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1. Introduction

1.1 OceanFlux GHG Overview

The air-sea flux of Greenhouse gases (GHGs) is a critical part of the climate system and a major factor in the development of the oceans (e.g. ocean acidification). More accurate and higher resolution calculations of these fluxes are required. We propose to deliver that improvement by bringing together expertise and capability in

- The physics of air-sea interaction and ocean waves.
- Marine Earth Observation
- Operational modelling of the oceans

A highly skilled and experienced international team has been constructed under the leadership of Dr. David Woolf from Heriot Watt University.

The main output from the project will be a global $1^{\circ} \times 1^{\circ}$ spatial resolution climatology and a higher spatial resolution subset of data for the European Shelf. This datasets will include information on data uncertainties and will be for the international SOLAS community to access and exploit.

Additional results and outputs from this project will include:

- Validated algorithms for studying air-sea gas interactions using Earth Observation.
- A number of key peer reviewed publications.

An end of project scientific workshop was held in September 2013 and this document provides a clear framework for future ESA involvement in SOLAS related studies.

1.2 Purpose and Scope of the final report

This is the OceanFlux Greenhouse Gases Final Report (FR). It is intended that this document presents the main aims and objectives of the project and then provides a detailed synopsis of the advancements and achievements.

1.3 Structure of this Report

The report is structured as follows:

- Section 1 (this section) the introduction gives an overview of the document aims and structure.
- Section 2 contains the original [SoW] objectives and benefits.



- Section 3 contains the OceanFlux GHG final report
- Section 4 contains the Scientific Impact Assessment Report as an annex.

1.4 Contributions

Table details the people who contributed to this report and the sections that they contributed to.

Section	Primary author(s)	Contributing author(s)
Section 1	Jamie Shutler (PML)	
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Section 5	David Woolf (Heriot Watt)	The whole OceanFlux project team.
	Jamie Shutler (PML)	

Table 1 Table of contributions.



1.5 Reference documents

This document makes reference to the documents listed in Table 2.

Reference	Document	
[SoW]	OceanFlux GHG Statement of Work ESRIN/AO/1-6668/11/I-AM 'Support to Science Element- OceanFlux'	
[RB]	OceanFlux GHG Requirements Baseline	
[TS]	OceanFlux GHG Technical Specification	
[GHG-WS]	OceanFlux Scientific workshop report.	

1.6 Definitions and acronyms

AATSR	Advanced Along Track Scanning Radiometer (ESA instrument)		
AMSR-E	Advanced Microwave Scanning Radiometer for EOS (NASA		
	instrument)		
ASAR	Advanced Synthetic Aperture Radar		
ATBD	Algorithm theoretical basis document		
AVHRR	Advanced Very High Resolution Radiometer (NOAA instruments)		
CO_2	Carbon dioxide		
DMS	Dimethylsulphide		
ECMWF	European Centre for Medium-Range Weather Forecasts		
Envisat	Environmental monitoring satellite		
EO	Earth observation		
EOS	Earth Observing System		
ERS	European Remote Sensing satellite (ESA instrument)		
ERSEM	European Regional Seas Ecosystem Model		
ESA	European Space Agency		
FTP	File transfer protocol		
GOTM	Generalised Ocean Turbulence Model		
IOWAGA	Integrated Ocean Waves for Geophysical and other Application		
IR	Infra-red (a piece of the electromagnetic spectrum)		
Jason-1	Altimetry mission (NASA/France instrument)		
Jason-2	Altimetry mission (NASA/France instrument)		
MERIS	Medium Resolution Imaging Spectrometer (ESA instrument)		
MODIS	Moderate Resolution Imaging Spectrometer (NASA instrument)		
NASA	National Aeronautics and Space Administration (US)		
NOAA	National Oceanographic and Atmospheric Administration (US)		
NOC	National Oceanography Centre (UK)		
OC-flux	ESA STSE project – Open ocean and Coastal CO ₂ fluxes in support		
	of carbon cycle monitoring		
OSTIA	Operational Sea Surface Temperature and Sea Ice Analysis (UK		
	Meteorological Office)		
PAR	Photosynthetically active radiation		
PML	Plymouth Marine Laboratory		



PMP	Project Management Plan
RA2	Radar altimeter 2 (ESA instrument)
SOLAS	Surface Ocean and Lower Atmosphere Study
STSE	Support to Science Element
TOPEX	TOPEX-Poseidon altimetry mission (NASA/France)
UHI	University of Highlands and Islands
WP	Work package
WPD	Work package description
1D	One dimensional
3D	Three dimensional
КО	Project kick off (November 2012)
SoW	ESA statement of work
GHRSST	Group for High-Resolution Sea Surface Temperature
GHRSST GDS	GHRSST Data Specification



2. The objectives and intended benefits

As defined in the original [SoW] the aim of the OceanFlux GHG study was to:

To improve quantitative air-sea flux estimates of CO_2 and other greenhouse gases using EO data in synergy in the Atlantic Ocean.

The objectives of the *OceanFlux GHG* study are to investigate the application of EO data in the Atlantic Ocean and European Shelf Seas and:

- 1. Develop novel or existing methodologies/algorithms and create new products derived from the use of EO data, *in situ* data and modelling for use by the SOLAS and other communities.
- 2. Estimate and reduce uncertainty in conventional gas transfer computations relative to EO driven computations,
- 3. Compute air sea gas transfer flux calculations using satellite derived mean square slope (MSS) estimates including a validated estimate of uncertainty,
- 4. Compute air sea gas transfer flux calculations using satellite derived surface waves and swells (white-capping) on bubble mediated gas transfer in high wind speed regimes including a validated estimate of uncertainty,
- 5. Compute the impact of biogenic surface slicks on EO derived air sea gas transfer flux calculations and their uncertainties,
- 6. Compute the impact of diurnal variability in SST, wind and other variables on EO derived air sea gas transfer flux calculations and their uncertainties,
- 7. Exploit modelling frameworks in synergy with satellite and *in situ* data to develop more dynamic and accurate estimates of air sea gas transfer on a sub-weekly timescale (including ecosystem components) and alleviate dependencies associated with the use of climatological data sets.

The expected benefits from the study are:

- 1. New dynamic and accurate estimates of GHG air sea gas transfer on a sub-weekly timescale based on the synergy between EO data, in situ data and models,
- 2. Improved understanding of the spatial and temporal variability in GHG air-sea gas transfer and the underlying processes governing flux rates,
- 3. New multi-sensor EO algorithms capitalising on the synergy between complementary EO data sets,
- 4. Novel data products and supporting documentation for use by the SOLAS and airsea interaction community,
- 5. Enhanced use and uptake of ESA and other Third Party EO Mission data by the SOLAS and air-sea interaction community,
- 6. New NOP model systems tuned to air-sea interaction and the carbon cycle,
- 7. A clear scientific roadmap for future activities to improve the quantitative understanding of the carbon cycle.

The remainder of this report is structured around the 7 objectives and presents the ways in which the project team addressed these objectives.



The work logic for the *OceanFlux GHG* project is shown in the Figure below. The *OceanFlux GHG* project shall be carried out within 24 months from the KO date. A mid term review (MTR) shall be held at KO+12 months.



Figure 2.3. Work logic diagram for the OceanFlux GHG project. Key meetings are shown in orange boxes.

Figure copied from the original [SoW] showing the different stages of the OceanFlux GHG project.

The OceanFlux GHG project is organised as seven tasks. In summary, these are:

- Task 1: Management and Coordination, Outreach, Communication and Promotion;
- Task 1.1. Management and Coordination;
- Task 1.2. Promotion and Scientific Outreach;
- Task 2: Technical Reference Baseline;
- Task 3: Technical Specifications;
- Task 4: Collection of Data Set;
- Task 5: Implementation, development and validation;
- Task 6: Scientific Analysis and Impact Assessment;
- Task 7: Scientific Roadmap, workshop and Study Closeout;



3. The OceanFlux Greenhouse Gases project

In late 2011, the OceanFlux GHG team started an ambitious programme of work to develop improve methods of calculating air-sea fluxes of greenhouse gases and to apply these methods for the creation of new flux climatologies. The research included quite fundamental research to place understanding of air-sea gas fluxes on a firmer scientific footing including a mechanistic understanding of air-sea exchange processes and the propagation of various uncertainties through to the finally calculated fluxes. The project also included an important technical element, primarily focussed on a versatile tool to enable broad participation in the calculation of air-sea gas fluxes, the FluxEngine (Abstract 7, Section 6). Within the bounds of the existing project, the FluxEngine has primarily been used internally (though not exclusively) and for prototype climatologies. The FluxEngine is an important initiative and needs to be developed and promoted to ensure its uptake and use by the international community (also see section 3.6)

The project continued contemporaneously with a large amount of related research, which fits under the umbrella of the International Surface Ocean Lower Atmosphere Study (SOLAS).

OceanFlux GHG was a recognised project of SOLAS and considerable interaction with SOLAS scientists and administrators occurred throughout the project, but as is the nature of things, the OceanFlux GHG team concentrated on their own immediate tasks for much of the project, as did other SOLAS teams. In this context, an international workshop organised by the OceanFlux GHG team and held by one of the partners, IFREMER, in September 2013 was critical in bringing the community together, presenting the OceanFlux outputs and identifying routes of future research and focus. The workshop was very successful in attracting the attendance of many of the leading practitioners in this area of science and much relevant research was presented and discussed. The workshop has also been important to the OceanFlux GHG team in developing a clear perspective on the broader scientific priorities of SOLAS with respect to this science area and particularly what developments we could make that would be most useful to the broader community.

The ESA OceanFlux GHG project focused primarily on interfacial transfer rates and thus, upon concentrations on either side of the sea surface and their corresponding airsea transfer coefficients. The significance of OceanFlux GHG extends more broadly for example to the global marine cycling of carbon. For example, the position of OceanFlux GHG in the broader context of marine carbon cycling is illustrated in Figure 1. A wide range of scientific activities are relevant to marine carbon cycling. These include the international SOLAS program spans the interface taking in processes also in the lower atmosphere and in the upper ocean. The international IMBER program overlaps with SOLAS in the upper ocean but is primarily concerned with marine biogeochemical cycles and ecosystems including the exchange of carbon between the upper ocean and the deep ocean.

The specific focus of OceanFlux-GHG is encapsulated in the air-sea gas flux equation (see Figure 1). The determination of the global fluxes, F, of carbon dioxide and other greenhouse gases is the primary objective and to reach that goal, the various parameters on the right-hand side of the equation must first be determined. OceanFlux-GHG spent much of its effort in the determination of the transfer velocity, k. Transfer is primarily a



result of stirring at and near the interface by the wind, but the process is complicated by wave physics generally, by breaking waves and bubbles at high wind speeds and by surfactants and convection at low wind speeds. The net flux, F, is also proportional to the concentration difference across the interface, written in Figure 1 as the product of solubility, α , and partial pressure, p, at either side of the interface. OceanFlux-GHG depended on measurements and archiving of partial pressures external to the project. In particular, it relied on SOCAT to provide measurements of oceanic partial pressure of carbon dioxide. OceanFlux-GHG also devoted a large amount of resource and time to the determination of solubilities (dependent on temperature and salinity) and to the correct calculation of the concentration difference.

OceanFlux GHG $f = k (a_w p CO_{2w} - a_s p CO_{2a})$ Surface ocean $p CO_{2w}$ F mix F biological pump F solubility pump IMBER

Carbon export to the deep ocean

Figure 1. A schematic of marine carbon cycling indicating the scope of OceanFlux GHG and of the large international programs SOLAS and IMBER.

3.1 Benefit and impact of EO data for SOLAS research

The ocean and atmosphere are major components of the Earth's surface, with reactions within and between them controlling many of the properties of the Earth's system. The air-sea interface represents a vital link between the oceans and the atmosphere by acting as the conduit for the transfer of heat, momentum, aerosols, and gases between the two phases. In particular, the flux of gases such as oxygen (O_2), dimethyl sulfide (DMS), carbon dioxide (CO_2), and volatile iodocarbons (VICs) across the interface is of fundamental importance to studies of marine productivity, biogeochemical cycles, atmospheric chemistry, Earth's climate, and human health. Furthermore, the surface exchange of heat and momentum is responsible for the dynamic circulation of the atmosphere and oceans. It is therefore important to quantify contemporary air-sea fluxes of gases and also to provide the understanding necessary to project possible future changes in these fluxes.

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Therefore understanding the pathways, sources, sinks, and impact of these gases on the Earth's climate system is essential for monitoring climate and predicting future scenarios. Space observations have an important role to play in such research through providing quasi-synoptic, reproducible and well-calibrated measurements for driving, parameterising and enhancing climate models. Indeed, Earth observation is potentially the only way of reliably monitoring global air-sea fluxes. In contrast, in situ data instrumentation provides spatially limited (sparse) data. The deployment and maintenance of environmental instrumentation on land is fairly routine, whereas the deployment of retrieval of instrumentation at sea is both challenging and orders of magnitude more expensive. Therefore remote methods, offered by satellite Earth observation, are the only practical way to efficiently monitor the Earth's marine surfaces and health.

The flux of gases between the atmosphere and the ocean (air-sea) is controlled by wind speed, sea state, sea surface temperature and surface processes including any biological activity (figure 2) and most of these processes can be studied using satellite Earth observation, either directly (e.g. sea state) or via proxies. Collectively this means that the following Earth observation data can be used to support air-sea gas studies: wind speed at 10m, significant wave height, sea surface temperature (skin and foundation), backscatter (sea surface roughness), ocean colour and sea-ice extent.



Figure 2 The air-sea flux of gases and the various processes that are believed to control these fluxes (Jayne Doucette, Woods Hole Oceanographic Institution, and Wade McGillis, Columbia University).

3.2 Challenges and advances – The OceanFlux GHG narrative

The OceanFlux-GHG project began by reviewing existing gas transfer velocity and whitecapping parameterisations (abstracts 1,2 below and annex of the SIAR). Focus then shifted towards unifying the methods for handling temperature and salinity within air-sea gas flux calculations (abstract 3 below). Many published studies had already used these methods, but others were ignoring the importance of near-surface effects,



therefore, the project focused on unifying the body of work to provide a clear path and approach for future studies. These methods were then used to produce a global climatology of fugacity measurements from the Surface Ocean CO₂ Atlas (SOCAT) (abstract 4). The project then highlighted the advances of the use of altimeters (both single and dual frequency) for characterising the direct component of the gas transfer velocity by using dimethylsulphide gas measurements to calibrate satellite retrievals of transfer velocity using two approaches (abstracts 5 and 6). The dual frequencyaltimeter approach developed by the project shows improved performance (reduced uncertainty) over that of purely wind-speed-based approaches. All of the methods and algorithms developed thus far were then combined within a data processing system. The project further developed this system (now called the FluxEngine) to support a large number of the scientific studies within the project (abstract 7). The focus of the project then shifted to the derivation of a full uncertainty budget for air-sea flux calculations. The FluxEngine was used to run a series of clearly defined ensemble runs to investigate the impact on global fluxes of the different components of the total uncertainty. This enabled the project to determine a new global climatology of air-sea carbon dioxide fluxes (Figure 3 and abstract 8) that includes for the first time a full uncertainty budget (abstract 9). The FluxEngine was then used to investigate the impact that rain can have on global air-sea CO₂ fluxes (abstract 10).

In parallel to all of this work the project also used Envisat datasets to study Arctic airsea CO_2 fluxes and their sensitivity to a changing climate (abstract 11). Towards removing the need to rely on *in situ* data, the performance of a hydrodynamic ecosystem model to derive shelf-sea and coastal partial pressure of CO_2 was also investigated. This work looked at issues including near-surface temperature gradients, biological slicks and data assimilation of satellite Earth observation data (abstract 12). The project published four peer reviewed journal articles and a further six journal papers are being prepared for submission to journals (see section 7 of this document and the annex of he SIAR). The use of a wave model to estimate whitecapping was also investigated and evaluated as an approach to parameterise bubble mediated gas transfer (abstract 13).

