A workflow for combining *in situ* and satellite data for CO_2 flux calculations

David K Woolf
Heriot-Watt University
d.k.woolf@hw.ac.uk

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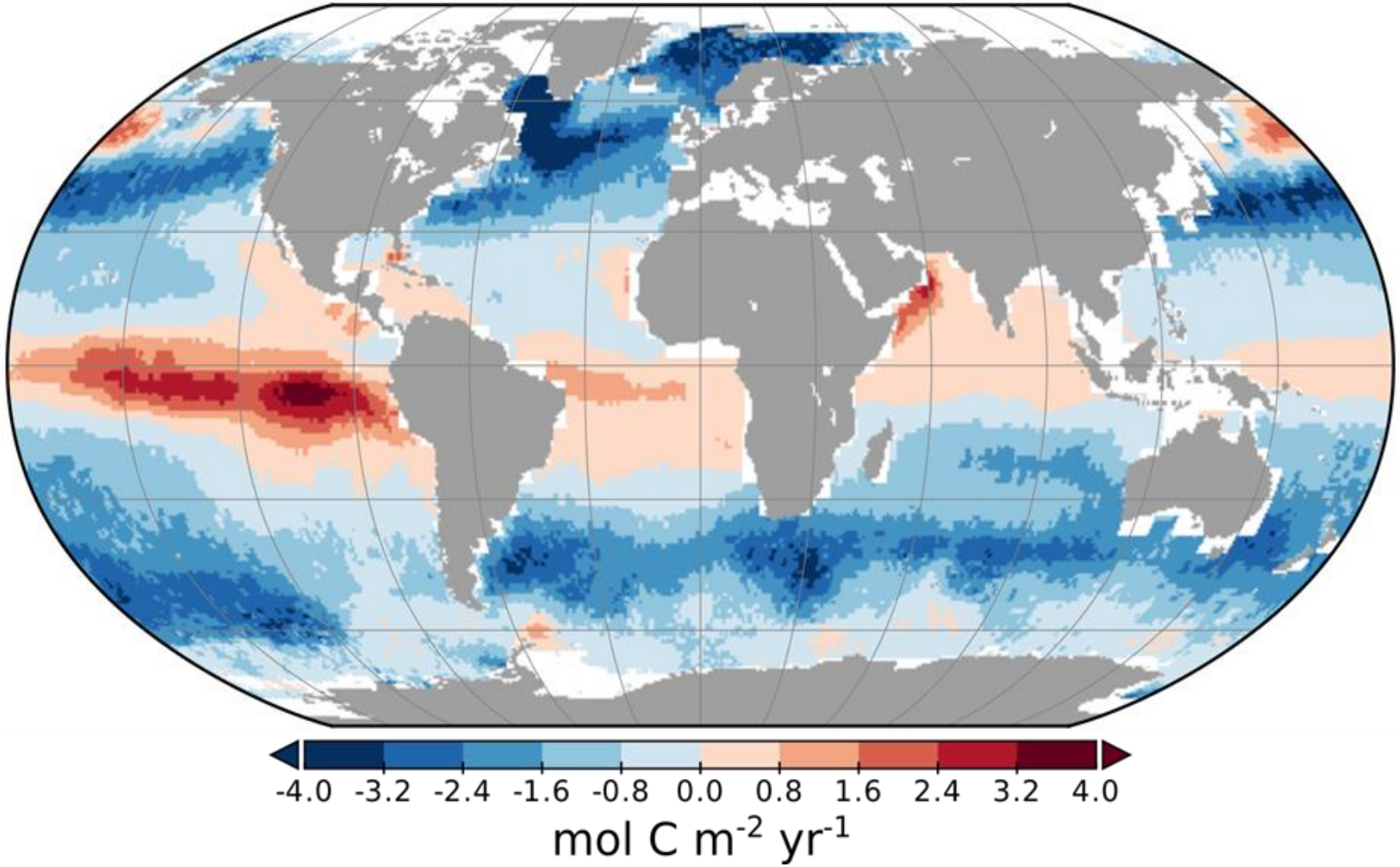

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Overview

- Bulk Air-Sea Gas Flux Formulae
- Sensitivity of Global Calculation to Temperature Handling
- Discrepancies between *in situ* and satellite-derived SSTs
- Systematic and Incidental relationships of CO_2 and temperature
- Data Products
- Options for combining data
- How robust is an “isochemical” correction?
- Knowledge Gaps and Priorities (1, 5 and 10 years)

Bulk Air-Sea Gas Flux Formulae

- Bulk air-sea flux formulae are a standard approach to estimating fluxes at the sea surfaces that depend on a primarily wind-driven and turbulent exchange across surface boundary layers. In the case of gas exchange this is often written:

