenhouse gas budget and perturbations”

For the ocean this means

Quantifying air-sea CO$_2$ fluxes
- Requires pCO$_2$ measurements
- Most suited for Carbon-VOS

Assessing variability and drivers
- Requires pCO$_2$, one of $A_T$, pH, or DIC, dissolved oxygen/nutrients
- Most suited for Fixed Ocean Stations
# Labelling scheme

<table>
<thead>
<tr>
<th>Carbon-VOS (Voluntary Observing Ship)</th>
<th>FOS (Fixed Ocean Station)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Class 2</strong></td>
<td><strong>Class 1</strong></td>
</tr>
<tr>
<td>(minimum required variables)</td>
<td>(additional variables)</td>
</tr>
<tr>
<td>pCO₂ (± 2 ppm)</td>
<td>Alkalinity of DIC</td>
</tr>
<tr>
<td></td>
<td>Oxygen</td>
</tr>
<tr>
<td></td>
<td>Surface:</td>
</tr>
<tr>
<td></td>
<td>Nutrients (nitrate, silicate, and phosphate)</td>
</tr>
</tbody>
</table>

*DIC = Dissolved Inorganic Carbon  
In addition, variables for validation must be sampled
Which precision do we actually need?

Target 14.3: minimize and address the impacts of ocean acidification
Which precision do we actually need?

**The weather goal**

- relative spatial patterns and short-term variations
- supporting mechanistic response to and impact on local, immediate ocean acidification dynamics.

Implies an uncertainty of:
- pH ~0.02
- TA, DIC ~10 μmol kg$^{-1}$
- pCO$_2$ ~2.5% relative uncertainty

**The climate goal**

- to assess long-term trends with a defined level of confidence,
- supporting detection of the long-term anthropogenically driven changes in hydrographic conditions and carbon chemistry over multi-decadal time scales.

Implies an uncertainty of:
- pH ~0.003
- TA, DIC ~2 μmol kg$^{-1}$
- pCO$_2$ ~0.5% relative uncertainty
FOS:

• Validation in-situ
  • Preferably monthly discrete samples from station site
  • At minimum, discrete samples during deployment and when the instruments are retrieved
  • Important with a sufficient amount of parallel samples (TRIPLICATES)

• Use of discrete samples for validation of pCO\textsubscript{2}
  • Use the pair $[\text{TA} + \text{pH}]$ or $[\text{DIC} + \text{pH}]$, do NOT use $[\text{TA} + \text{DIC}]$
  • Use $K1$ and $K2$ from Lueker et al. (2000) - Best practices from Dickson et al. (2007)
  • Use up to date calculation program
  • If you want to include error calculation (error.m) from Orr et al. (2018) you also need to use his CO2sys.m

• Discrete samples of TA, DIC, and/or pH - quality
  • OTC need statement from each laboratory regarding quality of measurement (accuracy of samples and how this is achieved, e.g. CRM from Dickson)
Saildrone

- Saildrone (Canadian) – 7 m long vessel
- Wind and wave driven, 2 to 8 knots
- Equipped with sensors for pCO₂, O₂, SST, SSS, wind, pH, etc.

(https://www.saildrone.com/)
Saildrone - in situ validation of FOS

• Joint proposal (Geomar/Cape Verde Observatory and OTC) submitted to Saildrone Nov 2018
• Aim to use Saildrones, equipped with calibration instruments to validate Fixed Ocean Stations within ICOS
• Mission supported by Saildrone
• Start in Cape Verde 1 November 2019
• Will arrive in Mediterranean early 2020 and Italian stations approx. February 2020
Data Lifecycle Within OTC

Data: L0, L1, L2
Metadata: L0, L1, L2
NRT vis.: L0, L1, L2
QuinCe: L0, L1, L2

- Data reduction;
- Automated QC
- NRT visualisation

Instrument Site PI OTC Carbon Portal Repository SOCAT and GLODAP User
QuinCe – general overview

- **online tool** developed by OTC for the submission, processing, data reduction, quality control and dissemination of data
- receives **raw data directly** from the stations’ instruments, performs all necessary calculations and performs automated quality control routines to highlight data that is likely to be of poor quality (like range checks and spike detection)
- station **PI** can **review** the data and perform their own **quality control** before approving it for submission to the OTC.
- once submitted, the data will automatically be archived at the CP and made available to other relevant external third level data products (e.g. the SOCAT - Surface Ocean CO2 Atlas, CMEMS).
1. Use QuinCe for automatic QC and data processing

2. Use the raw data and output from QuinCe to do more checks with R

Check atmospheric CO$_2$

Check drift in standards

Summarise QC results

Plot data
Quality Control for Biogeochemical Data - Workshop
September 24 and 25 at NOAA/PMEL in Seattle, WA

Objectives
- Workshop deliverables will be guidance that can be applied by the ICOS OTC and NOAA OAP developer groups towards an implementable solution
- Determine what degree of level 1 and level 2 quality control is acceptable for which variables, and what can be implemented by developer groups
- Determine what degree of QC automation is possible for both level 1 and level 2.
- SOCAT, GLODAP, ICOS, NOAA OAP, US BGC ARGO networks participated
1st ICOS OTC $pCO_2$ instrument inter-comparison exercise

When?  