The following sections are the abstracts from each of the journal manuscripts (published or in draft), published conference papers and in one case from the technical report that resulted from the project.





Air-sea CO2 flux using the unset unset gas transfer velocity (k) (g C m-2 day-1)

Figure 3 Mean air-sea flux of CO₂ for 2010 from the OceanFlux-GHG climatology.

3.3 Responding to the objectives

The follow sections details how the project addressed each of the original objectives set by ESA in the [SoW]. All of the abstracts that are referred to in this section can be found in section 4 (the SIAR annex).

Develop novel or existing methodologies/algorithms and create new products derived from the use of EO data, *in situ* data and modelling for use by the SOLAS and other communities.

One focus of the OceanFlux GHG project was to unify the methods for handling temperature and salinity within air-sea gas flux calculations (abstract 3). Many published studies had already used these methods, but others were ignoring the importance of near-surface effects, therefore, the project focused on unifying the body of work to provide a clear path and approach for future studies.

All of the methods and algorithms developed within the project were combined within a data processing system. The project further developed this system (now called the FluxEngine) to support a large number of the scientific studies within the project (abstract 7). The FluxEngine system is available for the community to use and is already being used within other UK and ESA projects (see section 3.6, point 5).

Within OceanFlux GHG, the FluxEngine was used to run a series of clearly defined ensemble runs to investigate the impact on global fluxes of the different components of the total uncertainty. This enabled the project to determine a new global climatology of air-sea carbon dioxide fluxes (Figure 3 and abstract 8) that includes for the first time a more complete uncertainty budget (abstract 9).

For a reference year of 2000, OceanFlux estimate a net global flux from air to sea of 2.0 Pg C yr⁻¹, but with a high bias uncertainty. An optimistic interpretation of existing uncertainty in gas transfer velocities leads to a bias uncertainty of ~0.5 Pg C yr⁻¹, while a more pessimistic interpretation implies a bias uncertainty > 1 Pg. Having identified and classified the errors we make a preliminary assessment of their significance to the bias uncertainty in global and basin-scale air-sea gas fluxes. While the limited number of measurements of dissolved gas concentration is certainly an issue for all gases, it appears that dispute over gas transfer velocities is a greater issue for carbon dioxide especially in basins such as the North Atlantic where observations of dissolved concentration are relatively common.



Estimate and reduce uncertainty in conventional gas transfer computations relative to EO driven computations

The OceanFlux-GHG project began by reviewing existing gas transfer velocity and whitecapping parameterisations (abstracts 1,2).

The FluxEngine (abstract 7) was used to run a series of clearly defined ensemble runs to investigate the impact on global fluxes of the different components of the total uncertainty. This enabled the project to determine a new global climatology of air-sea carbon dioxide fluxes (Figure 3, abstract 8 and 9). Initial results from this work were presented at the OceanFlux workshop and a draft journal paper is now complete (see Section 7).

The work has highlighted that the uncertainties (when taking into account the total uncertainty) is considerably larger than researchers had originally appreciated. While the limited number of measurements of dissolved gas concentration is certainly an issue for all gases, it appears that dispute over gas transfer velocities is a greater issue for carbon dioxide especially in basins such as the North Atlantic where observations of dissolved concentration are relatively common.

Compute air sea gas transfer flux calculations using satellite derived mean square slope (MSS) estimates including a validated estimate of uncertainty

The OceanFlux GHG work studying Arctic waters exploited the use of existing MSS and bubble mediated parameterisations and highlighted that re-calibration of these approaches was needed, as the estimates produced were significantly higher than wind speed based parameterisations (abstract 11, Land et al., 2012).

OceanFlux GHG then highlighted the advantages of the use of altimeters (both single and dual frequency) for characterising the direct component of the gas transfer velocity by using dimethyl-sulphide gas measurements to calibrate satellite retrievals of transfer velocity using two approaches (abstracts 5 and 6, Goddijn-Murphy et al., 2012; 2013). The dual frequency-altimeter approach developed by OceanFlux GHG shows improved performance (reduced uncertainty) over that of purely wind-speed-based approaches.

OceanFlux used experimental data from the same cruises to show that using the difference between the Ku-band and C-band signals, and thus reducing the contribution from longer waves, improved the *K* estimates. This is consistent with the theory that gas transfer is largely controlled by short capillary-gravity waves.

Compute air sea gas transfer flux calculations using satellite derived surface waves and swells (white-capping) on bubble mediated gas transfer in high wind speed regimes including a validated estimate of uncertainty

The FluxEngine (abstract 7) was used to run a series of clearly defined ensemble runs to investigate the impact on global fluxes of the different components of the total uncertainty. This work included estimates of total transfer using the OceanFlux GHG



re-calibrated direct transfer (as derived from altimeters) and an existing bubble mediated transfer parameterisation.

The use of a wave model to estimate whitecapping was also investigated and evaluated as an approach to parameterise bubble mediated gas transfer (abstract 13). However, in terms of calibrating the bubble mediated transfer, the work (after much effort) was inconclusive and this challenge still remains. Alternative approaches to parameterise bubble mediated transfer need to be investigated, potentially through the use of wind-wave tank experiments.

Compute the impact of biogenic surface slicks on EO derived air sea gas transfer flux calculations and their uncertainties

Towards removing the need to rely on *in situ* data, the performance of a hydrodynamic ecosystem model to derive shelf-sea and coastal partial pressure of CO_2 and air-sea fluxes was investigated. This work looked at issues including near-surface temperature gradients, biological slicks and data assimilation of satellite Earth observation data (abstract 12). The work highlighted that the impact on the air-sea fluxes due to biological slicks was very small. Impacts due SST diurnal cycle and near-surface SST gradients were much more important.

The OceanFlux Arctic study (abstract 11) highlighted that methods for estimating airsea fluxes which account for biogenic slicks should be used when studying air-sea CO_2 fluxes in the Kara Sea. We may conclude that using k parameterizations explicitly incorporating surface roughness, derived for example from satellite backscatter data should give a more accurate representation of Arctic CO_2 exchange than those based on wind speed alone. This conclusion supports the OceanFlux work on MSS parameterisations (abstracts 5 and 6). As minimum, uncertainty estimates that correctly account for the impact of biology on the CO_2 gas transfer estimate should be included in future air-sea CO_2 gas flux estimates for the Kara Sea.

Compute the impact of diurnal variability in SST, wind and other variables on EO derived air sea gas transfer flux calculations and their uncertainties

It was found that the impact on the air-sea fluxes due to biological slicks was very small. Resolving the near-surface temperature gradients had the largest impact at short, seasonal and annual time scales and results in improvements across all of the evaluated variables. This result highlights and supports the importance of the OceanFlux re-evaluation of the handling of temperature within air-sea gas flux studies (abstract 3).

The FluxEngine was used to investigate the impact that rain can have on global air-sea CO_2 fluxes (abstract 10). The Pacific and Southern ocean monthly net fluxes can be significantly modulated by rain with regular variations of $> \pm 15\%$. Instances of very large modulation of $> \pm 50\%$ are also possible. The impacts of rain should be included in the uncertainty analysis of studies that estimate net air-sea fluxes of CO_2 as the rain can have a considerable impact on the fluxes, dependent upon the region and timescale.



This work highlighted the need to include the impact of rain within the uncertainty estimate of the global and regional fluxes. The impact on regional air-sea fluxes can be significant, dependent upon the region of interest.

Exploit modelling frameworks in synergy with satellite and *in situ* data to develop more dynamic and accurate estimates of air sea gas transfer on a sub-weekly timescale (including ecosystem components) and alleviate dependencies associated with the use of climatological data sets.

Towards removing the need to rely on *in situ* data, the performance of a hydrodynamic ecosystem model to derive shelf-sea and coastal partial pressure of CO_2 and air-sea fluxes was investigated. This work looked at sub-weekly sir-sea gas fluxes, and issues including near-surface temperature gradients, the impact of diurnal SST cycles, biological slicks and data assimilation of satellite Earth observation data (abstract 12).

The model correctly reproduces the seasonality of nutrients (correlation > 0.80 for all three macronutrients silicate, nitrate and phosphate), surface chlorophyll (correlation > 0.43) and total biomass (corr>0.7) in a two year run for 2008-2009. The model simulates well the concentration of DIC, pH and in water partial pressure of CO_2 (pCO₂) with correlations between 0.4-0.5.

The use of a wave model to estimate whitecapping was also investigated and evaluated as an approach to parameterise bubble mediated gas transfer (abstract 13). The model generated whitecapping estimates were included in the project climatology within the process indicator data.

The OceanFlux work provided a useful validation test for model-derived whitecap coverages. We were able to conclude that both the model-derived whitecap coverages and the classical MW1979 parameterisations were credible inputs to transfer velocity parametrisations that required an estimate of whitecap coverage. However, the continuing difficulty in acquiring high-quality and reproducible estimates of whitecap coverage by in situ methods remains a brake on progress. Some initial objectives of the project (notably to investigate the temperature-dependence of whitecapping) proved to be impractical because the data passing QC were insufficient. Further progress in measuring whitecap coverage and evaluating environmental signals and quality control methods, preferably exploiting both in situ and satellite-based methods, remains a priority. Future work in this area would benefit from instrumentation on fixed platforms, enabling a much larger and consistent dataset to be collated and analysed.

3.4 Outputs

Listed below are the main outputs from the OceanFlux-GHG project. These outputs fall under the following six categories i) published journal papers, ii) draft journal papers, iii) published conference papers, iv) technical reports, v) community datasets and tools and vi) a youtube video.

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Published peer review journal papers

Goddijn-Murphy, L., D.K. Woolf and C.A. Marandino. (2012) Space-based retrievals of air-sea gas transfer velocities using altimeters: Calibration for dimethyl sulphide. *Journal of Geophysical Research* 117, C08028, doi:10.1029/2011JC007535.

Goddijn-Murphy, L., D.K. Woolf, B. Chapron and P. Queffeulou (2013) The enhancement of using dual-frequency, instead of single-frequency, altimeter backscatter for estimating air-sea gas transfer velocity, *Remote Sensing of the Environment*.

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Woolf, D., L. Goddijn-Murphy, J. Prytherch, M. Yelland, P. Nightingale, P., J. Shutler, J-F. Piolle, J. Hanafin and B. Chapron. (2013) Uncertainty and ambiguity in air-sea gas fluxes; a flexible system in response to a debate on transfer velocity. ESA Living Planet Symposium 2013, Edinburgh, UK, 9-13 September 2013.

Woolf, D.K. and Goddijn-Murphy L. (2012) The importance of whitecapping to air-sea interaction and earth observation approaches to its retrieval. In *"Earth Observation for Ocean-Atmosphere Interactions Science"* Symposium Proceedings, SP-703 (CD), ESA.

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Quartly, G., J. Shutler and D. Woolf. (2013) A global study of the correlation properties of wind and rain. ESA Living Planet Symposium 2013, Edinburgh, UK, 9-13 September 2013.

Technical reports

J. Hanafin, F. Ardhuin, B. Chapron, M. Yelland, B. Moat. (2013) Comparison of WAVEWATCH-III ® model output whitecap fraction with *in situ* observations, ESA OceanFlux-GHG technical report.

Community datasets and tools

OceanFlux Greenhouse Gases global climatology of air-sea CO_2 fluxes version 0.95 (v0.95)

FluxEngine air-sea flux data processing tool.

youTube video

Sea, satellites and CO₂ <u>http://www.youtube.com/watch?v=4uak0vVGgGY</u>



3.5 Benefit and impact of close collaboration with the international community

OceanFlux-GHG has benefitted from close collaboration with the a number of different international communities and initiatives. In most cases the collaboration has been mutually beneficial for all those involved (i.e. ESA, OceanFlux and the initiative in question). OceanFlux-GHG has collaborated with the following international groups and initiatives:

1. The International Surface Ocean - Lower Atmosphere Study (SOLAS) project is an international research initiative aiming to understand the key biogeochemical-physical interactions and feedbacks between the ocean and atmosphere. International SOLAS has supported the OceanFlux projects from their gestation. It remains an important vehicle for ensuring both that this and similar projects are genuinely targeted to recognised scientific priorities and for enabling the promotion of the project and its interactions with related projects. We would expect any future projects to benefit from an active involvement with and from SOLAS.

2. The Surface Ocean CO_2 Atlas (SOCAT) is an international initiative to establish a global surface CO₂ data set that would bring together, in a common format, all publicly available fCO₂ data for the surface oceans. SOCAT is in some senses a complementary activity to OceanFlux GHG that has developed broadly in parallel. A genuine (two-way) interaction has only developed slowly and there should be more interaction in any future projects. It is also important to note that SOCAT has primarily been a voluntary activity with very limited funding. Since the continued flourishing of SOCAT is important to OceanFlux and the broader scientific community, it would be appropriate (if future OceanFlux projects are funded) that ESA STSE and SOLAS contribute to the funding of SOCAT by some means. Since the SOCAT data is important to flux estimates and also SOCAT and OceanFlux participants have to a large extent complementary expertise it will be important to build a stronger relationship. SOCAT should have input to future FluxEngine developments including the estimation of fCO₂ gridded fields from the sparse SOCAT measurements. OceanFlux participants and ESA scientists may be able to provide useful input to SOCAT, from data quality control with respect to uncertain temperature, through processing with respect to temperature and salinity and to the correct application of Earth observation data.

3. The Global Carbon Project (GCP) was established in 2001 in recognition of the large scientific challenges and critical nature of the carbon cycle for Earth's sustainability. The scientific goal of the project is to develop a complete picture of the global carbon cycle, including both its biophysical and human dimensions together with the interactions and feedbacks between them. Thus, the Global Carbon Project has a much broader remit with respect to CO_2 than OceanFlux GHG; it extends to the entire global carbon budget, not just the air-sea flux. Within this context the air-sea fluxes are important since they help to close the global carbon budget. At least in some basins, e.g. North Atlantic it is generally assumed that the air-sea flux is better constrained than neighbouring terrestrial sources and sinks. Thus the terrestrial budgets are often inferred



by closing the budget using estimates of the marine flux. We have shown in OceanFlux-GHG however that existing estimates of the marine flux are not as secure as sometimes supposed. There should be a role for a future project both to improve the estimates of the basin-scale air-sea fluxes (as estimated via the air-sea flux equation) and to communicate both the central estimates and realistic uncertainties to those involved in the broader global carbon budget. That interaction may be best pursued through interaction with the Global Carbon Project who have already expressed an interest.

4. Support for more joint meetings was highlighted in the OceanFlux-GHG scientific workshop minutes. There is always some risk of a "silo mentality" and while those meeting at OceanFlux GHG workshop were generally not strangers at the beginning of the workshop, some significant miscommunication and misinformation was made apparent by the workshop. While large established meetings such as the International SOLAS Open Science Conference play a large role, they may not be sufficiently focussed or attract the appropriate cross-disciplinary community to address specific issues. It is proposed that future workshops should be organised with highly focussed aims, but also solicit the support of SOLAS, GCP, EGU or similar.

5. Close collaboration with the Group on High Resolution Sea Surface Temperature (GHRSST) community meant that the project could access SST experts and datasets, which were key to generating the fCO2 climatology, the basis of the OceanFlux air-sea gas flux climatology and also key for refining methods.

6. Close collaboration with the ESA Climate Change Initiative (CCI, SST and Ocean Colour) and ESA GlobWave projects meant that OceanFlux could exploit all of the datasets from these projects. The ESA CCI SST and GlobWave datasets were key for all of the OceanFlux research and outputs. The CCI projects benefitted, as the OceanFlux outputs were an early example how multiple CCI project outputs could be exploited in synergy.