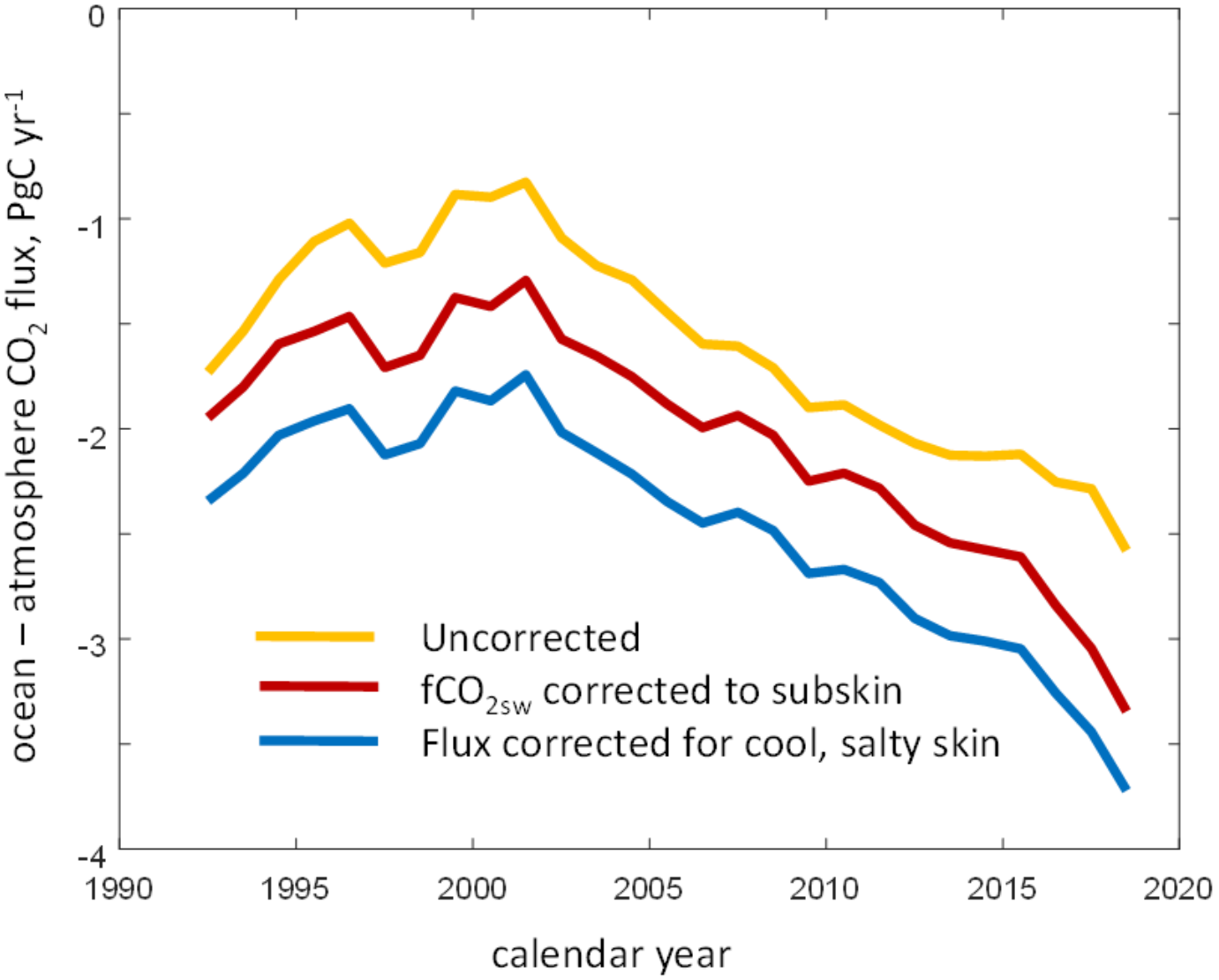
$$F = Tr\,\Delta pCO_2$$

- There are two flaws in this simple expression
  - An assumption of symmetrical and direct transfer
  - Omission of the complexity of temperature distribution

- Fixing the latter only:

$$\text{Sea-to-air flux, } F_{CO2} = k.(C_{sw} - C')$$

Sensitivity of Global Calculation to Temperature Handling



Watson et al. 2020; https://www.nature.com/articles/s41467-020-18203-3

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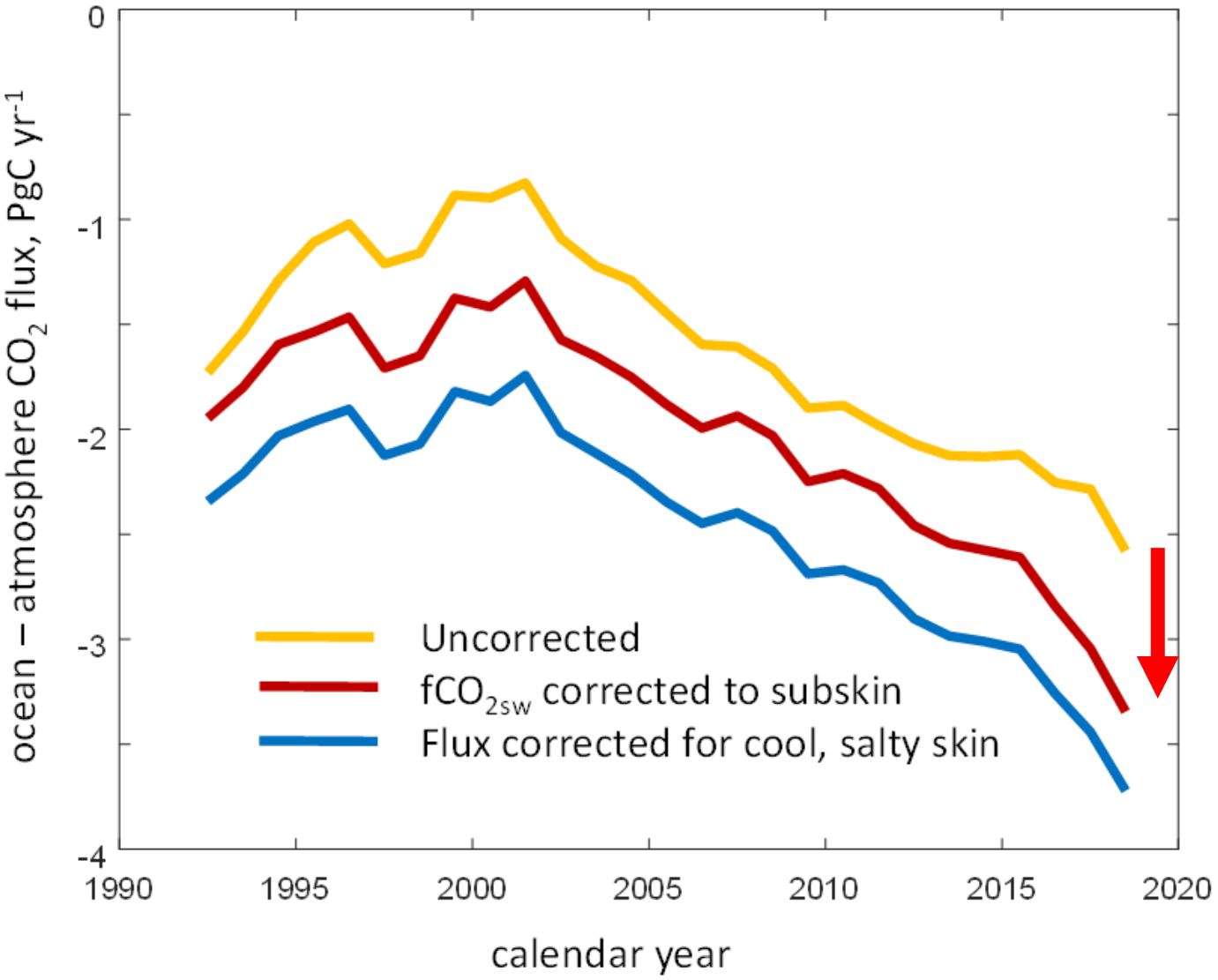

"Sampling Correction"

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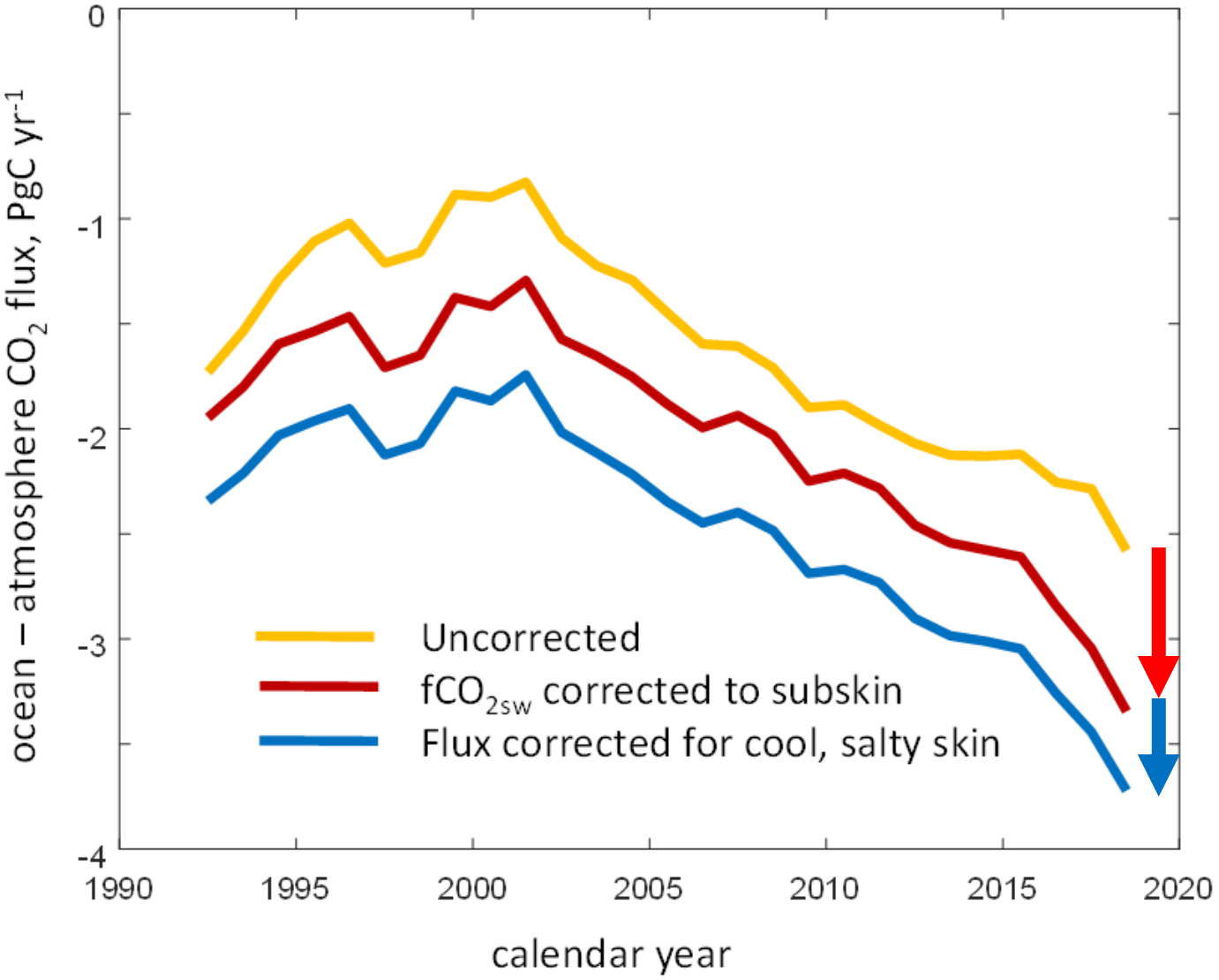