Where?  
Flanders Marine Institute (VLIZ) in Oostende/Belgium

What?  
In the recent years new technologies are involving and a whole new generation of sensors and instruments measuring $pCO_2$ the surface ocean and below entered the market. This spans from "classical" equilibrator based systems with new $CO_2$ detectors to membrane based sensors that can be submerged.

The aim of this exercise is:
- the comparison of instruments and sensors that are (or will be) used within the ICOS community over a range of temperatures and $pCO_2$.
- to engage instrument suppliers to work together with the observational community to reach a high level of standardization in operating $pCO_2$ sensors and instruments.
- to give answers to the community of choosing the appropriate sensor for their application.

Contact:  
ICOS OTC, Tobias Steinhoff  
tost@nrcresearch.no
Thank you!
For more information please visit https://otc.icos-cp.eu
ICOS Oceans CO$_2$ sensors - moorings

Contros HydroC CO$_2$
- Membrane equilibration
- IR CO$_2$ detection
- Auto zeroing
- Pre/post calibration necessary

Pro Oceanus CO$_2$-Pro
- Membrane equilibration
- IR CO$_2$ detection
- Auto zeroing

Sunburst SAMI-CO$_2$
- Membrane equilibration
- Colorimetric reagent method

Recommendations for ocean stations

- If a station does not follow SOPs, the station must provide evidence that their station meet the OTC requirements.

**Carbon-VOS**

- **Calibration frequency**
  - Temperature and pressure sensors - every two years at calibration facility, in-house every two years
  - LICOR - every five year at calibration facility

- **Equilibrator pressure**
  - Should be measured by an absolute pressure sensor in the Wet Box /equilibrator

- **Atmospheric xCO₂ measurements**
  - Compared with nearby atmospheric station (Global View)
  - Wait for outcome from RINGO

- **Atmospheric pressure**
  - Changed to a core parameter, accuracy ±1 mbar
Fixed Ocean Station (FOS):

- **pCO$_2$ accuracy**
  - Changed from ±5 µatm to ±10 µatm

- **Dissolved oxygen** - requirements released to 2%

- **Calibration frequency**
  - pCO$_2$ - at factory or calibration facility prior to deployment (Contros, Pro-Oceanus, SAMI)
  - Post deployment calibration for Contros
  - O$_2$/temperature/salinity - prior to deployment

- **Equilibration time for pCO$_2$ sensor** (Contros and Pro-Oceanus, IR detection)
  - If no equilibration evidence during deployment, such evidence should be provided from a laboratory test prior to deployment
Network design

- Evolve the network towards a state of high level robustness and optimal structure

-Deliverable Network Design (continuous):
Production and implementation of a roadmap aimed at helping the MSA produce a robust and optimally structured network.

-refreshed annually
According to GOOS EOV’s and the GOA-ON (Newton et al., 2014):

The “weather” goal is defined as measurements of quality sufficient to identify
• relative spatial patterns and short-term variations,
• supporting mechanistic response to and impact on local, immediate ocean acidification dynamics.
This implies an uncertainty of:
\[ \text{pH} \sim 0.02 \]
\[ \text{TA and DIC} \sim 10 \, \mu\text{mol kg}^{-1} \]
\[ \text{pCO}_2 \sim 2.5\% \text{ relative uncertainty} \]

The “climate” goal is defined as measurements of quality sufficient
• to assess long-term trends with a defined level of confidence,
• supporting detection of the long-term anthropogenically driven changes in hydrographic conditions and carbon chemistry over multi-decadal time scales.
This implies an uncertainty of:
\[ \text{pH} \sim 0.003 \]
\[ \text{TA and DIC} \sim 2 \, \mu\text{mol kg}^{-1} \]
\[ \text{pCO}_2 \sim 0.5\% \text{ relative uncertainty} \]
Carbon-VOS  Calculated carbon system using fCO2 and a 2nd carbon variable and uncertainties $u(fCO2) = 2 \mu$atm, $u(DIC) = u(TA) = 2 \mu$mol kg$^{-1}$; $u(pH) = 0.001$
Carbon-VOS  Calculated carbon system using fCO2 and a 2nd carbon variable and uncertainties \( u(f\text{CO}_2) = 2 \ \mu\text{atm}, u(\text{DIC}) = u(\text{TA}) = 2 \ \mu\text{mol kg}^{-1}; u(\text{pH}) = 0.001 \)
Calculated carbon variables using fCO₂ and a 2nd carbon variable and uncertainties $u(\text{fCO}_2) = 10 \, \mu\text{atm}$, $u(\text{DIC}) = u(\text{TA}) = 2 \, \mu\text{mol kg}^{-1}$; $u(\text{pH}) = 0.001$. 