7. Close collaboration with Prof. Andy Watson FRS and Prof. Jonathan Sharples and their research groups at the University of Exeter and the University of Liverpool repectively has enabled the exploitation of FluxEngine within four major UK NERC projects (RAGNARoCC, Deliverable D, CANDYFLOSS and Blue Carbon see point 5 in section 6). This has helped OceanFlux gain further exposure and these projects have benefitted through exploiting the FluxEngine community tool.

3.6 Lessons learnt and feedback to ESA

The following section describes a number of lessons that have been learnt, or became apparent during the project.

1. Throughout the project one of main aims has to be maximise peer-reviewed publications. However, the need for many ESA documents can direct effort away from science and project advancement. It would benefit all (both funder and contractors) if all deliverables could be based around scientific publications. In this way the main ESA deliverable can effectively become a 'wrapper' for the draft scientific publication. The OceanFlux project team tried to do this, but most of the time the focus was always on providing the ESA deliverable as the main priority, so the deliverables were not always structured or focussed in a way that would enable easy publication. Viewing each deliverables as a publication first and ESA deliverable second, will help in future



projects. The ESA 'wrapper' can then pick out the ESA specific information from the draft publication (annex) or add to it where the draft publication has insufficient information or detail.

2. The OceanFlux Greenhouse project has clearly made a large amount of progress in a relatively short period of time with a comparatively small budget. For instance, the project has published 4 journal papers and has another 6 in draft. This Equates to a cost of \in 35000 per journal paper (ie \in 350000/10) whereas UK government research council funded research (e.g. NERC) is assumed to have a cost of \geq 70000 per journal paper. The main reason for the low cost per journal paper within the OceanFlux-GHG project is that by building on previous work, efforts and experience has greatly increased and accelerated the outputs from the project. The high level of output from the OceanFlux-GHG would not have been possible if the team had started completely from the beginning. Examples of this include:

- Much of the altimeter algorithm development exploited previous work funded UK National Centre for Earth observation (NCEO) projects.
- The source code for the FluxEngine heavily exploited a previous ESA fellowship (fellow Shutler) source code and work.
- Pre-processing of all data benefitted from Nephelae cloud and ESA GlobWave tools.
- Data formats exploited ESA GlobWave NetCDF formats.
- The use of generic data formats across projects eased their use within the project ie OceanFlux-GHG used ESA Ocean Colour CCI, ESA Sea surface temperature CCI and ESA GlobWave, all data that were available in NetCDF formats.

3. Journal papers motivate scientists, therefore deliverables based on journal papers is a good approach to encourage and ensure a high level of scientific and technological output. Journal papers do not have to be solely based on scientific outputs. It is just as valid to publish technological advances (e.g. the FluxEngine journal paper from this study). Therefore even technology driven projects (or technology aspects of scientific projects) can, and should be, expected to publish journal papers.

4. The contractor should be wary of trying to do too much and ESA should be wary of asking for too much additional work. A balance needs to be met. Substantially increasing work can have unexpected and indirect impacts e.g. work can get dropped and staff fall ill. Within OceanFlux-GHG there was often a tendency to try and develop all ideas and leads that arose from discussions at the various meetings. Doing so can result in too much extra work being generated and a loss of focus from the main tasks. Care should be taken in this respect. e.g. some work (whilst potentially beneficial long term) should be recorded and put on hold for future investigation, and the main focus of the study should be prioritised.

5. The FluxEngine system is already being used within the following projects:

• UK NERC/Defra CANDYFLOSS (2014-2017) (European shelf sea air-sea fluxes).



- UK NERC RAGNARoCC (2013-2017) (open ocean air-sea fluxes).
- UK NERC Deliverable D (2013-2017) (open ocean air-sea fluxes)
- UK NERC/Defra Blue Carbon (2013-2017) (shelf sea air-sea fluxes)
- A PhD project (supervisors: Goddijn-Murphy and Woolf).
- ESA Pathfinders-Ocean Acidification (2014 2016).

Further exploitation of the FluxEngine and the project outputs are expected when the key journal papers have been published (ie the kriging, FluxEngine and climatology papers). Full exploitation is not expected until these papers are published, as the science community will want peer-review process go happen before fully relying on the project data and systems.

4. Scientific priority areas for future work

The following sections detail the priority areas identified within discussion at the OceanFlux scientific workshop in 2013 and during the final project meeting.

Scientific Workshop

Here follows an analysis of the issues that either provoked intensive discussions and/or issues that came up in discussion multiple times during the project scientific workshop. The evidence for this analysis is found in the minutes for the discussion sessions in the Annexes (Section 3) of the [GHG-WS]. The following text has been copied from the [GHG-WS].

1. There is a need to understand and evaluate air-sea exchange in high winds (> 15 ms⁻¹) and related uncertainties. Empirical relationships have been developed for estimating k in hurricane conditions, however the impact of such systems on net-integrated fluxes in the Atlantic and Pacific have yet to be fully studied as most global flux studies concentrate on monthly fluxes that may miss such events (examples of high wind phenomena include hurricanes and polar lows). The limited understanding of air-sea exchange in strong winds was discussed and it seems timely to address the remaining uncertainties with the wide range of tools (ranging from Earth Observation through in situ measurement, physical modelling and numerical modelling to new theoretical paradigms) now available.

2. There is a need for a marine carbon observing system i.e. as part of the International Carbon Observing System (ICOS). EO has a clear role to play in developing a capability. The OceanFlux-GHG data processing system (FluxEngine) could be a component of such a system. The continued development of a "marine carbon observing system" was strongly endorsed by delegates. It was noted that the marine component lags behind other elements of the global carbon observing system, while accurate estimates of the North Atlantic sink, for example, are a realistic goal and can provide tight constraints on the terrestrial budget.



3. Air-sea gas flux work needs to further exploit EO, models, and in situ data (see 5 and 6 below). In situ data from fixed platforms is an under exploited resource. Environmental monitoring platforms exist in the Gulf of Mexico. Offshore oil rigs and wind farms also offer great potential.

4. There is a need to study other gases and not just CO_2 . e.g. behaviour or characteristics of gases other than CO_2 can help to interpret CO_2 fluxes or indirectly infer carbon cycling. Some research cruises are now addressing a multiplicity of gases including in situ data collection and process studies.

5. There is a clear need for the community to support the SOCAT (Surface Ocean CO_2 Atlas) initiative. This initiative is already producing very valuable outputs and it needs the community support (both time and funding) to continue.

6. Different mapping and interpolation methods can hide and/or create problems when interpreting data. The impacts of this on global net integrated air-sea fluxes are unclear as yet. The SOCAT community have begun to look at this by organising a community inter-comparison.

7. It was identified that very little EO work has concentrated on Ocean acidification. This could be an opportunity for future work. Note: ESA STSE have a funding call open at the time of the workshop focussed on developing novel EO ocean acidification products.

8. The issues of freshwater inputs from large river systems and rain and their impact on CO_2 other gases was discussed. This also links with the Ocean Acidification case already discussed. This is one area where EO could clearly help. E.g. use of SMOS or Aquarius data for freshwater inputs from large river systems.

9. There is a clear need for the community to use standard techniques and data formats. Other scientific communities are doing this, whereas the flux community has been slow to take this up. OceanFlux-GHG is using Climate Forcing (CF) compliant NetCDF format data.

10. There appears to be a need to develop clear routes for communication of scientific developments and results through to policy.

11. There is a clear need to identify the sources of and reduce the size of uncertainties in current air-sea flux estimates and approaches. OceanFlux-GHG has been working on this and David Woolf gave a presentation on this at the workshop. The use of ensembles can be used to study uncertainties in air-sea gas fluxes. This is an approach that has been used with some success in the climate modelling community. It is not always possible to quantify all of the uncertainties, but it is still important to provide a reasonable range in the values on those that can't be quantified.

12. A number of disciplinary communities are interested in the air-sea flux of CO_2 . There is a clear need for the broader air-sea CO_2 flux community to meet frequently to learn from each others' work and advances. This workshop has highlighted the benefit of such communication. This approach can be used to help pool resources and focus effort (and to avoid duplication).



13. The in situ gas flux community needs to start collecting SSTskin data and mean square slope data. The skin data should be used for the air-sea flux calculation and the mean square slope data will help support efforts to investigate more physically explained methods to parameterise the gas transfer velocity. If we want to exploit EO more, then we need to collect in situ data that is directly comparable to the EO data and the processes of interest.

Final project meeting

The following information resulted from the final project meeting. All of the information has been copied with minor amendments from the final meeting minutes.

1. Further study of diurnal impacts is really needed. OceanFlux-GHG only really touched upon this (ie methods development and 1D modeling study in coastal waters).

Typical diurnal SST signals could be used along with a range of other shapes to study the impact of warming cycles. There is a PhD thesis of potential use – A global study of diurnal warming, Alice Stuart-Menteth, University of Southampton PhD 2004 (Cosupervised by Craig Donlon while at the University of Southampton). Available on request from

http://www.southampton.ac.uk/library/resources/documents/thesisrequestform.pdf.

Some potential examples for upwelling work could be the impact on monthly fluxes, sensitivity and to highlight need for high resolution sampling in the future. As a starting point we could use the diurnal variability via day/night differences. There is the potential to use SEVIRI data in the Atlantic, and the potential to link this with N. Atlantic work. IFREMER have SEVIRI data due to GHRSST involvement.

2. Ocean Think Tank: a potential approach to determine links and highlight where future ESA STSE work can go. We would need people with broad overviews of science and not just specialists, so could include engineers and scientists. Possible questions, what is feasible, what is missing, what can be achieved quickly, strategy for the future and you would need to include young people (ie to provide a fresh perspective on issues).

3. Gas exchange within regions of melting/breaking pack ice have yet to be quantified. Cryosat data could be used to evaluate this e.g. using ku band derived k that OceanFlux-GHG has developed. This could be used to illustrate the advances of OceanFlux and this would also link with project's published Arctic work to make a nice web story/impact study. This would also be of interest to ESA STSE Pathfinders Ocean Acidification project. The work should study the same Arctic seas as those already studied so that the two studies can be linked (ie Kara, Barents and Greenland Seas).

4. The spread in k parameterisations is similar to spreads of many other physical sea variables against U10. There is potential to illustrate/investigate whether or not the spread in k is due to sea state (e.g. significant wave height). Also how does time impact the spread? ie is some of the spread in the in situ data due to a temporal mismatch? e.g. fast sampling after initial patch dispersal as storm is brewing or delay between patch release and sampling as there was no rush? Could these temporal delays help explain



some of the spread ? A model could be used. Could go back to altimeter derived k_d 's to investigate it. 3D plots of k versus U10 versus Hs may help explain.

5. Can we investigate trends (in components of the flux calculation and the net sink) ? e.g. try different trends in pCO2 prior to kriging and then run ensembles to see the impact. This could lead to involvement in global carbon project outputs. The evolution of k has been reported by Fangohr and Woolf (2008, JGR paper). Some work should be carried out to look at extreme cases first and this will help reduce errors in trend work. i.e. hurricane seasons and their forcing of k. Some work could be done in the North Atlantic as this is where the data is most dense. i.e. extend work of Watson et al science paper but make use of EO.

6. There is a need to update the Data Access Requirements Document (DARD) datasets and make use of data in more recent years.

7. Kriging and SOCAT strategic work is needed to build relationships and support the SOCAT initiative. Improved and/or more advanced Kriging methods are required.

8. Extraordinary air-sea exchange (i.e. hurricanes, polar lows). The use of monthly data to quantify global air-sea fluxes would miss these events as they will be averaged out. We could look at the impact of hurricanes on the CO_2 budget using published parameterisations. The FluxEngine system could be used to quantify their impact. Upwelling in the wake of hurricanes could be studied and this work could exploit links with ESA STSE SMOS storms.

9. Need to parameterise/validate (in some way) the bubble component of k, so that OceanFlux can publish a climatology with a physically justified, defined and validated total k. Could we determine the latitudinal component of k? Could a tank experiment or wave model be used to advance this ?. Could AMRS-E and cloudmap combination be exploited? Climatology of foam thickness and wave breaking and then relate latitudinal variation with U10, Hs etc and then use this to parameterise wave breaking.

4.1 Strategies for integration with large scientific initiatives

It is clear that there are multiple routes that can be exploited to increase the uptake and exploitation of OceanFlux-GHG outputs. It is also intended that these routes will provide mutual benefit for all those involved (i.e. ESA, OceanFlux and the initiative in question).

1. The International Surface Ocean - Lower Atmosphere Study (SOLAS) project is an international research initiative aiming to understand the key biogeochemical-physical interactions and feedbacks between the ocean and atmosphere. International SOLAS has supported the OceanFlux projects from their gestation. It remains an important vehicle for ensuring both that this and similar projects are genuinely targeted to recognised scientific priorities and for enabling the promotion of the project and its interactions with related projects. We expect any future projects to benefit from an active involvement with and from SOLAS.



2. SOCAT is an international initiative to establish a global surface CO_2 data set that would bring together, in a common format, all publicly available fCO₂ data for the surface oceans. SOCAT is in some senses a complementary activity to OceanFlux GHG that has developed broadly in parallel. A genuine (two-way) interaction has only developed slowly and there should be more interaction in the future. It is also important to note that SOCAT has primarily been a voluntary activity with very limited funding. Since the continued flourishing of SOCAT is important to OceanFlux and the broader scientific community, it is appropriate that ESA STSE and SOLAS contribute to the funding of SOCAT by some means. Since the SOCAT data is important to flux estimates and also SOCAT and OceanFlux participants have to a large extent complementary expertise it will be important to build a stronger relationship. SOCAT should have input to future FluxEngine developments including the estimation of fCO₂ gridded fields from the sparse SOCAT measurements. OceanFlux participants and ESA scientists may be able to provide useful input to SOCAT, from data quality control with respect to uncertain temperature, through processing with respect to temperature and salinity and to the correct application of earth observation data.

3. The Global Carbon Project (GCP) was established in 2001 in recognition of the large scientific challenges and critical nature of the carbon cycle for Earth's sustainability. The scientific goal of the project is to develop a complete picture of the global carbon cycle, including both its biophysical and human dimensions together with the interactions and feedbacks between them. Thus, the Global Carbon Project has a much broader remit with respect to CO₂ than OceanFlux GHG; it extends to the entire global carbon budget, not just the air-sea flux. Within this context the air-sea fluxes are important since they help to close the global carbon budget. At least in some basins, e.g. North Atlantic it is generally assumed that the air-sea flux is better constrained than neighbouring terrestrial sources and sinks. Thus the terrestrial budgets are often inferred by closing the budget using estimates of the marine flux. We have shown in OceanFlux however that existing estimates of the marine flux are not as secure as sometimes supposed. There should be a role for a future project both to improve the estimates of the basin-scale air-sea fluxes (as estimated via the air-sea flux equation) and to communicate both the central estimates and realistic uncertainties to those involved in the broader global carbon budget. That interaction may be best pursued through interaction with the Global Carbon Project who have already expressed an interest.

4. Support for more joint meetings was highlighted in the workshop minutes [GHG-WS]. There is always some risk of a "silo mentality" and while those meeting at OceanFlux GHG workshop were generally not strangers at the beginning of the workshop, some significant miscommunication and misinformation was made apparent by the workshop. While large established meetings such as the International SOLAS Open Science Conference play a large role, they may not be sufficiently focussed or attract the appropriate cross-disciplinary community to address specific issues. It is proposed that future workshops should be organised with highly focussed aims, but also solicit the support of SOLAS, GCP, EGU or similar.



4.2 Scientific and software engineering development strategy

The following development activities and potential aims have been identified during the scientific workshop and project meetings.

The following aims or strategies are scientific related:

1. Parameterise bubble-mediated gas transfer in order to produce a climatology that uses a physically-based gas transfer relationship. Latitudinal variations, foam thickness, breaking wave distribution, relationship of Hs to k curves (direct and indirect method curves) may all be important aspects to study.

2. Work with the SOCAT team (especially D. Bakker, UEA, UK) to help quality control and exploit new versions of SOCAT data. There are too few data in upwelling regions, The Mediterranean and Arctic areas and we may be able to help support data collation and/or quality control in these areas.