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"Skin Effect"

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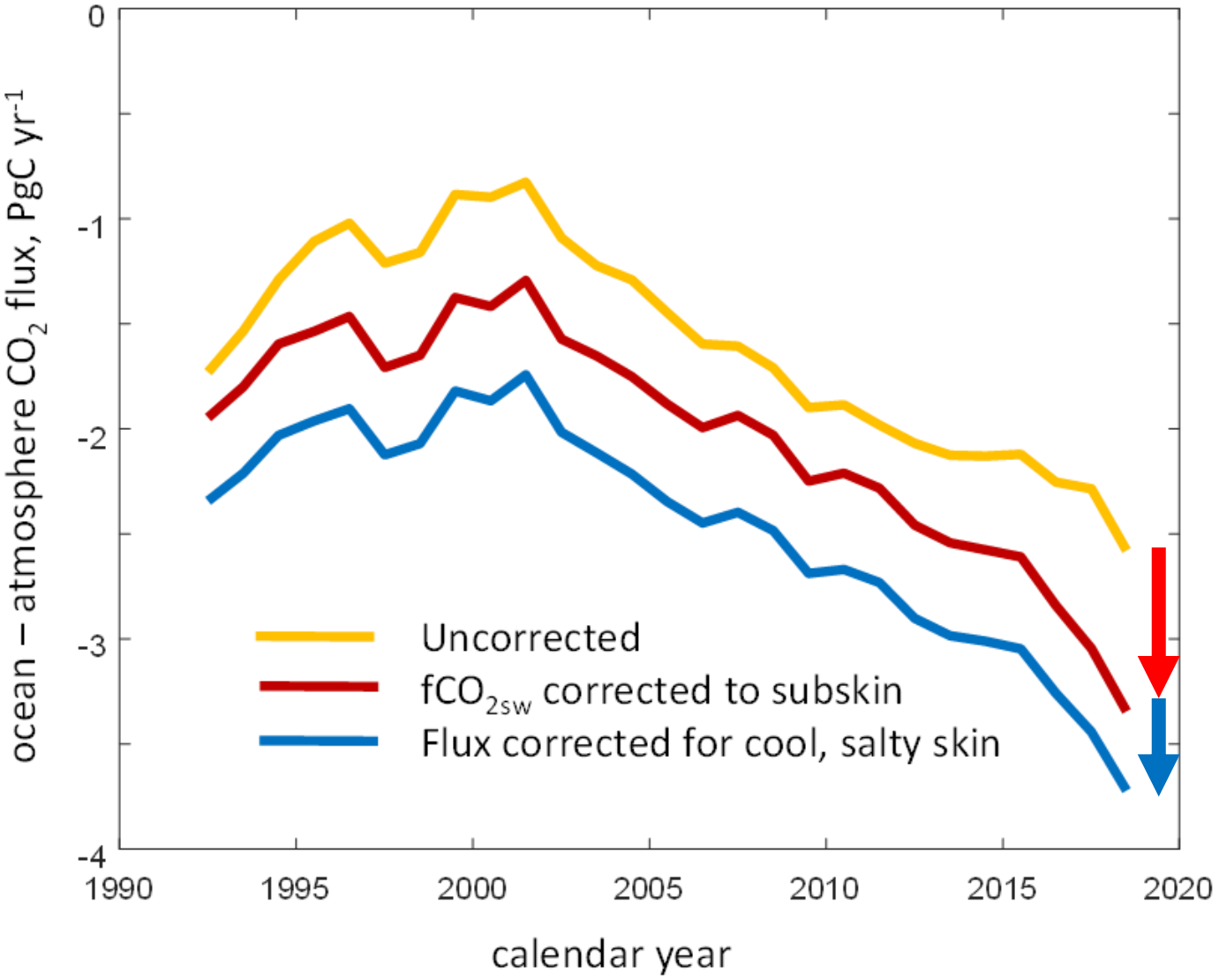