Ocean MSA and OTC meeting, Southampton 18 March
Calculated carbon variables using fCO2 and a 2nd carbon variable and uncertainties $u(fCO2) = 10 \mu$atm, $u(DIC) = u(TA) = 2 \mu$mol kg$^{-1}$; $u(pH) = 0.001$
ICOS Oceans CO$_2$ sensors – Carbon-VOS

Water/air equilibrator based systems
- Standard: General Oceanics
- Several custom built systems
- Bubble/spray... equilibration
- IR CO$_2$ detection (other detectors possible)

SubCtech OceanPack pCO$_2$
- Membrane equilibration
- IR CO$_2$ detection
- Auto zeroing, standard gases possible

Contros HydroC CO$_2$ FT
- Membrane equilibration
- IR CO$_2$ detection
- Auto zeroing
- Pre/post calibration necessary
QuinCe - online tool for data reduction and quality control of surface ocean fCO2 data
QuinCe - Motivation

- A single, centralised tool - data from all sources is treated with the same community-approved algorithms
- Removes code development responsibilities from scientists
- Open Source code increases traceability and transparency
- Reduces data handling work required by scientists
- Flexible architecture will allow shorter development time for new projects using different types of data
QuinCe - Features

- Upload data in any text format
- Individual sensor calibration adjustments can be applied
- Data reduction is performed automatically, with calibration to gas standards
- Automated QC routines detect common issues
- Extensive plotting and mapping tools for manual QC
- All QC decisions (automatic and manual) are recorded for future traceability
- Automatic submission to ICOS, CMEMS INSTAC and SOCAT

Near Real Time processing allows fully automatic data flow from ship to publication within minutes
QuinCe - Future developments

• Complete metadata integration
• More intelligent automatic QC routines based on previous data sets and external data sources
• Uncertainty propagation
• Longitudinal study of instrument performance
• More variables (pH, O2 ...
QuinCe – status: quality control

Follows SOCAT quality control procedures

In its current version, QuinCe performs checks on:

• File format
• Monotonically increasing timestamps
• Range (bad/impossible and questionable)
• Constant values for a certain period (may indicate instrument malfunction).
• Outliers (standard deviation range checks)
• Excessive gradients during a certain period

Excessive gradients during a certain period
Benguela Stream (Labelling) - Standard Concentrations

### Deployment Date
Select the date on which the standards were deployed

- **2014-06-24**

### Standard Concentrations
Enter the concentration for each gas standard

<table>
<thead>
<tr>
<th>Standard</th>
<th>Concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td>000</td>
<td>0.00</td>
</tr>
<tr>
<td>250</td>
<td>260.36</td>
</tr>
<tr>
<td>350</td>
<td>361.14</td>
</tr>
<tr>
<td>450</td>
<td>460.69</td>
</tr>
</tbody>
</table>

### Calibration Date
Select the date on which the calibration was performed

- **2015-04-28**

### Calibration coefficients
Enter the calibration coefficients for each sensor

<table>
<thead>
<tr>
<th>Sensor</th>
<th>Intercept</th>
<th>( x )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Intake Temperature: Aanderaa</td>
<td>0.0</td>
<td>1.0</td>
</tr>
<tr>
<td>Salinity: Seabird</td>
<td>0.0</td>
<td>1.0</td>
</tr>
<tr>
<td>Equilibrator Temperature: PT100 (Top)</td>
<td>0.9721</td>
<td>9.8304</td>
</tr>
<tr>
<td>Equilibrator Temperature: PT2000 (Bottom)</td>
<td>0.0</td>
<td>1.0</td>
</tr>
<tr>
<td>Equilibrator Pressure: Omega</td>
<td>878.41</td>
<td>40.377</td>
</tr>
<tr>
<td>Date</td>
<td>Longitude</td>
<td>Latitude</td>
</tr>
<tr>
<td>--------------</td>
<td>-----------</td>
<td>----------</td>
</tr>
<tr>
<td>2019-04-14 12:03:07</td>
<td>-25.537</td>
<td>59.076</td>
</tr>
<tr>
<td>2019-04-14 12:06:11</td>
<td>-25.515</td>
<td>59.079</td>
</tr>
<tr>
<td>2019-04-14 12:07:43</td>
<td>-25.505</td>
<td>59.081</td>
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<tr>
<td>2019-04-14 12:09:15</td>
<td>-25.494</td>
<td>59.083</td>
</tr>
<tr>
<td>2019-04-14 12:10:47</td>
<td>-25.483</td>
<td>59.084</td>
</tr>
<tr>
<td>2019-04-14 12:12:19</td>
<td>-25.473</td>
<td>59.086</td>
</tr>
<tr>
<td>2019-04-14 12:15:23</td>
<td>-25.452</td>
<td>59.088</td>
</tr>
<tr>
<td>2019-04-14 12:16:55</td>
<td>-25.442</td>
<td>59.090</td>
</tr>
</tbody>
</table>