3. Design, implement and publish a series of tailored global ensemble experiments using the FluxEngine.

4. Produce regional CO₂ flux estimates using the FluxEngine in the North Atlantic to study trends (potentially with A. Watson, University of Exeter, UK)

5. Use Cryosat to study gas fluxes in the Arctic seas as sea ice is breaking up (e.g. Kara, Barentz, Laptev Seas where we have new open water/fetch conditions).

6. Develop a strategy and implement a method to enable local/regional extreme events to be studied (e.g. Upwelling, strong ETC and TC, biological blooms, Diurnal variation) and conduct sensitivity studies on impacts to CO_2 fluxes using the FluxEngine.

The following aims or strategies are software engineering and/or web related:

1. There is a need to study other gases and not just CO_2 . The behaviour or characteristics of gases (other than CO_2) can help to interpret CO_2 fluxes or indirectly infer carbon cycling. Some research cruises are now addressing a multiplicity of gases including in situ data collection and process studies. To increase the potential of the FluxEngine to support CO_2 flux work, there is a need to extend the FluxEngine to calculate fluxes and/or methods to study other climatically important gases e.g. DMS, N₂O and O₂ and NOAA COARE support into the FluxEngine. This will also have the additional bonus of making the FluxEngine useful for a much wider air-sea exchange community.

2. Implement and validate NOAA-COARE gas transfer model within the FluxEngine. This is linked to the previous aim. However it also distinct as it would encourage greater US exploitation of the FluxEngine. We could augment the work by producing new climatologies and sensitivity studies based on COARE algorithms.

3. Provide tools to promote and manage OceanFlux science users (graphics and web resources, improve the web interface, focussing on promoting OceanFlux and the



FluxEngine to scientists. Tools should include methods for user feedback and a bug tracking system, code to read and display climatology and diagnostics, documentation that Masters students could follow to use the system, improvements of the interface to the FluxEngine system.

4.3 Transition from OceanFlux research to international community exploitation

The FluxEngine is about to be used in the following 2 UK funded projects: UK NERC CANDYFLOSS (2014-2017) to study European shelf sea air-sea fluxes and UK NERC RAGNARoCC (2013-2017) to study open ocean air-sea fluxes. It is also to be used by a UK PhD student (co-supervised by L. Goddijn-Murphy and D. Woolf). The OceanFlux-GHG data and methods are also to be used within ESA STSE Pathfinders Ocean Acidification for the same reasons. However, it is noted that this usage is because OceanFlux-GHG team members are involved in all of these projects.

It is anticipated that the use of the project datasets and the FluxEngine will only increase once the methods are published in a peer-reviewed journals. The FluxEngine and the main climatology papers are currently in draft and will be submitted in April 2014. These papers would need to be published before we would expect to see any transition from solely project use to being exploited by the international community.

Once the papers are published, the ESA/EGU/SOLAS workshop in ESRIN in October 2014 could be used to encourage and market the publications and the use of the FluxEngine. A live demonstration of the FluxEngine could be given at the workshop to encourage workshop participants to take part in a crowd-sourced ensemble run. The demonstration could also be used to illustrate how to access and analyse the resultant netcdf data output. The results of this crowd-sourced ensemble could then be presented during the conference and the final dataset will be made available. This could be achieved by using the ESRIN training room. A set of simple diagnostic tools could be applied to each run (e.g. to difference maps to Takahashi, calculated global and basin values with uncertainties). and a standard script applied (for example, to open files s and to calculate and plot monthly fluxes).

Prior to the workshop, an instruction manual for the FluxEngine suitable for an MSc student to use would need to be written. A way in which users can report discovered errors and problems would also be needed. A forum is the obvious solution to this.

4.4 Conclusions on the future directions and foci

In common with other scientific and technical endeavours, it is far too easy to write an ever expanding list of future objectives. The study of the air-sea flux of gases has been slowed by some substantial and technical obstacles. It is also the case that retrieving the most appropriate information by earth observation is not simple. Nevertheless, a road map has been established that identifies strategically significant tasks with tractable solutions. We have established a "long list" of major objectives and also a shorter list where earth observation, air-sea interaction and technical expertise can be immediately brought to bear. The development and promulgation of FluxEngine is central to much of



the proposed road map. We have also highlighted the importance of cementing our mechanistic understanding of air-sea exchange, especially in strong winds when bubblemediated processes are important. We have also outlined a process by which future projects can work with major umbrella organisations and initiatives (e.g. SOLAS, SOCAT, GCP) and with individual scientists with varying backgrounds.

5. Overall conclusions

The study of the air-sea flux of gases has been slowed by some substantial and technical obstacles. It is also the case that retrieving the most appropriate information by Earth observation is not simple. Nevertheless, the OceanFlux-GHG project has made some significant advances and contributions to the area of science. The project has highlighted the importance of cementing our mechanistic understanding of air-sea exchange, especially in strong winds when bubble-mediated processes are important. Advancements within the project have highlighted how such an approach can reduce the uncertainties in the resultant air-sea fluxes and net sink estimates through the use of data that describes the surface turbulence (backscatter) rather than relying on wind as proxy for describing the surface turbulence. The project has developed a powerful community tool that can be used to generate global climatologies and ensemble experiments. The team composition of modellers, Earth observation, computing, carbonate and in situ specialists was key to the success of the project. The project has also identified and constructed the first near-complete uncertainty budget for gas flux climatologies; key information that will help focus future international efforts in reducing these uncertainties.



6. Annex 1 – abstracts for each of the outputs

Abstract 1. Reviewing gas transfer velocity parameterisations

The Oceanflux Greenhouse Gases project is concerned with the calculation of the airsea flux of greenhouse gases, especially carbon dioxide, using an air-sea flux equation. Within the flux equation, fluxes are proportional to a transfer velocity, k. We can use Earth observation or in situ data for the calculation of the fluxes, only if we adopt a suitable algorithm that typically describes the dependence of k on wind speed and water temperature. Unfortunately, appropriate algorithms for the transfer velocity of carbon dioxide are hotly debated. The debate is not limited to an uncertainty in one or more parameters, "parameter uncertainty", but extends to a structural uncertainty arising from both conflicting data and rival theories. Measurements and parameterisations of gas transfer velocities are critically reviewed. Two substantially different empirical algorithms for k are arrived at by separate approaches. The most established algorithm is based on a simple Schmidt number dependence (and thus temperature dependence) and a simple quadratic dependence on wind speed. An alternative "cubic" algorithm shares the same temperature dependence, but predicts much higher transfer velocities in high wind speeds. Those high values in strong winds are primarily, but not solely, supported by micrometeorological measurements of carbon dioxide flux and are assumed to be the result of a roughly cubic wind speed dependence of wave breaking. Each empirical algorithm has strong proponents, but is contradicted by some data and criticised by other experts. Since there is a large body of data, but the perceived information is contradictory, more data is unlikely to resolve the debate swiftly. This ambiguity poses a dilemma for estimation of fluxes and their uncertainty. A twofold approach is adopted. Firstly, we examine critically both algorithms and pursue an alternative more mechanistic approach. Secondly, we construct an open system for the calculation of air-sea fluxes that enables a very broad range of algorithms to be applied.

Abstract 2. Reviewing whitecapping and air-sea interaction

A number of geochemical processes are dependent on bubbles primarily produced by "whitecapping" breaking waves, notably primary marine aerosol production, bubblemediated gas exchange and the renewal of the organically rich surface marine microlayer. It is convenient to predict the magnitude of these processes through a "whitecap method" that then requires whitecap coverage to be measured or predicted. Whitecap coverage is difficult to define and harder to measure. There is adequate evidence that whitecap coverage (and thus by implication, the processes driven by it) do not simply depend on wind speed. Typically whitecap coverage may vary by a factor of two either side of a geometric mean for a given wind speed in response to changes in sea state. Both parametric and relatively direct methods of retrieving whitecap coverage require further development



Abstract 3. Unifying the methods for handling thermal and haline effects in air-sea gas flux calculations

The presence of vertical temperature and salinity gradients in the upper ocean and the occurrence of variations in temperature and salinity on time scales from hours to many years complicate the calculation of the flux of carbon dioxide (CO₂) across the sea surface. Temperature and salinity affect the interfacial concentration of aqueous CO₂ primarily through their effect on solubility with lesser effects related to saturated vapour pressure and the relationship between fugacity and partial pressure. The effects of temperature and salinity profiles in the water column and changes in the aqueous concentration act primarily through the partitioning of the carbonate system. Climatological calculations of flux require attention to variability in the upper ocean and to the limited validity of assuming "constant chemistry" in transforming measurements to climatological values. Contrary to some recent analysis, it is shown that the effect on CO_2 fluxes of a cool skin on the sea surface is large and ubiquitous. An opposing effect on calculated fluxes is related to the occurrence of warm layers near the surface; this effect can be locally large but will usually coincide with periods of low exchange. A salty skin and salinity anomalies in the upper ocean also affect CO_2 flux calculations, though these haline effects are generally weaker than the thermal effects.

Abstract 4. Deriving a sea surface climatology of CO₂ fugacity in support of air-sea gas flux studies.

Climatologies, or long-term averages, of essential climate variables are useful for evaluating models and providing a baseline for studying anomalies. The Surface Ocean Carbon Dioxide (CO₂) Atlas (SOCAT) has made millions of global underway sea surface measurements of CO_2 publicly available, all in a uniform format and presented as fugacity, fCO_2 . fCO_2 is highly sensitive to temperature and the measurements are only valid for the instantaneous sea surface temperature (SST) that is measured concurrent with the in-water CO₂ measurement. To create a climatology of fCO₂ data suitable for calculating air-sea CO_2 fluxes it is therefore desirable to calculate fCO_2 valid for climate quality SST. This paper presents a method for creating such a climatology. We recomputed SOCAT's fCO₂ values for their respective measurement month and year using climate quality SST data from satellite Earth observation and then extrapolated the resulting fCO₂ values to reference year 2010. The data were then spatially interpolated onto a 1° x 1° grid of the global oceans to produce 12 monthly fCO_2 distributions for 2010. The partial pressure of CO_2 (pCO₂) is also provided for those who prefer to use pCO₂. The CO₂ concentration difference between ocean and atmosphere is the thermodynamic driving force of the air-sea CO₂ flux, and hence the presented fCO₂ distributions can be used in air-sea gas flux calculations together with climatologies of other climate variables.

Abstract 5. Single frequency altimeters for deriving air-sea gas transfer velocity

This study is the first to directly correlate gas transfer velocity, measured at sea using the eddy-correlation (EC) technique, and satellite altimeter backscattering. During eight research cruises in different parts of the world, gas transfer velocity of dimethyl sulphide (DMS) was measured. The sample times and locations were compared with



overpass times and locations of remote sensing satellites carrying Ku-band altimeters: ERS-1, ERS-2, TOPEX, POSEIDON, GEOSAT Follow-On, JASON-1, JASON-2 and ENVISAT. The result was 179 pairs of gas transfer velocity measurements and backscattering coefficients. An inter-calibration of the different altimeters significantly reduced data scatter. The intercalibrated data was best fitted to a quadratic relation between the inverse of the backscattering coefficients and the gas transfer velocity measurements. A gas transfer parameterization based on backscattering, corresponding with sea surface roughness, might be expected to perform better than wind speed-based parameterizations. Our results, however, did not show improvement compared to direct correlation of shipboard wind speeds. The relationship of gas transfer velocity to satellite-derived backscatter, or wind speed, is useful to provide retrieval algorithms. Gas transfer velocity (cm/hr), corrected to a Schmidt number of 660, is proportional to wind speed (m/s). The measured gas transfer velocity is controlled by both the individual water-side and air-side gas transfer velocities. We calculated the latter using a numerical scheme, to derive water-side gas transfer velocity. DMS is sufficiently soluble to neglect bubble-mediated gas transfer, thus, the DMS transfer velocities could be applied to estimate water-side gas transfer velocities through the unbroken surface of any other gas.

Abstract 6. Dual frequency altimeters for deriving air-sea gas transfer velocity

A previous study shows a significant relation between Ku-band backscattering from satellite altimeters and field estimates of gas transfer velocity, *K*. Recently C-band backscatter data were made available for altimeters on board the JASON-1 and JASON-2 satellites. In this paper we used experimental data from the same cruises to show that using the difference between the Ku-band and C-band signals, and thus reducing the contribution from longer waves, improved the *K* estimates. This is consistent with the theory that gas transfer is largely controlled by short capillary-gravity waves. For satellite data closer than 2 hr and 0.5° from the *K* sample stations, the dual-frequency parameterization is found to perform better than a wind speed parameterization that uses in situ wind speed.

Abstract 7. FluxEngine: A flexible processing system for calculating air-sea carbon dioxide gas fluxes and climatologies

The air-sea flux of Greenhouse gases (e.g. carbon dioxide, CO_2) is a critical part of the climate system and a major factor in the biogeochemical development of the oceans. More accurate and higher resolution calculations of these gas fluxes are required if we are to fully understand and predict our future climate. Satellite Earth observation is able to provide large spatial scale datasets that can be used to study gas fluxes. However, the large storage requirements needed to host such data can restrict its use by the scientific community. Fortunately, the development of cloud-computing can provide a solution. Here we describe a cloud-computing based air-sea CO_2 flux processing toolbox called the 'FluxEngine'. The toolbox allows users to easily generate global and regional air-sea CO_2 flux data from model, *in situ* and Earth observation data. The air-sea gas flux calculation is user configurable and the toolbox allows users to easily exploit more than 8 terabytes of climate quality Earth observation data for the derivation of gas fluxes.



The resultant NetCDF data output can be easily downloaded and each file contains >20 data layers containing the various stages of the flux calculation along with process indicator layers to aid interpretation of the data. The toolbox exploits a cloudcomputing platform that provides efficient and fast data processing. This paper describes the toolbox design, the verification of the air-sea CO₂ flux calculations, demonstrates the use of the tools for studying global and shelf sea air-sea fluxes and discusses future developments.

Abstract 8. The contemporary air-sea flux of carbon dioxide, II Scenario and ensemble estimates of global fluxes in the OceanFlux climatology.

A global flux of CO₂ of ~80 Pg C yr⁻¹ is exchanged between atmosphere and ocean annually with a net flux in recent years of $\sim 2 \text{ Pg C yr}^{-1}$ into the oceans. While other methods are available to estimate global and basin-scale fluxes, regional and subseasonal estimates are only practical through application of an air-sea flux equation that requires concentrations in atmosphere and ocean and estimates of transfer velocity. Uncertainties arise throughout the calculation and the propagation of these errors through to a final flux estimate of flux. Various data sets (in situ, Earth Observation and modelling) and algorithms are used to compute air-sea gas flux. Fluxes are calculated at monthly and one-degree resolution for a reference year of 2010, but the analysis presented here focusses on annual fluxes for the global oceans. A large number of calculations are presented representing different scenarios and formal ensembles. The results suggest relatively high uncertainty in global and regional carbon dioxide flux. For a reference year of 2000, we estimate a net global flux from air to sea of 2.0 Pg C yr^{-1} , but with a high bias uncertainty. An optimistic interpretation of existing uncertainty in gas transfer velocities leads to a bias uncertainty of ~ 0.5 Pg C yr⁻¹, while a more pessimistic interpretation implies a bias uncertainty $> 1 \text{ Pg C yr}^{-1}$. Similarly, a set of simulated upper ocean CO₂ fields created by a bootstrap method are also used to study the uncertainty in flux. Some ensemble members suggest a very large uncertainty in global net flux. Some of the scenarios and ensemble members may be contradicted by global and regional estimates by other methods, but they cannot be easily dismissed directly.

Abstract 9. The contemporary air-sea flux of carbon dioxide I: Sources and types of uncertainty in the OceanFlux Climatology.