"Sampling Correction" Discussed Here

"Skin Effect" Not Discussed Here

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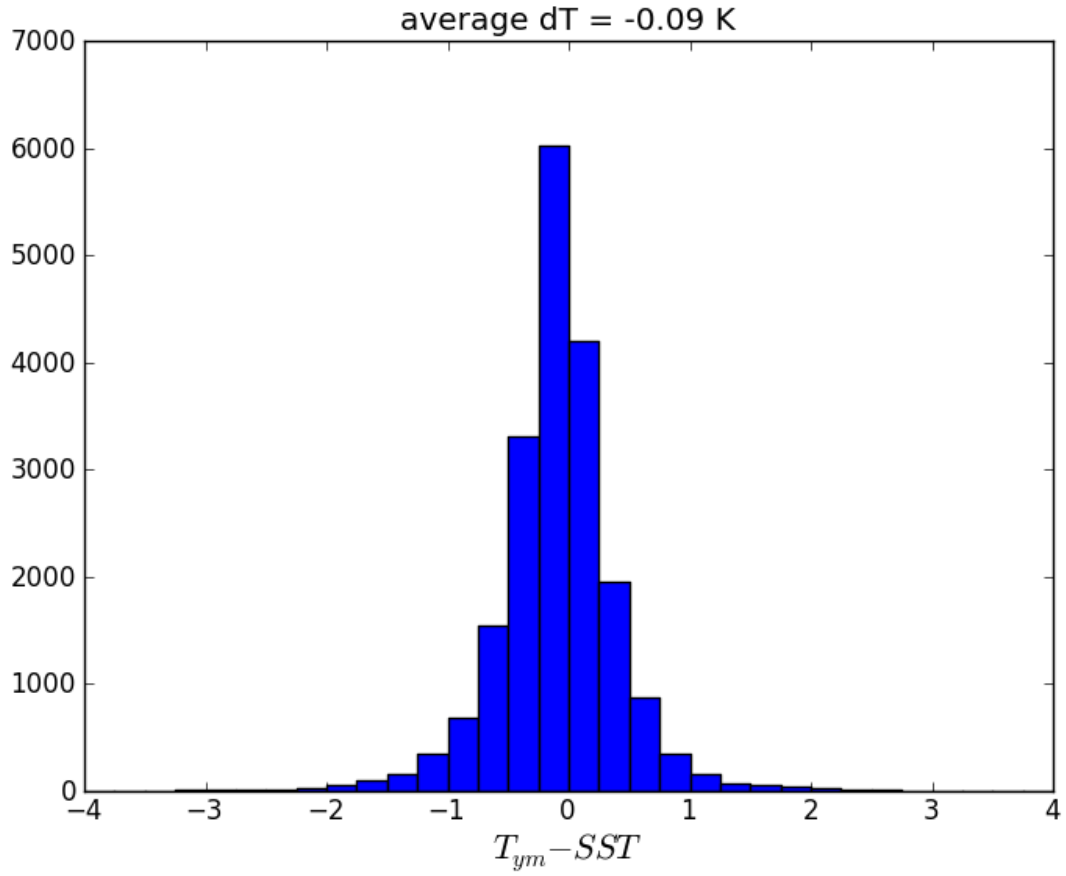
Discrepancies between *in situ* and satellite-derived SSTs

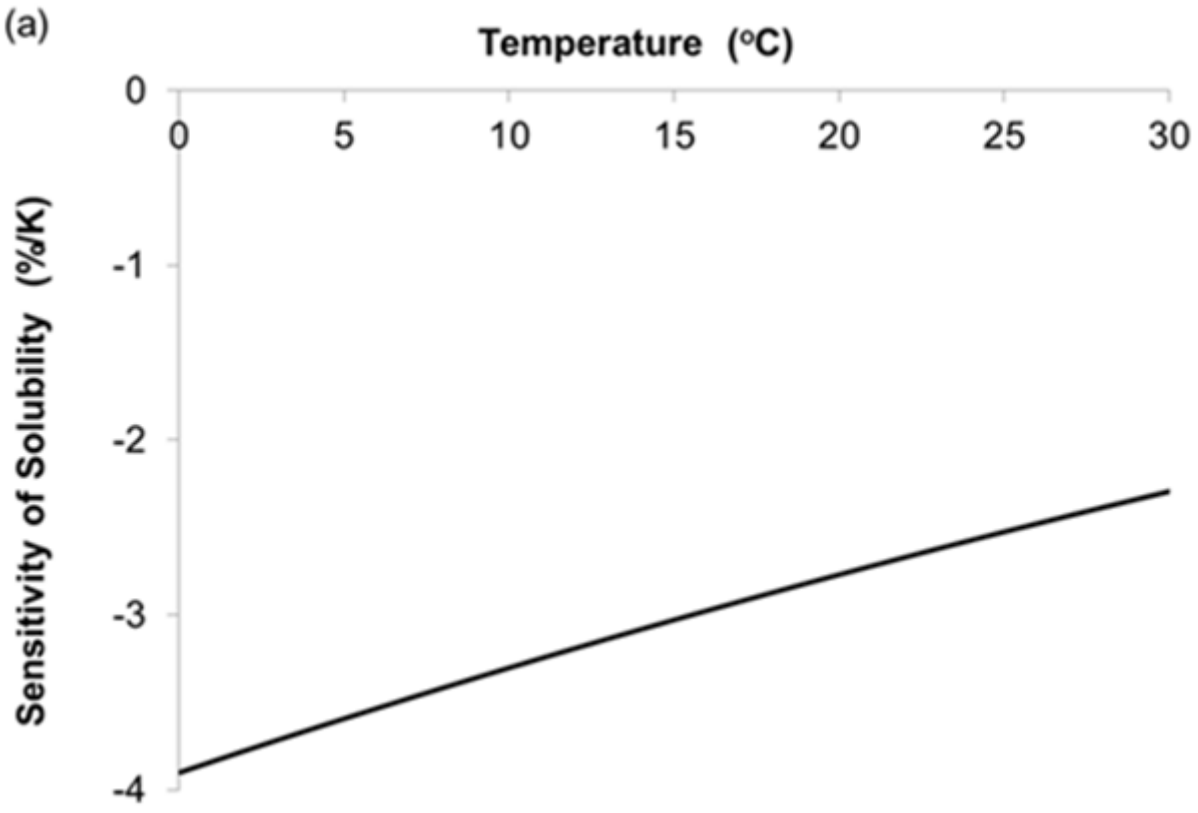
- Takahashi et al. (2009) described a difference between “climatological” and “interpolated” temperature of -0.08 ^{o}C
- Goddijn-Murphy et al. (2015) described a difference between “ARC SST” (satellite) and in situ temperature of -0.09 ^{o}C
- This bias (see figure) is on average with much larger positive and negative values