Set WOCE flag for 4 rows

WOCE Flag: **Bad**

Comment: Moisture value invalid

Save  Cancel
<table>
<thead>
<tr>
<th>Variable</th>
<th>Frequency</th>
<th>Accuracy</th>
<th>Required for Class</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sea surface fCO₂</td>
<td>Quasi-continuous</td>
<td>±2 μatm</td>
<td>2</td>
</tr>
<tr>
<td>Intake temperature (SST)</td>
<td>Continuous</td>
<td>±0.05 °C</td>
<td>2</td>
</tr>
<tr>
<td>Water vapour pressure</td>
<td>Continuous</td>
<td>±0.5 mbar</td>
<td>2</td>
</tr>
<tr>
<td>Equilibrator pressure</td>
<td>Continuous</td>
<td>±2.0 mbar</td>
<td>2</td>
</tr>
<tr>
<td>Equilibrator temperature</td>
<td>Continuous</td>
<td>±0.05 °C</td>
<td>2</td>
</tr>
<tr>
<td>Delta-T (Intake/Equilibrator temperature difference)</td>
<td>Continuous</td>
<td>&lt; 1.5 °C (normal)</td>
<td>2</td>
</tr>
<tr>
<td></td>
<td></td>
<td>&lt; 3 °C (ice edge)</td>
<td></td>
</tr>
<tr>
<td>Sea surface salinity (SSS)</td>
<td>Continuous</td>
<td>± 0.1 psu</td>
<td>2</td>
</tr>
<tr>
<td>Atmospheric xCO₂</td>
<td>Quasi-continuous</td>
<td>±1 μatm</td>
<td>1</td>
</tr>
<tr>
<td>Alkalinity (TA)</td>
<td></td>
<td></td>
<td>1**</td>
</tr>
<tr>
<td>Dissolved Inorganic Carbon (DIC)</td>
<td></td>
<td></td>
<td>1**</td>
</tr>
<tr>
<td>pH</td>
<td></td>
<td></td>
<td>1**</td>
</tr>
<tr>
<td>Dissolved oxygen</td>
<td></td>
<td>±2% #</td>
<td>1</td>
</tr>
<tr>
<td>Dissolved nutrients</td>
<td></td>
<td>±1%* #</td>
<td>1</td>
</tr>
</tbody>
</table>

* Currently no sensors available with this accuracy
** At least one of these variables must be measured
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<table>
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<tr>
<th>Variable</th>
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<th>Required for Class</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sea surface fCO₂</td>
<td>&gt;1 day⁻¹/3 day⁻¹</td>
<td>±10 μatm</td>
<td>2</td>
</tr>
<tr>
<td>Sea surface temperature</td>
<td>&gt;1 day⁻¹/3 day⁻¹</td>
<td>±0.02 °C</td>
<td>2</td>
</tr>
<tr>
<td>Sea surface salinity</td>
<td>&gt;1 day⁻¹/3 day⁻¹</td>
<td>±0.03 psu</td>
<td>2</td>
</tr>
<tr>
<td>Alkalinity</td>
<td>&gt;1 day⁻¹/3 day⁻¹</td>
<td></td>
<td>2**</td>
</tr>
<tr>
<td>Dissolved Inorganic Carbon</td>
<td></td>
<td></td>
<td>2**</td>
</tr>
<tr>
<td>pH</td>
<td></td>
<td></td>
<td>2**</td>
</tr>
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<td>Dissolved oxygen</td>
<td>±2%</td>
<td></td>
<td>1</td>
</tr>
<tr>
<td>Dissolved nutrients</td>
<td>±1%*</td>
<td></td>
<td>1</td>
</tr>
</tbody>
</table>

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** At least one of these variables must be measured