We consider the problem of producing air-sea gas flux climatologies with a complete and traceable description of uncertainties. We start with a consideration of the generic problem of calculating the uncertainties inherent in a system and then focus on the particular sources of error for calculating air-sea gas fluxes from a flux equation. The approach to the generic problem starts with the identification of errors, each of which is categorised according to location, level, nature and randomness. The first three categories follow the definitions proposed by Warmink et al. (2010). "Randomness" separates errors into a consistent bias and a wholly random error. Having identified and classified the errors we make a preliminary assessment of their significance, first to the error in individual estimates of flux and secondly, to the bias uncertainty in averaged air-sea gas fluxes. While the limited number of measurements of dissolved gas



concentration is certainly an issue for all gases, the dispute over gas transfer velocities may be a greater issue for averaged fluxes of carbon dioxide, especially in basins such as the North Atlantic where observations of dissolved concentration are relatively common.

Abstract 10. The impact of rain on air-sea fluxes

The global oceans are considered a major sink of atmospheric carbon dioxide (CO_2) . Rain is known to alter the physical and chemical conditions at the sea surface, and thus influences the transfer of CO_2 between the ocean and atmosphere. However, to date no quantification of these effects on global net air-sea fluxes exists. Rain can influence gas exchange through surface layer dilution, enhanced gas transfer velocity, altering the sea skin temperature and through the direct export of carbon from the atmosphere to the ocean. We investigate the impact of all of these processes using a 20+ year archive of monthly global climate quality satellite Earth observation (EO) data. Globally rain can increase the annual oceanic integrated net sink of CO_2 by up to 6 %. Regionally, the annual variations can be larger, the largest of which is in the Southern Ocean where rain can increase the net sink by up to 13%. The regional monthly variations can be much higher. The Pacific and Southern ocean monthly net fluxes can be significantly modulated by rain with regular variations of $> \pm 15\%$. Instances of very large modulation of $> \pm 50\%$ are also possible. The impacts of rain should be included in the uncertainty analysis of studies that estimate net air-sea fluxes of CO2 as the rain can have a considerable impact on the fluxes, dependent upon the region and timescale.

Abstract 11. Characterising air-sea fluxes of carbon dioxeide in Arctic waters

We applied coincident Earth observation data collected during 2008 and 2009 from multiple sensors (RA2, AATSR and MERIS, mounted on the European Space Agency satellite Envisat) to characterise environmental conditions and integrated sea-air fluxes of CO_2 in three Arctic seas (Greenland, Barents, Kara). We assessed net CO_2 sink sensitivity due to changes in temperature, salinity and sea ice duration arising from future climate scenarios. During the study period the Greenland and Barents seas were net sinks for atmospheric CO₂, with integrated sea–air fluxes of -36 ± 14 and -11 ± 5 Tg C yr⁻¹, respectively, and the Kara Sea was a weak net CO₂ source with an integrated sea-air flux of $+2.2 \pm 1.4$ Tg C yr⁻¹. The combined integrated CO₂ sea-air flux from all three was -45 ± 18 Tg C yr⁻¹. In a sensitivity analysis we varied temperature, salinity and sea ice duration. Variations in temperature and salinity led to modification of the transfer velocity, solubility and partial pressure of CO_2 taking into account the resultant variations in alkalinity and dissolved organic carbon (DOC). Our results showed that warming had a strong positive effect on the annual integrated sea-air flux of CO_2 (i.e. reducing the sink), freshening had a strong negative effect and reduced sea ice duration had a small but measurable positive effect. In the climate change scenario examined, the effects of warming in just over a decade of climate change up to 2020 outweighed the combined effects of freshening and reduced sea ice duration. Collectively these effects gave an integrated sea-air flux change of +4.0 Tg C in the Greenland Sea, +6.0 Tg C in the Barents Sea and +1.7 Tg C in the Kara Sea, reducing the Greenland and Barents sinks by 11% and 53%, respectively, and increasing the weak Kara Sea source by 81%.



Overall, the regional integrated flux changed by +11.7 Tg C, which is a 26% reduction in the regional sink. In terms of CO₂ sink strength, we conclude that the Barents Sea is the most susceptible of the three regions to the climate changes examined. Our results imply that the region will cease to be a net CO₂ sink in the 2050s.

Abstract 12. Modelling the carbonate system and pCO₂ in shelf seas

This work evaluates the sensitivity of CO₂ air-sea gas exchange in a coastal site to four different model system configurations of the 1D coupled hydrodynamic-ecosystem model GOTM-ERSEM. The European Sea Regional Ecosystem Model (ERSEM) is a biomass and functional group based biogeochemical model that resolves the time evolution of the pelagic ecosystem including the nutrient and carbon cycle within the planktonic trophic chain of primary producers (picophytoplankton, nanoflagellates, dinoflagellates and diatoms), consumers (meso- and micro- zooplankton and heterotrophic nanoflagellates) and decomposers (heterotrophic bacteria). ERSEM includes a comprehensive carbonate system and explicitly simulates the production of dissolved organic carbon (DOC), dissolved inorganic carbon (DIC) and organic matter (DOM). The model was implemented at the coastal station L4 (4 nutical miles south of Plymouth, 50°15.00'N, 4°13.02'W, depth of 51 m). The model performance was evaluated using more than 1500 hydrological and biochemical observations routinely collected at L4 through the Western Coastal Observatory activities of 2008-2009.

The 1D model resolves well the physical environment (sea surface temperature has a correlation of 0.94 when comparing hourly data from the L4 monitoring buoy, all values given with a p>0.95). Overall, the model captures the seasonal signal in most biogeochemical variables including the air-sea flux of CO₂ and primary production and can capture some of the intra-seasonal variability and short-lived blooms. The model correctly reproduces the seasonality of nutrients (correlation > 0.80 for all three macronutrients silicate, nitrate and phosphate), surface chlorophyll (correlation > 0.43) and total biomass (corr>0.7) in a two year run for 2008-2009. The model simulates well the concentration of DIC, pH and in water partial pressure of CO₂ (pCO₂) with correlations between 0.4-0.5. The model result suggest that L4 is a weak net sink of CO₂ (0.3-1.8 molC m⁻² year⁻¹)

We ran three distinct experiments to investigate the sensitivity of the carbonate system and modelled air-sea fluxes to i) the SST diurnal cycle, ii) biological suppression of gas exchange and iii) data assimilation using satellite Earth observation data. Resolving the near-surface temperature gradients has the largest impact at short, seasonal and annual time scales and results in improvements across the evaluated variables that are comparable to the results from the assimilation of chlorophyll experiment. The correlation of carbonate system variables (DIC, pCO2 and pH) improve by up to 19% while annually integrated values of CO₂ exchange with the atmosphere changed by up to 50% with respect to the standard simulation, increasing the net sink nature of L4. At the L4 site, the introduction of a dependence of the CO₂ gas transfer velocity on gross production as a proxy for the production of surface slicks has a non-significant impact on the dynamics of CO₂, including the air-sea annual exchange estimates. The assimilation of surface Chlorophyll has an overall mixed effect on the ability of the model to reproduce the observations. As expected the simulation of chlorophyll improves and while the correlation for nutrients do not significantly change, their bias



decreases. The effect on the carbonate system variables is similar; the bias decreases for DIC and pH but so do the correlations. The largest impact of assimilation is on the net Air-sea gas exchange where the results indicate the potential for L4 to be a weak source $(1.3 \pm 1.7 \text{ molC m}^{-2} \text{ year}^{-1})$.

Abstract 13. Parameterising whitecapping within wave models

Ardhuin and colleagues have developed two model parameterisations of breaking wave parameters (T451 and T570), both of which is based on a physics-based relationship of wave slope to breaking probability. These parameterisations have been implemented in the spectral wave model WAVEWATCH-III (WW3). Reul and Chapron (2013) have reported a method to convert those breaking statistics to an estimate of whitecap coverage. Both T451 and T570 agree reasonably well with classical empirical fits of whitecap coverage against wind speed.

Within the OceanFlux GHG project, participating scientists from IFREMER and NOC collaborated to bring together model hindcasts using T451 and T570 with collocated in situ observations of whitecap coverage and ancillary data (e.g. wind speed). Output from the model includes whitecap fraction, whitecap thickness dissipation-related parameters such as mean-squared sloe, friction velocity, atmosphere-ocean energy flux and ocean-wave energy flux. Comparisons were made with in situ data collected during research cruises in the North and South Atlantic and in the Norwegian Sea in 2007, 2008 and 2009. A number of CFD corrections were applied to the data and Quality Control (QC) procedures applied. Two of the original cruises (DOGEE 2 (D320) and WAGES) were excluded, because a systematic bias low appeared to be related to a technical innovation (the use of polarising filters on the cameras to reduce sunglint). All of the QC procedures drastically reduced the amount of data, however inclusion of more risked introducing spurious environmental signals. Both model values and the data passing QC ware shown to be broadly consistent with a classical empirical parameterisation (Monahan and Woolf, 1989; "MW1989"). T570 model values exceed both the in situ data and MW1979 at wind speeds up to 16m/s. Above 16m/s T70 values are lower than both MW1979 and the in situ data, but are consistently closer to MW1979 than to the in situ data at higher wind speeds. Some of the inconsistencies between model and in situ values of whitecap coverage could be traced to differences in the in situ and model wind speeds. This work currently exists as a OceanFlux GHG technical report.

The OceanFlux GHG provided a useful validation test for model-derived whitecap coverages. We were able to conclude that both the model-derived whitecap coverages and the classical MW1979 parameterisations were credible inputs to transfer velocity parametrisations that required an estimate of whitecap coverage. However, the continuing difficulty in acquiring high-quality and reproducible estimates of whitecap coverage by in situ methods remains a brake on progress. Some initial objectives of the project (notably to investigate the temperature-dependence of whitecapping) proved to be impractical because the data passing QC were insufficient. Further progress in measuring whitecap coverage and evaluating environmental signals and quality control methods, preferably exploiting both in situ and satellite-based methods, remains a priority.



7. Annex 2 Scientific Impact Assessment Report

This is a summary of OceanFlux GHG Deliverable 2.17, Version 2.0 30th September 2014. It is included in the Final Report for completeness in this version.

7.1 Purpose and Scope of the Scientific Impact Assessment Report

This is the Scientific Impact Assessment Report (SIAR) (deliverable D2.17) for the OceanFlux GHG project. It is intended to satisfy the requirement of the contract to provide a compendium of the outputs of the project, in the form of papers (published, in review or in draft form) arising from the project. It also supports the Scientific Roadmap by providing a more detailed explanation of the underpinning science.

Each of the following section concludes with a reference, abstract and the status of each publication or report. The status of each output fall into one of three categories: published, in-press or in draft.

7.2 Structure of this Report

The report is structured as follows:

- Section 1 (this section) the introduction gives an overview of the document aims and structure.
- Section 2 A brief summary of the anticipated progress and future prospects organized by sub-topic
- Section 3 and following: Annexes providing supporting material to one or more of the sub-topics

7.3 Contributions

Table details the people who contributed to this report and the sections that they contributed to.

Section	Primary author(s)	Contributing author(s)
Section 1	Jamie Shutler (PML)	
Section 2	David Woolf (HW)	Jamie Shutler (PML)
Section 3	David Woolf (HW)	Jamie Shutler (PML)
Section 4	David Woolf (HW), Jamie Shutler (PML), Lonneke Goddijn-Murphy (ERI), Ricardo Torres (PML)	The whole OceanFlux GHG project team.

Table 3 Table of contributions.



7.4 Introduction and overview

The Scientific Impact Assessment Report (SIAR) is based around a number of publications produced by the OceanFlux GHG project. Each of the subsections below describe one aspect of the scientific work and refer to journal publications which are either in-preparation, in-review or published.

OceanFlux GHG is focussed primarily on interfacial transfer rates and thus upon concentrations on either side of the sea surface, and air-sea transfer coefficients. The significance of OceanFlux GHG extends more broadly for example to the global marine cycling of carbon. The position of OceanFlux GHG in the broader context of marine carbon cycling is illustrated in Figure 1. A wide range of scientific activities are relevant to marine carbon cycling. For example, the international SOLAS program spans the interface taking in processes also in the lower atmosphere and in the upper ocean. The international IMBER program overlaps with SOLAS in the upper ocean but is primarily concerned with marine biogeochemical cycles and ecosystems including the exchange of carbon between the upper ocean and the deep ocean.



Carbon export to the deep ocean

Figure 1. A schematic of marine carbon cycling indicating the scope of OceanFlux GHG and of the large international programs SOLAS and IMBER.

The specific focus of OceanFlux GHG is encapsulated in the air-sea gas flux equation (see Figure 1). The determination of the global fluxes, F, of carbon dioxide and other greenhouse gases is the primary objective and to reach that goal, the various parameters on the right-hand side of the equation must first be determined. OceanFlux GHG expends much of its effort in the determination of the transfer velocity, k. Transfer is primarily a result of stirring at and near the interface by the wind, but the process is



complicated by wave physics generally, by breaking waves and bubbles at high wind speeds and by surfactants and convection at low wind speeds. The net flux, F, is also proportional to the concentration difference across the interface, written in Figure 1 as the product of solubility, **G**, and partial pressure, p, at either side of the interface. OceanFlux GHG depends on measurements and archiving of partial pressures external to the project. In particular, it relies on SOCAT to provide measurements of oceanic partial pressure of carbon dioxide. OceanFlux GHG has devoted more of its own resource to the determination of solubilities (dependent on temperature and salinity) and to the correct calculation of the concentration difference.

The outputs are ordered in this document by category, starting with papers on the background and processing methods, followed by several outputs pertaining to the transfer velocity. The key objective of the project, the calculation and presentation of global climatologies, is described next, followed by outputs relating to a subsidiary objective, the coastal climatology. Several "special cases" follow later, looking at the particular effects of temperature gradients, rain, slicks and ice on air-sea fluxes. Finally a few "associated papers" are reported; the chosen outputs do not directly arise from the project, but are relevant, involve project personnel and are contemporary to the project.

The outputs are summarised below. More detail on each output is contained in the following sub-sections. A version of each output (the most complete available) will be included as an annex to the final version of this document.

No.	Title/section	Lead author	Works hop	Journal special iss.	Confer. paper	Other journal paper	Need for FR	Status
1	Review of transfer velocities	Woolf			~		✓	Published
2	Review of whitecapping	Woolf			✓		~	Published (CP)
3	Thermal and haline effects	Woolf	√			~	~	In draft (JP)
4	Gridded conc. fields and methods	Goddijn- Murphy	V		~	✓ (data journal)	√	In draft (JP) Published (CP)
5	Altimetry single frequency	Goddijn- Murphy				~	~	Published (JP)
6	Altimetry dual frequency	Goddijn- Murphy				✓	~	Published (JP)
7	In situ vs model whitecapping	Hanafin		✓ (or other)		~	~	Complete (TR)
8	Sources of uncertainty	Woolf	~					In draft. (Part of 11.)
9	Data processing	Shutler	~			✓	✓	In draft (JP)

Key: Journal Paper (JP), 'Workshop' column refers to 'workshop presentation will be given', Final Report (FR).



	system							
10	Global	Woolf	✓	✓			✓	In draft
	climatology							(JP)
11	Model derived	Torres	✓	\checkmark			\checkmark	In draft
	pCO2							(JP)
12	Thermal and	Land				\checkmark	\checkmark	Published
	haline in							(JP)
	Arctic and							
	their sensitvity							
13	Impact of rain	Shutler	\checkmark	\checkmark			\checkmark	In draft
	on fluxes							(JP)
14	Impact of	Chapron				\checkmark	\checkmark	Published
	wind waves on							(JP)
	air-sea fluxes							
Adde	ed extras (not form	hally part of	the project	<u>()</u>		-		
15	Book review –	Woolf					\checkmark	Published
	transfer across							(book)
	air-sea							
	interface							
16	Correlation of	Shutler			\checkmark		\checkmark	Published
	wind and rain							(CP)
17	Statistical	Chapron					\checkmark	Published
	properties of							(CP)
	breaking							
	waves							

7.5 Review of Transfer velocities

This work investigates how different methods and models lead to different fields of k. and looks at model/parameter uncertainty in k. This is primarily a building block for the key papers on uncertainties (Sect. 2.9) and the global climatology (Sect. 2.10).