Goddijn-Murphy et al., 2015 (ARC subskin SST and SOCAT v 1.5)

Systematic and Incidental relationships of CO_2 and temperature

- Systematic dependence (thermodynamics) of carbonate system in seawater
  - Solubility of CO_2 decreases with increasing temperature (-2.7 %/^{o}C)
  - Concentration of CO_2 changes with temperature in “isochemical transformation” due to repartitioning (1.5 %/^{o}C)
  - pCO2 increases (2.7 + 1.5 = 4.2 %/^{o}C) with temperature isochemically
- Empirical (non-isochemical) relationships
  - Local and scale-dependent correlations are common

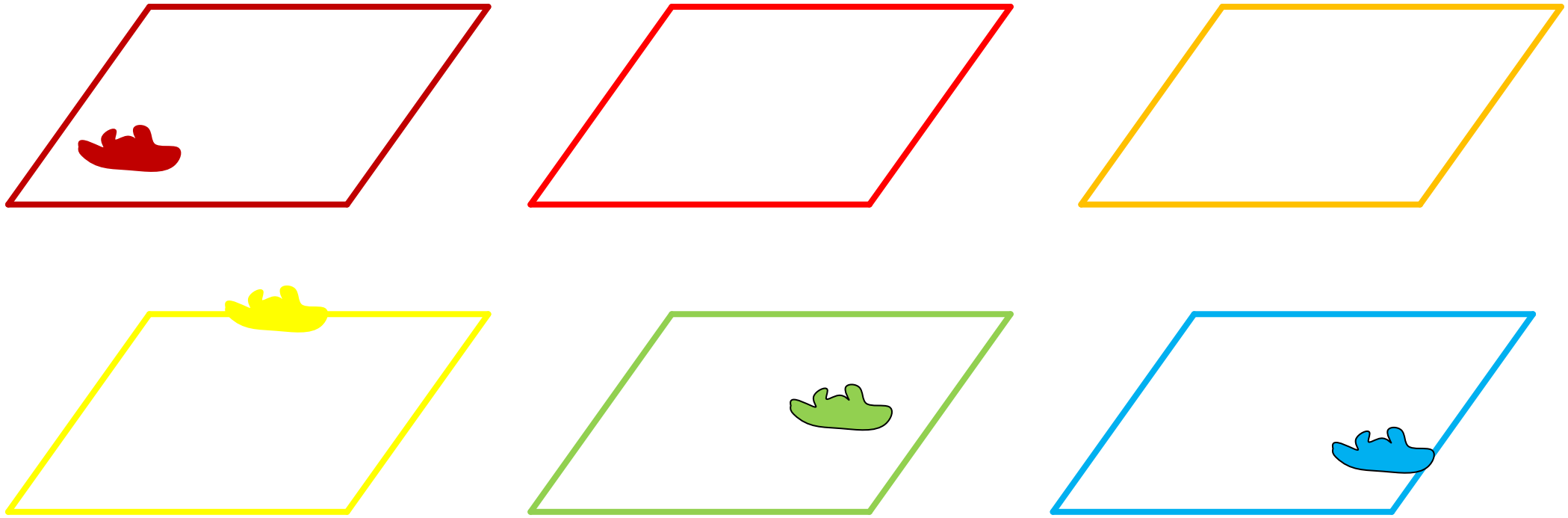


Woolf et al., 2016

Systematic and Incidental relationships of CO_2 and temperature II

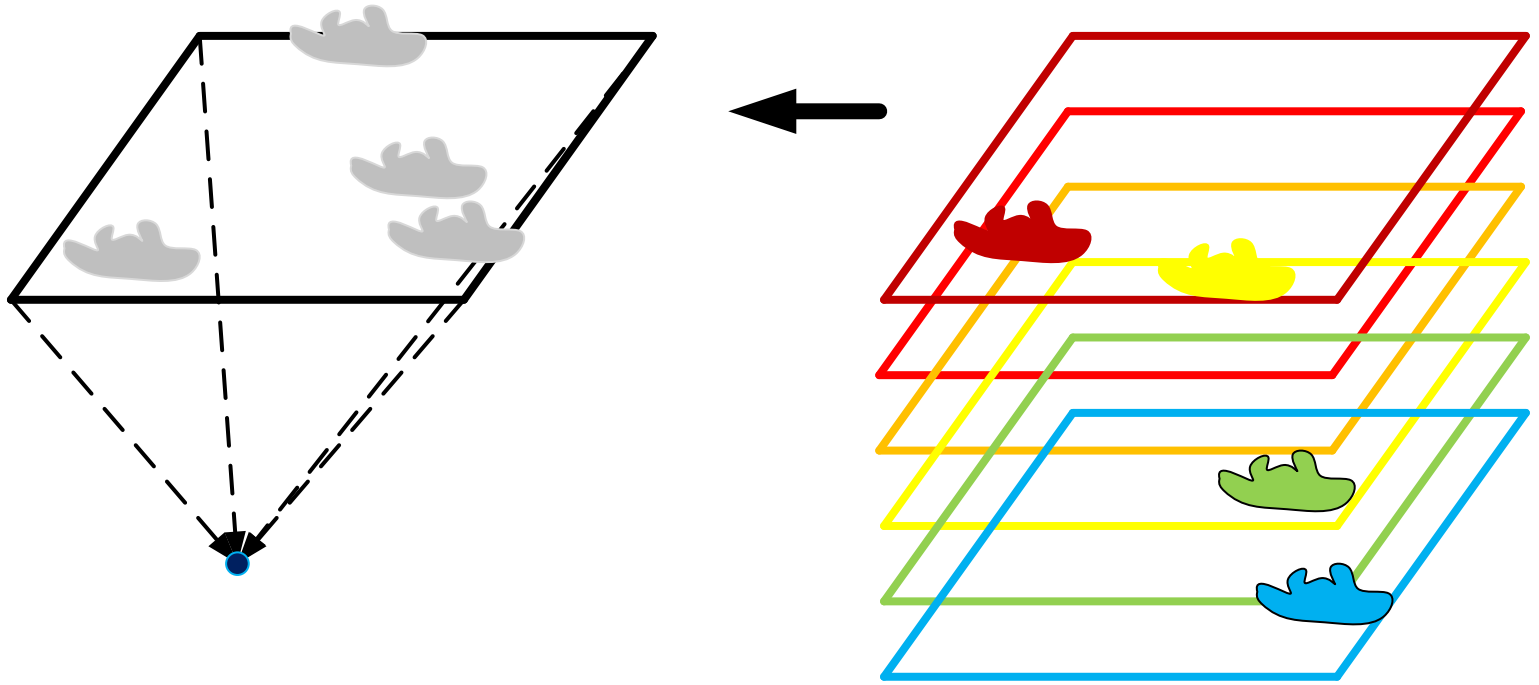
- A platform measures temperature and CO_2 at a particular location. What is the best estimate of CO_2 at a “neighbour” where the measured temperature is different? Options include
  - Assume pCO_2 is the same
  - Assume concentration of CO_2 is the same
  - Assume DIC is the same
  - Use a local empirical relationship
- With some elaboration this is the conundrum set by the combination of in situ, sparse and autocorrelated measurements of CO_2 from platforms (mainly underway ships) and relatively robust “gridded” measurements of SST from satellites.

Data Products; Scenes, grids and platforms



A grid square (e.g. 1° latitude x 1° longitude appears in scenes of one or more satellite instruments over each day of a month. On some of those days a measuring platform is somewhere within the grid square.

Data Products; Scenes, grids and platforms



Stack data from many times to form a monthly composite, further reduced to a single value **representative** of a “cube”, month x 1 degree latitude x 1 degree longitude