Here we look at the spread of different k parameterisations and study which ones give plausible global and region values. This is essentially a sensitivity study on different parameters within the gas flux calculation. E.g. sst, fugacity, wind averaging methods etc and is addressed by constructing an ensemble of different runs.

A major source of uncertainty in greenhouse gas fluxes is related to controversy in the transfer velocity. Woolf et al. (2013) characterised that debate as follows:

The Oceanflux GHG project is concerned with the calculation of the air-sea flux of greenhouse gases, especially carbon dioxide, using an air-sea flux equation. Within the flux equation, fluxes are proportional to a transfer velocity, k. We can use Earth observation or in situ data for the calculation of the fluxes, only if we adopt a suitable algorithm that typically describes the dependence of k on wind speed and water temperature. Unfortunately, appropriate algorithms for the transfer velocity of carbon dioxide are hotly debated. The debate is not limited to an uncertainty in one or more parameters, "parameter uncertainty", but extends to a structural uncertainty arising from both conflicting data and rival theories. Measurements and parameterisations of gas transfer velocities are critically reviewed. Two substantially different empirical algorithms for k are arrived at by separate approaches. The most established algorithm is based on a simple Schmidt number dependence (and thus temperature dependence) and a simple quadratic dependence on wind speed. An alternative "cubic" algorithm



shares the same temperature dependence, but predicts much higher transfer velocities in high wind speeds. Those high values in strong winds are primarily, but not solely, supported by micrometeorological measurements of carbon dioxide flux and are assumed to be the result of a roughly cubic wind speed dependence of wave breaking. Each empirical algorithm has strong proponents, but is contradicted by some data and criticised by other experts. Since there is a large body of data, but the perceived information is contradictory, more data is unlikely to resolve the debate swiftly. This ambiguity poses a dilemma for estimation of fluxes and their uncertainty.

Following from that review of the situation, Woolf et al. (2013) discuss whether each proposed empirical parameterisation is credible. They also discuss more mechanistic and semi-empirical parameterisations such as NOAA-COARE (Hare et al. 2004) or modifications of NOAA-COARE (e.g. Jeffery et al., 2010). While some tentative conclusions about which parameterisations are more consistent with available data are reached, the choice of parameterisation remains a subject of expert judgment (see discussion of ambiguity in Section 2.8). Therefore several different parameterisations, or "model structures" for transfer velocity were included in the architecture for calculating air-sea fluxes. Additionally, for each model structure, one or more parameters need to be set and only a range can be set on the basis of experimental data.

Woolf et al (2013) presents an ensemble approach for the calculation of global fields of transfer velocity. Experiments include using a variety of model structures and using a range of parameters for the same model structure. This approach is shown to be useful, firstly since it gives a far more realistic picture of the uncertainty in transfer velocities, gross flux of CO_2 and net flux of CO_2 . Secondly, the gross flux and net flux of CO_2 can be inferred by independent means, therefore it can be demonstrated that some combinations of model structures and parameters contradict other credible evidence, which is significant evidence against those combinations.

The OceanFlux GHG project yields a realistic assessment of the uncertainty in transfer velocities and demonstrates that further progress is necessary. Some recommendations of related research priorities are described.

Abstract:

Woolf, D., L. Goddijn-Murphy, J. Prytherch, M. Yelland, P. Nightingale, P., J. Shutler, J-F. Piolle, J. Hanafin and B. Chapron. 2013. Uncertainty and ambiguity in air-sea gas fluxes; a flexible system in response to a debate on transfer velocity. ESA Living Planet Symposium 2013, Edinburgh, UK, 9-13 September, 2013.

The Oceanflux Greenhouse Gases project is concerned with the calculation of the airsea flux of greenhouse gases, especially carbon dioxide, using an air-sea flux equation. Within the flux equation, fluxes are proportional to a transfer velocity, k. We can use Earth observation or in situ data for the calculation of the fluxes, only if we adopt a suitable algorithm that typically describes the dependence of k on wind speed and water temperature. Unfortunately, appropriate algorithms for the transfer velocity of carbon dioxide are hotly debated. The debate is not limited to an uncertainty in one or more parameters, "parameter uncertainty", but extends to a structural uncertainty arising from both conflicting data and rival theories. Measurements and parameterisations of gas transfer velocities are critically reviewed. Two substantially different empirical algorithms for k are arrived at by separate approaches. The most established algorithm



is based on a simple Schmidt number dependence (and thus temperature dependence) and a simple quadratic dependence on wind speed. An alternative "cubic" algorithm shares the same temperature dependence, but predicts much higher transfer velocities in high wind speeds. Those high values in strong winds are primarily, but not solely, supported by micrometeorological measurements of carbon dioxide flux and are assumed to be the result of a roughly cubic wind speed dependence of wave breaking. Each empirical algorithm has strong proponents, but is contradicted by some data and criticised by other experts. Since there is a large body of data, but the perceived information is contradictory, more data is unlikely to resolve the debate swiftly. This ambiguity poses a dilemma for estimation of fluxes and their uncertainty. A twofold approach is adopted. Firstly, we examine critically both algorithms and pursue an alternative more mechanistic approach. Secondly, we construct an open system for the calculation of air-sea fluxes that enables a very broad range of algorithms to be applied.

Status: published.

7.6 Review of Whitecapping and air-sea interaction

Abstract:

Woolf, D.K. and Goddijn-Murphy L. 2012. The importance of whitecapping to air-sea interaction and earth observation approaches to its retrieval. In *"Earth Observation for Ocean-Atmosphere Interactions Science"* Symposium Proceedings, SP-703 (CD), ESA.

A number of geochemical processes are dependent on bubbles primarily produced by "whitecapping" breaking waves, notably primary marine aerosol production, bubblemediated gas exchange and the renewal of the organically rich surface marine microlayer. It is convenient to predict the magnitude of these processes through a "whitecap method" that then requires whitecap coverage to be measured or predicted. Whitecap coverage is difficult to define and harder to measure. There is adequate evidence that whitecap coverage (and thus by implication, the processes driven by it) do not simply depend on wind speed. Typically whitecap coverage may vary by a factor of two either side of a geometric mean for a given wind speed in response to changes in sea state. Both parametric and relatively direct methods of retrieving whitecap coverage require further development.

Status: Published. Potential to upgrade from conference paper to journal paper with new material.

7.7 Thermal and haline effects on calculation of fluxes

Abstract:

Woolf, D. K., P. E. Land, J. D. Shutler and L. M. Goddijn-Murphy. (draft). The calculation of air-sea fluxes of carbon dioxide; thermal and haline effects revisited.

The presence of vertical temperature and salinity gradients in the upper ocean and the occurrence of variations in temperature and salinity on time scales from hours to many years complicate the calculation of the flux of carbon dioxide (CO2) across the sea



surface. Temperature and salinity affect the interfacial concentration of aqueous CO2 primarily through their effect on solubility with lesser effects related to saturated vapour pressure and the relationship between fugacity and partial pressure. The effects of temperature and salinity profiles in the water column and changes in the aqueous concentration act primarily through the partitioning of the carbonate system. Climatological calculations of flux require attention to variability in the upper ocean and to the limited validity of assuming "constant chemistry" in transforming measurements to climatological values. Contrary to some recent analysis, it is shown that the effect on CO2 fluxes of a cool skin on the sea surface is large and ubiquitous. An opposing effect on calculated fluxes is related to the occurrence of warm layers near the surface; this effect can be locally large but will usually coincide with periods of low exchange. A salty skin and salinity anomalies in the upper ocean also affect CO2 flux calculations, though these haline effects are generally weaker than the thermal effects.

Status: Draft ready for submission.

7.8 Gridded concentration fields methods and processing

This work is primarily a building block for the key papers on uncertainties (Sect. 2.9) and the global climatology (Sect. 2.10).

While gridded concentration fields have been generated previously both for the Takahashi climatology (Takahashi et al., 2009) and based on the SOCAT database (Sabine et al., 2012), this project has produced its own monthly, 1° x 1° global fields for the chosen reference year of 2010. This work was undertaken primarily on the basis of identifying preferred methods for estimating fugacity and concentration fields, which will inevitably result in differing fields from Sabine et al. even when both start from the same SOCAT data. The preferred methods build on the work of Woolf et al. (2012) who have described the necessary corrections for thermal and haline effects. The later work takes the largely theoretical directives from Woolf et al., and defines the practical processes of applying these directives to a real database, SOCAT. The work is presented in two papers. The first paper (Goddijn-Murphy et al., 2013) describes the processing of data from the basic SOCAT formats for in situ data, through to "transformed values" appropriate to the reference year. A second paper (?, 201?) describes using the transformed values to generate gridded maps for each month of the reference year. The maps are generated using kriging and optimal interpolation methods that calculate implicit sampling uncertainties in addition to "best estimates".

The method of Goddijn-Murphy et al, (2013) is outlined below. This description is based on an abstract submitted to the Living Planet symposium. Since then the work has been written up into a draft journal paper.

In the Oceanflux Greenhouse Gases project, satellite Earth Observation, in situ and model data are combined to obtain a climatology of key parameters that can be used to determine atmosphere-ocean CO_2 fluxes. A main goal is to produce a monthly 1° x 1° global climatology data. Because the CO_2 concentration difference between ocean and atmosphere is the thermodynamic driving force of the CO_2 flux, one of the scientific challenges concerns the estimation of oceanic CO_2 concentration. This CO_2 concentration is related to the partial pressure (pCO2) or fugacity (fCO2). The Surface



Ocean CO_2 Atlas (SOCAT) has made millions of global underway sea surface measurements of CO_2 publicly available, all in a uniform format and presented as fCO_2 . However, these fCO_2 values are valid strictly only for the in situ sea surface instantaneous temperature at measurement, SST, measurements and are not ideal for climatology. We recomputed SOCAT's these fCO2 values to be applicable to monthly averages of SST on a 1° x 1° grid derived from the Advanced Along-Track Scanning Radiometer (AATSR; Re-processing for Climate (ARC) Dataset of Sea Surface Temperature Retrievals). Concentrations for the measurement month can than be calculated using a solubility calculated from the climatological temperature and salinity. Concentrations in a reference year are calculated by applying an assumed secular trend and then using a solubility appropriate to the reference year. We detail the methodology of in situ fCO2 to climatological fCO2 data conversion.for calculating transformed "climatological" concentrations from SOCAT values and climatological estimates of temperature.

Sabine, C. L., Hankin, S., Koyuk, H., Bakker, D. C. E., Pfeil, B., Olsen, A., Metzl, N., Kozyr, A., Fassbender, A., Manke, A., Malczyk, J., Akl, J., Alin, S. R., Bellerby, R. G. J., Borges, A., Boutin, J., Brown, P. J., Cai, W.-J., Chavez, F. P., Chen, A., Cosca, C., Feely, R. A., González-Dávila, M., Goyet, C., Hardman-Mountford, N., Heinze, C., Hoppema, M., Hunt, C. W., Hydes, D., Ishii, M., Johannessen, T., Key, R. M., Körtzinger, A., Landschützer, P., Lauvset, S. K., Lefèvre, N., Lenton, A., Lourantou, A., Merlivat, L., Midorikawa, T., Mintrop, L., Miyazaki, C., Murata, A., Nakadate, A., Nakano, Y., Nakaoka, S., Nojiri, Y., Omar, A. M., Padin, X. A., Park, G.-H., Paterson, K., Perez, F. F., Pierrot, D., Poisson, A., Ríos, A. F., Salisbury, J., Santana-Casiano, J. M., Sarma, V. V. S. S., Schlitzer, R., Schneider, B., Schuster, U., Sieger, R., Skjelvan, I., Steinhoff, T., Suzuki, T., Takahashi, T., Tedesco, K., Telszewski, M., Thomas, H., Tilbrook, B., Vandemark, D., Veness, T., Watson, A. J., Weiss, R., Wong, C. S., and Yoshikawa-Inoue, H.: Surface Ocean CO2 Atlas (SOCAT) gridded data products, Earth Syst. Sci. Data Discuss., 5, 781-804, doi:10.5194/essdd-5-781-2012, 2012.

While substantial progress has been made within the OceanFlux GHG project, there are clear limitations of global gridded fields of oceanic CO_2 . It is readily apparent that a large part of the problem is that - notwithstanding the enormous international effort that has gone into generating very large databases of high quality oceanic CO₂ data sampling remains insufficient to directly infer accurate global fields of oceanic CO₂. This problem is quite general, though it is clearly exacerbated in regions and seasons (such as the local winter in the Southern Ocean) where sampling is particularly sparse. We have deliberately limited interpolation to direct numerical interpolation methods. It is possible to arrive at more "appealing" fields by using indirect methods of interpolation, for example based on knowledge of ocean circulation (e.g. Takahashi et al., 2009) or based on empirical relationships of CO₂ to environmental variables that are better sampled (e.g. SST, Park et al., 2010). It is possible that the appeal of these fields is matched by a genuine improvement in the products, but that depends on the implied relationships (of for example CO₂ to circulation or temperature) being genuinely robust, which in our opinion has not been clearly demonstrated. For future progress, we identify two essential lines of research. Firstly, it is essential to maintain (and preferably enhance) the in situ measurement of oceanic CO₂. Secondly, robust methods of indirect interpolation clearly are very valuable and it is imperative to test the validity of techniques proposed to date and to seek more robust methods if necessary.



Abstract:

Goddijn-Murphy, L., D. Woolf, P. Land and J. Shutler 2013. The derivation of a CO₂ fugacity climatology from SOCAT's global in situ data. ESA Living Planet Symposium 2013, Edinburgh, UK, 9-13 September, 2013.

In the Oceanflux Greenhouse Gases project, Earth Observation, in situ and model data are combined to obtain a climatology of key parameters that can be used to determine atmosphere-ocean CO2 fluxes. A main goal is to produce a monthly 1° x 1° global climatology data. Since the CO2 concentration difference between ocean and atmosphere is the thermodynamic driving force of the CO2 flux, one of the scientific challenges concerns the estimation of oceanic CO2 concentration. This CO2 concentration is related to the partial pressure (pCO2) or fugacity (fCO2). The Surface Ocean CO2 Atlas (SOCAT) has made millions of global underway sea surface measurements of CO2 publicly available, all in a uniform format and presented as fCO2. However, these fCO2 values are valid strictly only for the instantaneous temperature at measurement and are not ideal for climatology. We recomputed these fCO2 values to be applicable to monthly averages of SST on a 1° x 1° grid derived from the Advanced Along-Track Scanning Radiometer (AATSR) Re-processing for Climate (ARC) Dataset of Sea Surface Temperature Retrievals. Concentrations for the measurement month can then be calculated using a solubility calculated from the climatological temperature and salinity. Concentrations in a reference year are calculated by applying an assumed secular trend and then using a solubility appropriate to the reference year. We detail the methodology for calculating "climatological" CO2 concentrations from SOCAT values and climatological estimates of temperature.

Status: published.

Abstract:

L. M. Goddijn-Murphy, D. K. Woolf, P. E. Land, J. D. Shutler, C. J. Donlon (inreview) Deriving a sea surface climatology of CO2 fugacity in support of air-sea gas flux studies, submitted to Ocean Sciences.