Options for combining data

- Assume pCO_2 is the same
  - $F = Tr\,\Delta pCO_2$
- Assume concentration of CO_2 is the same
  - $F_{CO2} = k.(C_{sw} - C')$
- Assume DIC is the same
  - As argued by Woolf et al. (2016)
- Use a local empirical relationship
  - But beware that those relationships will be time- and space-scale dependent

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They Give Different Answers

Why are there discrepancies in temperature?

- Sparse sampling of temperature by platform
- Disturbance of both temperature and CO_2 vertical profiles by the ship
- Estimates of warming between outside hull and equilibrator are incorrect

How should we correct?

- Sparse sampling of temperature by platform

Isochemical correction may be best within each month, but this needs testing

- Disturbance of both temperature and CO_2 vertical profiles by the ship

☹ Maybe only a substantial effect in warm layers; data will be very flawed

- Estimates of warming between outside hull and equilibrator are incorrect

☺ Isochemical correction is wholly appropriate (use equilibrator data, ignoring outside of hull estimates)

How can we know?

- Disturbance of both temperature and CO_2 vertical profiles by the ship

Detection and deletion or substitution of warm-layer data

- Sparse sampling of temperature by platform
- Estimates of warming between outside hull and equilibrator are incorrect

Return to the data.

On each platform, is there a similar bias between more localized subskin SST and in situ temperature? In that case, a poor estimate of warming is implied. Isochemical correction is appropriate.

How do CO_2 and SST correlate along track? This can provide insight into the appropriate correction.