Climatologies, or long-term averages, of essential climate variables are useful for evaluating models and providing a baseline for studying anomalies. The Surface Ocean Carbon Dioxide (CO₂) Atlas (SOCAT) has made millions of global underway sea surface measurements of CO₂ publicly available, all in a uniform format and presented as fugacity, fCO_2 . fCO_2 is highly sensitive to temperature and the measurements are only valid for the instantaneous sea surface temperature (SST) that is measured concurrent with the in-water CO₂ measurement. To create a climatology of fCO₂ data suitable for calculating air-sea CO_2 fluxes it is therefore desirable to calculate fCO_2 valid for climate quality SST. This paper presents a method for creating such a climatology. We recomputed SOCAT's fCO₂ values for their respective measurement month and year using climate quality SST data from satellite Earth observation and then extrapolated the resulting fCO₂ values to reference year 2010. The data were then spatially interpolated onto a 1° x 1° grid of the global oceans to produce 12 monthly fCO_2 distributions for 2010. The partial pressure of CO_2 (pCO₂) is also provided for those who prefer to use pCO_2 . The CO_2 concentration difference between ocean and atmosphere is the thermodynamic driving force of the air-sea CO₂ flux, and hence the presented fCO₂ distributions can be used in air-sea gas flux calculations together with



climatologies of other climate variables.

Status: submitted and in review.

7.9 Altimeter single-frequency algorithms

Abstract:

Goddijn-Murphy, L., D.K. Woolf and C.A. Marandino. 2012. Space-based retrievals of air-sea gas transfer velocities using altimeters: Calibration for dimethyl sulphide. *Journal of Geophysical Research* 117, C08028, doi:10.1029/2011JC007535.

This study is the first to directly correlate gas transfer velocity, measured at sea using the eddy-correlation (EC) technique, and satellite altimeter backscattering. During eight research cruises in different parts of the world, gas transfer velocity of dimethyl sulphide (DMS) was measured. The sample times and locations were compared with overpass times and locations of remote sensing satellites carrying Ku-band altimeters: ERS-1, ERS-2, TOPEX, POSEIDON, GEOSAT Follow-On, JASON-1, JASON-2 and ENVISAT. The result was 179 pairs of gas transfer velocity measurements and backscattering coefficients. An inter-calibration of the different altimeters significantly reduced data scatter. The intercalibrated data was best fitted to a quadratic relation between the inverse of the backscattering coefficients and the gas transfer velocity measurements. A gas transfer parameterization based on backscattering, corresponding with sea surface roughness, might be expected to perform better than wind speed-based parameterizations. Our results, however, did not show improvement compared to direct correlation of shipboard wind speeds. The relationship of gas transfer velocity to satellite-derived backscatter, or wind speed, is useful to provide retrieval algorithms. Gas transfer velocity (cm/hr), corrected to a Schmidt number of 660, is proportional to wind speed (m/s). The measured gas transfer velocity is controlled by both the individual water-side and air-side gas transfer velocities. We calculated the latter using a numerical scheme, to derive water-side gas transfer velocity. DMS is sufficiently soluble to neglect bubble-mediated gas transfer, thus, the DMS transfer velocities could be applied to estimate water-side gas transfer velocities through the unbroken surface of any other gas.

Status: Published.

7.10 Altimeter dual-frequency algorithms

Abstract:

Goddijn-Murphy, L., D.K. Woolf, B. Chapron and P. Queffeulou. 2013. The enhancement of using dual-frequency, instead of single-frequency, altimeter backscatter for estimating air-sea gas transfer velocity, *Remote Sensing of the Environment*.

A previous study shows a significant relation between Ku-band backscattering from satellite altimeters and field estimates of gas transfer velocity, *K*. Recently C-band backscatter data were made available for altimeters on board the JASON-1 and JASON-2 satellites. In this paper we used experimental data from the same cruises to show that using the difference between the Ku-band and C-band signals, and thus reducing the



contribution from longer waves, improved the *K* estimates. This is consistent with the theory that gas transfer is largely controlled by short capillary-gravity waves. For satellite data closer than 2 hr and 0.5° from the *K* sample stations, the dual-frequency parameterization is found to perform better than a wind speed parameterization that uses in situ wind speed.

Status: Published.

Additional Output as follows:

Using satellite altimetry to measure air-sea gas transfer velocity

The relationship of gas transfer velocity to satellite-derived backscatter, or wind speed, is useful to provide retrieval algorithms. Gas transfer velocity is controlled by both the individual water-side and air-side gas transfer velocities. In practice, for insoluble gases the rate limiting step is transfer through the water side and water-side gas transfer velocity is often taken as an adequate estimation of gas transfer velocity. We calculated air-side transfer velocities using a numerical scheme, in order to estimate water-side gas transfer velocities from measurements of the total transfer velocity for DMS. Relationships between water-side transfer velocity and altimeter-derived variables are derived. Using Ku-band backscattering or altimeter derived wind speed give equally good results. Using the difference between the Ku-band and C-band signals, and thus reducing the contribution from longer waves, improves the gas transfer velocity estimates. Since DMS was used to calibrate the relationship, and DMS is sufficiently soluble to neglect bubble-mediated gas transfer, the relationship could be applied to estimate water-side gas transfer velocities through the unbroken surface of any other gas. For less soluble gases, such as CO₂, the contribution of breaking waves to waterside air-sea gas transfer velocity has to be taken into account. An option is to use satellite observations or models of whitecapping, and apply a relation between whitecap fraction and bubble mediated gas transfer.

Status: Presented at the scientific workshop. Ideally will form basis of EGU special issue paper.

7.11 Whitecapping

Ardhuin and colleagues have developed two model parameterisations of breaking wave parameters (T451 and T570), both of which is based on a physics-based relationship of wave slope to breaking probability. These parameterisations have been implemented in the spectral wave model WAVEWATCH-III (WW3). Reul and Chapron (2013) have reported a method to convert those breaking statistics to an estimate of whitecap coverage. Both T451 and T570 agree reasonably well with classical empirical fits of whitecap coverage against wind speed.

Within the OceanFlux GHG project, participating scientists from IFREMER and NOC collaborated to bring together model hindcasts using T451 and T570 with collocated in situ observations of whitecap coverage and ancillary data (e.g. wind speed). Output from the model includes whitecap fraction, whitecap thickness dissipation-related parameters such as mean-squared sloe, friction velocity, atmosphere-ocean energy flux



and ocean-wave energy flux. Comparisons were made with in situ data collected during research cruises in the North and South Atlantic and in the Norwegian Sea in 2007, 2008 and 2009. A number of CFD corrections were applied to the data and Quality Control (QC) procedures applied. Two of the original cruises (DOGEE 2 (D320) and WAGES) were excluded, because a systematic bias low appeared to be related to a technical innovation (the use of polarising filters on the cameras to reduce sunglint). All of the QC procedures drastically reduced the amount of data, however inclusion of more risked introducing spurious environmental signals. Both model values and the data passing QC ware shown to be broadly consistent with a classical empirical parameterisation (Monahan and Woolf, 1989; "MW1989"). T570 model values exceed both the in situ data and MW1979 at wind speeds up to 16m/s. Above 16m/s T70 values are lower than both MW1979 and the in situ data, but are consistently closer to MW1979 than to the in situ data at higher wind speeds. Some of the inconsistencies between model and in situ values of whitecap coverage could be traced to differences in the in situ and model wind speeds. This work currently exists as a OceanFlux GHG technical report.

The OceanFlux GHG provided a useful validation test for model-derived whitecap coverages. We were able to conclude that both the model-derived whitecap coverages and the classical MW1979 parameterisations were credible inputs to transfer velocity parametrisations that required an estimate of whitecap coverage. However, the continuing difficulty in acquiring high-quality and reproducible estimates of whitecap coverage by in situ methods remains a brake on progress. Some initial objectives of the project (notably to investigate the temperature-dependence of whitecapping) proved to be impractical because the data passing QC were insufficient. Further progress in measuring whitecap coverage and evaluating environmental signals and quality control methods, preferably exploiting both in situ and satellite-based methods, remains a priority.

Abstract:

J. Hanafin, F. Ardhuin, B. Chapron, M. Yelland, B. Moat. (2013) Comparison of WAVEWATCH-III ® model output whitecap fraction with *in situ* observations, ESA OceanFlux-GHG technical report.

Recently, modeling of whitecap properties was implemented in the spectral wave model WAVEWATCH-III ® (WW3). The two different wave breaking parameterizations which have been developed for WW3 were implemented in special hindcasts over the period 2006-2009 for comparison with in situ observations in the context of the OceanFlux-GHG project. The model parameterizations use different approaches related to the steepness of the carrying waves to estimate breaking wave probabilities. That of Ardhuin et al. (2010), denoted as T451 in the following, is based on the hypothesis that breaking probabilities become significant when the saturation spectrum exceeds a threshold, and includes a modification to allow for greater breaking in the mean wave direction, to agree with observations. In the second, denoted as T570 (Filipot and Ardhuin, 2012), breaking probabilities are defined at different scales by using wave steepness and then the breaking wave height distribution is integrated over all scales. A further adaptation of the latter to make it self-consistent is described in (Leckler et al, 2012, manuscript in review by Ocean Modelling) which was also implemented in the



hindcasts. Comparisons were made with in situ data collected during research cruises in the North and South Atlantic, and the Norwegian Sea in 2007, 2008 and 2009. The model values follow the Monahan and Woolf (1989) parameterisation for combined static and dynamic breakers quite well, with a tendency to overestimate at wind speeds up to 16m/s and underestimate at higher wind speeds. The error due to the fact that model winds may have a wind speed dependent bias compared to the in situ winds, and have less spatial and temporal variability is presented.

Status: technical report complete.

7.12 Sources of uncertainty

This section gives a brief outline (in the form of an abstract) of a planned paper on sources of uncertainties in CO_2 fluxes. It is partly informed by preceding papers (for example on uncertainties in transfer velocity and on corrections for thermal and haline effects). This paper also feeds into another paper described in the following section (2.9) describing a new CO_2 climatology. Both of of these sections are supported by a longer document (Section 3) that provides a more detailed discussion of errors and uncertainties from the general and theoretical to the practical examples of previous climatologies and the new climatology. A further section (2.10) provides an abstract of an additional output focussing on the effects of rain.

Woolf et al. (2014) consider the problem of producing air-sea gas flux climatologies with a complete and traceable description of uncertainties. The paper starts with a consideration of the generic problem of calculating the uncertainties inherent in a modelling system (see also, the first two subsections of Section 3) and then focussing on the particular sources for air-sea gas fluxes. The approach to the generic problem starts with the identification of errors, each of which is categorised according to location, level, nature and randomness. The first three categories follow the definitions proposed by Warmink et al. (2010). "Randomness" separates errors into a consistent bias and a wholly random error. Having identified the errors that are most likely to be significant to the problem of air-sea gas fluxes, we attempt to estimate their importance to air-sea fluxes. The emphasis is on global fluxes of CO₂; both the global flux (80-100 Pg C yr⁻¹ is exchanged between atmosphere and ocean) and the net flux (1-2 Pg C yr⁻¹ into the oceans). Some errors are noted to be peripheral to the uncertainty in global fluxes, but may be relatively important regionally or locally.

A large source of uncertainties relate the uncertainty in inputs, for example:

- Epistemic uncertainty and natural variability in inputs (e.g. wind speed)
- Epistemic uncertainty in parameters (e.g. in the traditional quadratic model of the transfer velocity)
- Scenario uncertainty due to ambiguity in model structure (opposing expert opinions for the transfer velocity).

A preliminary estimate of these errors is summarised in the Table.



Identifier	Location	Level	Nature	Randomness	Uncertainty in Gross Flux	Uncertainty in Net Flux
k kerfuffle	Model structure	Scenario	Ambiguity	Bias	50%	>100%
k parameter	Parameter	Statistical or scenario	Epistemic	Bias	20%	50%
Wind speed (products)	Input	Statistical or scenario	Epistemic	Bias	10%	10%
Wind speed (sampling)	Input	Statistical	Natural Variability	Random	<5%, a	<5%
Cool skin and warm layers	Model structure	Statistical or scenario	Epistemic	Bias	<5%, a	25%
Temperature (products)	Input	Statistical or scenario	Epistemic	Bias	<5%, a	<5%
Temperature (sampling)	Input	Statistical	Natural Variability	Random	<5%, a	<5%
Temperature – wind speed covariance (sampling)	Input	Statistical	Natural Variability	Random	<5%, a	<5%
Temperature – wind speed covariance	Model Structure	Statistical or scenario	Natural Variability	Random	<5%, a	<5%
pCO2 (bias)	Input	Statistical or scenario	Epistemic	Bias	<5%, a	25%
pCO2 (random)	Input	Statistical	Epistemic	Random	<5%, a	<5%
Asymmetry	Model Structure	Statistical or scenario	Epistemic	Bias	<5%	25%

a, likely to be minor errors at global level, but much more important locally

Table: identification of sources of error within the flux calculation and tentative estimates of the uncertainty they contribute to the gross and net fluxes.

Abstract:

David K. Woolf, Lonneke M. Goddijn-Murphy, Jamie D. Shutler, Peter E. Land, Craig J. Donlon, John Prytherch, Margaret J. Yelland, Phil D. Nightingale, Ricardo Torres, Bertrand Chapron, Jean-Francois Piolle, Sylvain Herledan, Jenny Hanafin, Fanny Girard-Ardhuin, Fabrice Ardhuin and Ben Moat (in-draft) The contemporary air-sea flux of carbon dioxide I: Sources and types of uncertainty in the OceanFlux Climatology



We consider the problem of producing air-sea gas flux climatologies with a complete and traceable description of uncertainties. We start with a consideration of the generic problem of calculating the uncertainties inherent in a system and then focus on the particular sources of error for calculating air-sea gas fluxes from a flux equation. The approach to the generic problem starts with the identification of errors, each of which is categorised according to location, level, nature and randomness. The first three categories follow the definitions proposed by *Warmink et al.* (2010). "Randomness" separates errors into a consistent bias and a wholly random error. Having identified and classified the errors we make a preliminary assessment of their significance, first to the error in individual estimates of flux and secondly, to the bias uncertainty in averaged air-sea gas fluxes. While the limited number of measurements of dissolved gas concentration is certainly an issue for all gases, the dispute over gas transfer velocities may be a greater issue for averaged fluxes of carbon dioxide, especially in basins such as the North Atlantic where observations of dissolved concentration are relatively common.

Status: In draft (it forms part I of the main climatology paper)

7.13 Global climatology of sea-air CO₂ fluxes

Abstract:

David K. Woolf, Jamie D. Shutler, Lonneke Goddijn-Murphy, Craig J. Donlon, Phil D. Nightingale, Peter E. Land, Ricardo Torres, Bertrand Chapron, Jean-Francois Piolle, Sylvain Herledan, Jenny Hanafin, Fanny Girard-Ardhuin, Fabrice Ardhuin, John Prytherch, Ben Moat and Margaret Yelland (in-draft) The contemporary air-sea flux of carbon dioxide, II Scenario and ensemble estimates of global fluxes in the OceanFlux climatology.

A global flux of CO₂ of \sim 80 Pg C yr⁻¹ is exchanged between atmosphere and ocean annually with a net flux in recent years of $\sim 2 \text{ Pg C} \text{ yr}^{-1}$ into the oceans. While other methods are available to estimate global and basin-scale fluxes, regional and subseasonal estimates are only practical through application of an air-sea flux equation that requires concentrations in atmosphere and ocean and estimates of transfer velocity. Uncertainties arise throughout the calculation and the propagation of these errors through to a final flux estimate of flux. Various data sets (in situ, Earth Observation and modelling) and algorithms are used to compute air-sea gas flux. Fluxes are calculated at monthly and one-degree resolution for a reference year of 2010, but the analysis presented here focusses on annual fluxes for the global oceans. A large number of calculations are presented representing different scenarios and formal ensembles. The results suggest relatively high uncertainty in global and regional carbon dioxide flux. For a reference year of 2000, we estimate a net global flux from air to sea of 2.0 Pg C yr⁻¹, but with a high bias uncertainty. An optimistic interpretation of existing uncertainty in gas transfer velocities leads to a bias uncertainty of ~0.5 Pg C yr⁻¹, while a more pessimistic interpretation implies a bias uncertainty > 1 Pg C yr⁻¹. Similarly, a set of simulated upper ocean CO₂ fields created by a bootstrap method are also used to study the uncertainty in flux. Some ensemble members suggest a very large uncertainty in global net flux. Some of the scenarios and ensemble members may be contradicted by global and regional estimates by other methods, but they cannot be easily dismissed directly.