Knowledge Gaps and Priorities (1, 5 and 10 years)

- 1 Year
  - Engage with Community
    - Data Providers; CO_2 and SST
    - Global Carbon Project (Contingent estimates)
  - Finalise Data Workflow
- 5 Years
  - Data collection and processing by proposed methods
  - ? Converge on agreed historical flux estimates ?
- 10 Years
  - Historical time series as a means to understand how the oceanic carbon sink works; and how it will behave in the future
  - New platforms, instruments, methods

Acknowledgments

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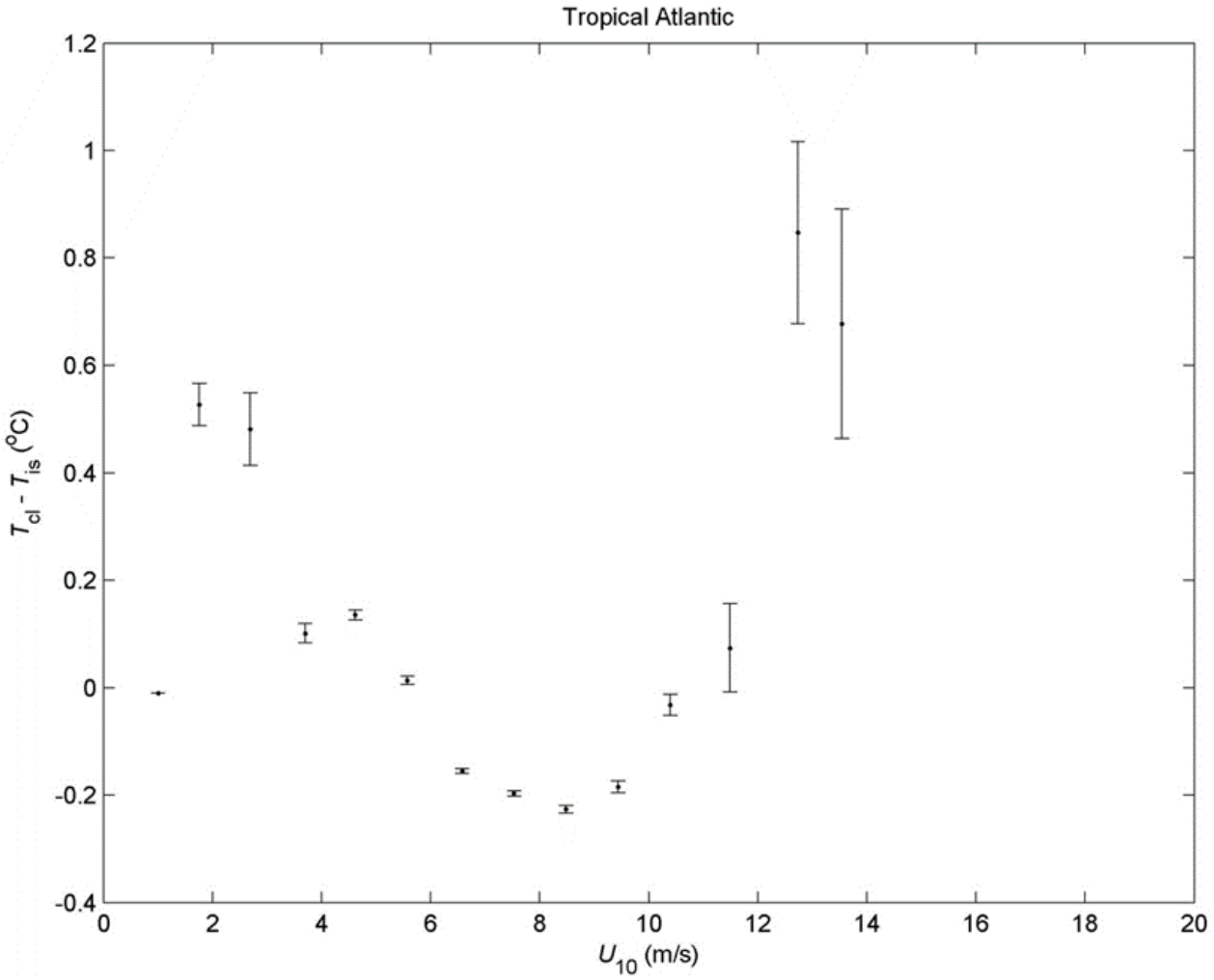
- European Space Agency OCEANFLUX Greenhouse Gases projects (contract numbers 4000104762/11/I-AM and 4000112091/14/I-LG).
- The Surface Ocean CO_2 Atlas (SOCAT) is an international effort, endorsed by the International Ocean Carbon Coordination Project (IOCCP), the Surface Ocean Lower Atmosphere Study (SOLAS) and the Integrated Marine Biosphere Research (IMBeR) program, to deliver a uniformly quality-controlled surface ocean CO_2 database. The many researchers and funding agencies responsible for the collection of data and quality control are thanked for their contributions to SOCAT.

Extra – some exploratory data analysis

Regional, Seasonal and Environmental Dependence of Temperature Discrepancy

- Discrepancies are very variable
- Depend on region and season
- Depend on wind speed



Goddijn-Murphy (unpublished from SOCAT v2)