Status: In draft.

7.14 Data processing system architecture and approach

Two novel aspects of the OceanFlux GHG project are the system architecture used for calculations of fluxes and an "open door" to the SOLAS community to implement their own calculations. These two aspects are closely related. The open door policy is only practical by supplying access to all the basis data sets and open source tools for calculation and display, and also sufficient computational power to enable the calculations. Those facilities are supplied by the chosen system architecture, which is based on the cloud computing capability at IFREMER with programming in open source languages (primarily Python, but also R).

The architecture developed and tested for the OceanFlux GHG is novel and the experience should inform future projects that need to use cloud computing, enable open access or both. Similarly, the experience of managing an open door policy was invaluable and demonstrates advantages and pitfalls of this approach. An important project outcome is a number of recommendations for similar projects in the future.

Abstract:

Jamie D. Shutler, Jean-Francois Piolle, Peter Land, David K. Woolf, Lonneke Goddijn-Murphy,Frederic Paul, Fanny Girard-Ardhuin, Bertrand Chapron, Craig J. Donlon (in draft) FluxEngine: A flexible processing system for calculating air-sea carbon dioxide gas fluxes and climatologies, *to be submitted to Journal of Atmospheric and Oceanic Technology*.

The air-sea flux of Greenhouse gases (e.g. carbon dioxide, CO₂) is a critical part of the climate system and a major factor in the biogeochemical development of the oceans. More accurate and higher resolution calculations of these gas fluxes are required if we are to fully understand and predict our future climate. Satellite Earth observation is able to provide large spatial scale datasets that can be used to study gas fluxes. However, the large storage requirements needed to host such data can restrict its use by the scientific community. Fortunately, the development of cloud-computing can provide a solution. Here we describe a cloud-computing based air-sea CO₂ flux processing toolbox called the 'FluxEngine'. The toolbox allows users to easily generate global and regional airsea CO₂ flux data from model, in situ and Earth observation data. The air-sea gas flux calculation is user configurable and the toolbox allows users to easily exploit more than 8 terabytes of climate quality Earth observation data for the derivation of gas fluxes. The resultant NetCDF data output can be easily downloaded and each file contains >20 data layers containing the various stages of the flux calculation along with process indicator layers to aid interpretation of the data. The toolbox exploits a cloudcomputing platform that provides efficient and fast data processing. This paper describes the toolbox design, the verification of the air-sea CO₂ flux calculations, demonstrates the use of the tools for studying global and shelf sea air-sea fluxes and discusses future developments.

Status: In draft.



7.15 Model derived pCO₂

OceanFlux GHG project used coupled ecosystem-hydrodynamic models as a method for producing estimates of pCO_2 in shelf and coastal waters. This approach is complementary to the global approach based on gridding and interpolating in situ data. The latter method is less credible in coastal waters where it is known the autocorrelation length and time scales of pCO_2 are drastically reduced. For example, Jones et al. (2012) estimate a global median spatial autocorrelation (e-folding) length of 400 km, but reports lengths as low as 50 km in coastal regions. In situ data sets are mostly sufficient to interpolate with search radii of O(400 km), but a search radii of only 50 km would leave a large number of "empty cells".

The specific research within OceanFlux GHG builds on a large body of work previously and currently undertaken by PML scientists and their collaborators. A specific contribution within OceanFlux GHG is based on the implementation of a 1D model system (GOTM-ERSEM) at station L4 in UK coastal waters (western English Channel). This station is ~10nm south of Plymouth at a depth of 51 m. Observations have been sustained at L4 for more than 20 years and sampling is weekly. Model experiments for EO data assimilation and the impact of biogenic slicks and diurnal warming were performed. The data assimilation system implemented in this work is the 1D version of the Ensemble Kalman Filter described by Torres et al. (2006) and Ciavatta et al. (2011). The EO data used in the assimilation experiments was from MODIS-Aqua and included both chlorophyll-a and SST. Higher frequency temperature data from the L4 autonomous buoy was also used for comparison.

The capability to accurately predict coastal CO_2 parameters is developing and OceanFlux GHG has made a distinct contribution to developing that capability.

The comparison of model-generated CO_2 parameters with interpolated in situ values in an overlapping region provides useful insights into the limitations of both.

Abstract:

R. Torres, V. Kitidis, Y. Artioli, S. Ciavatta, M. Villareal, J. D. Shutler, L. Polimene, V. Martinez, C. Widdicombe and E. M. S Woodward (draft) Sensitivity of modelled CO₂ Air-Sea flux in a coastal environment using a complex ecosystem model.

This work evaluates the sensitivity of CO₂ air-sea gas exchange in a coastal site to four different model system configurations of the 1D coupled hydrodynamic-ecosystem model GOTM-ERSEM. The European Sea Regional Ecosystem Model (ERSEM) is a biomass and functional group based biogeochemical model that resolves the time evolution of the pelagic ecosystem including the nutrient and carbon cycle within the planktonic trophic chain of primary producers (picophytoplankton, nanoflagellates, dinoflagellates and diatoms), consumers (meso- and micro- zooplankton and heterotrophic nanoflagellates) and decomposers (heterotrophic bacteria). ERSEM includes a comprehensive carbonate system and explicitly simulates the production of dissolved organic carbon (DOC), dissolved inorganic carbon (DIC) and organic matter (DOM). The model was implemented at the coastal station L4 (4 nutical miles south of



Plymouth, 50°15.00'N, 4°13.02'W, depth of 51 m). The model performance was evaluated using more than 1500 hydrological and biochemical observations routinely collected at L4 through the Western Coastal Observatory activities of 2008-2009.

The 1D model resolves well the physical environment (sea surface temperature has a correlation of 0.94 when comparing hourly data from the L4 monitoring buoy, all values given with a p>0.95). Overall, the model captures the seasonal signal in most biogeochemical variables including the air-sea flux of CO₂ and primary production and can capture some of the intra-seasonal variability and short-lived blooms. The model correctly reproduces the seasonality of nutrients (correlation > 0.80 for all three macronutrients silicate, nitrate and phosphate), surface chlorophyll (correlation > 0.43) and total biomass (corr>0.7) in a two year run for 2008-2009. The model simulates well the concentration of DIC, pH and in water partial pressure of CO₂ (pCO₂) with correlations between 0.4-0.5. The model result suggest that L4 is a weak net sink of CO₂ (0.3-1.8 molC m⁻² year⁻¹)

We ran three distinct experiments to investigate the sensitivity of the carbonate system and modelled air-sea fluxes to i) the SST diurnal cycle, ii) biological suppression of gas exchange and iii) data assimilation using satellite Earth observation data. Resolving the near-surface temperature gradients has the largest impact at short, seasonal and annual time scales and results in improvements across the evaluated variables that are comparable to the results from the assimilation of chlorophyll experiment. The correlation of carbonate system variables (DIC, pCO₂ and pH) improve by up to 19% while annually integrated values of CO₂ exchange with the atmosphere changed by up to 50% with respect to the standard simulation, increasing the net sink nature of L4. At the L4 site, the introduction of a dependence of the CO₂ gas transfer velocity on gross production as a proxy for the production of surface slicks has a non-significant impact on the dynamics of CO₂, including the air-sea annual exchange estimates. The assimilation of surface Chlorophyll has an overall mixed effect on the ability of the model to reproduce the observations. As expected the simulation of chlorophyll improves and while the correlation for nutrients do not significantly change, their bias decreases. The effect on the carbonate system variables is similar; the bias decreases for DIC and pH but so do the correlations. The largest impact of assimilation is on the net Air-sea gas exchange where the results indicate the potential for L4 to be a weak source $(1.3 \pm 1.7 \text{ molC m}^{-2} \text{ year}^{-1}).$

Status: In draft. Presentation given at the science workshop.

7.16 Calculations of sensitivity of Arctic air-sea fluxes to climate, exploiting thermal and haline methods.

Abstract:

Land, P. E., Shutler, J. D., Cowling, R. D., Woolf, D. K., Walker, P., Findlay, H. S., Upstill-Goddard, R. C., and Donlon, C. J.: Climate change impacts on sea–air fluxes of CO₂ in three Arctic seas: a sensitivity study using Earth observation, Biogeosciences, 10, 8109-8128, doi:10.5194/bg-10-8109-2013, 2013, http://www.biogeosciences.net/10/8109/2013/bg-10-8109-2013.html



We applied coincident Earth observation data collected during 2008 and 2009 from multiple sensors (RA2, AATSR and MERIS, mounted on the European Space Agency satellite Envisat) to characterise environmental conditions and integrated sea-air fluxes of CO_2 in three Arctic seas (Greenland, Barents, Kara). We assessed net CO_2 sink sensitivity due to changes in temperature, salinity and sea ice duration arising from future climate scenarios. During the study period the Greenland and Barents seas were net sinks for atmospheric CO₂, with integrated sea-air fluxes of -36 ± 14 and -11 ± 5 Tg C yr⁻¹, respectively, and the Kara Sea was a weak net CO₂ source with an integrated sea-air flux of $+2.2 \pm 1.4$ Tg C yr⁻¹. The combined integrated CO₂ sea-air flux from all three was -45 ± 18 Tg C yr⁻¹. In a sensitivity analysis we varied temperature, salinity and sea ice duration. Variations in temperature and salinity led to modification of the transfer velocity, solubility and partial pressure of CO_2 taking into account the resultant variations in alkalinity and dissolved organic carbon (DOC). Our results showed that warming had a strong positive effect on the annual integrated sea-air flux of CO_2 (i.e. reducing the sink), freshening had a strong negative effect and reduced sea ice duration had a small but measurable positive effect. In the climate change scenario examined, the effects of warming in just over a decade of climate change up to 2020 outweighed the combined effects of freshening and reduced sea ice duration. Collectively these effects gave an integrated sea-air flux change of +4.0 Tg C in the Greenland Sea, +6.0 Tg C in the Barents Sea and +1.7 Tg C in the Kara Sea, reducing the Greenland and Barents sinks by 11% and 53%, respectively, and increasing the weak Kara Sea source by 81%. Overall, the regional integrated flux changed by +11.7 Tg C, which is a 26% reduction in the regional sink. In terms of CO_2 sink strength, we conclude that the Barents Sea is the most susceptible of the three regions to the climate changes examined. Our results imply that the region will cease to be a net CO_2 sink in the 2050s.

Status: published.

7.17 The effect of rain on sea-air CO₂ fluxes

Abstract:

J. D. Shutler, P. E. Land, D. K. Woolf, G. Quartly, C. J. Zappa and W. R. McGillis (draft) Characterising the impact of rain on global and regional air-sea fluxes of CO₂: a 20 year global sensitivity analysis, *to be submitted to JGR Biogeosciences*.

The global oceans are considered a major sink of atmospheric carbon dioxide (CO₂). Rain is known to alter the physical and chemical conditions at the sea surface, and thus influences the transfer of CO₂ between the ocean and atmosphere. However, to date no quantification of these effects on global net air-sea fluxes exists. Rain can influence gas exchange through surface layer dilution, enhanced gas transfer velocity, altering the sea skin temperature and through the direct export of carbon from the atmosphere to the ocean. We investigate the impact of all of these processes using a 20+ year archive of monthly global climate quality satellite Earth observation (EO) data. Globally rain can increase the annual oceanic integrated net sink of CO₂ by up to 6 %. Regionally, the annual variations can be larger, the largest of which is in the Southern Ocean where rain can increase the net sink by up to 13%. The regional monthly variations can be much higher. The Pacific and Southern ocean monthly net fluxes can be significantly modulated by rain with regular variations of $> \pm 15\%$. Instances of very large

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modulation of $> \pm 50\%$ are also possible. The impacts of rain should be included in the uncertainty analysis of studies that estimate net air-sea fluxes of CO2 as the rain can have a considerable impact on the fluxes, dependent upon the region and timescale.

Status: partial draft.

7.18Impact of wind waves on the air-sea fluxes: A coupled model

Abstract:

Kudryavtsev V. K., Chapron B., Makin V (in-press) Impact of wind waves on the airsea fluxes: A coupled model, *Journal of Geophysical Research*.

A revised wind-over-wave-coupling model is developed to provide a consistent description of the sea surface drag and heat/moister transfer coefficients, and associated wind velocity and temperature profiles. The spectral distribution of short wind waves in the decimeter to a few millimeters range of wavelengths is introduced based on the wave action balance equation constrained using the Yurovskaya et al. (2013) optical field wave measurements. The model is capable to reproduce fundamental statistical properties of the sea surface such as the mean square slope and the spectral distribution of breaking crests length. The surface stress accounts for the effect of airflow separation due to wave breaking, which enables a better fit of simulated form drag to observations. The wave breaking controls the overall energy losses for the gravity waves, but also the generation of shorter waves including the parasitic capillaries, thus enhancing the form drag. Breaking wave contribution to the form drag increases rapidly at winds above 15 m/s where it exceeds the non-breaking wave contribution. The overall impact of wind waves (breaking and non-breaking) leads to a sheltering of the near surface layer where the turbulent mixing is suppressed. Accordingly, the air temperature gradient in this sheltered layer increases to maintain the heat flux constant. The resulting deformation of the air temperature profile tends to lower the roughness scale for temperature compared to its value over the smooth surface.

Status: in-press.

7.19 Review, "Transfer across the air-sea interface"

The following is not a project deliverable, so is an added extra.

Garbe, C.S., A. Rutgersson, J. Boutin, B. Delille, C.W. Fairall, N. Gruber, J. Hare, D. Ho, M. Johnson, G. de Leeuw, P. Nightingale, H. Petterson, J. Piskozub, E. Sahlee, W.-T. Tsai, B. Ward, **D.K. Woolf** and C. Zappa. 2013. Transfer across the air-sea interface. In **Ocean-Atmosphere Interactions of Gases and Particles,** edited by Peter Liss and Martin Johnson, Springer-Verlag. (2014)

Status: published.



7.20A global study of the correlation properties of wind and rain

This is not a project deliverable, so is considered an added extra as it credits the project.

Quartly, G., **J. Shutler** and **D. Woolf**. 2013. A global study of the correlation properties of wind and rain. ESA Living Planet Symposium 2013, Edinburgh, UK, 9-13 September, 2013.

Both wind and rain have major impacts on the surface ocean, but in many cases their contributions are treated independently, parametrizing the output of processes as separate components dependent upon the mean fields of wind speed and rain rate, without regard for any interaction terms. Here we make use of the two decades of dual-frequency altimetry, which provide simultaneous measurements of wind speed and rain rate. Whilst the primary Ku-band channel is sensitive to both wind and rain, the secondary frequency (S-band for Envisat; C-band for Topex, Jason-1 and Jason-2) is relatively unaffected by rain, permitting the effects of rain and wind on the altimeter record to be separated. Data are subdivided into key oceanographic regions and the conditional probability of rain calculated for different wind speed conditions. Whilst in many cases rain is associated with strong winds in storms, in lower latitudes convective rain predominantly occurs in calmer conditions. We quantify these effects and discuss their relevance for sound generation at sea (where wind can diminish the signal due to rain) and the flux of greenhouse gases between atmosphere and ocean.

Status: published.

7.21 Statistical properties of breaking waves in field condition: A Gaussian field approach

This is not a project deliverable, so is an added extra as it credits the project.

Alexey Mironov, **Bertrand Chapron** and Vladimir Dulov (2013) Statistical properties of breaking waves in field condition: A Gaussian field approach, Brest Scientific workshop.

Breaking of the wind waves play a dominant role in the dynamics of upper ocean layer, air-sea interactions and energy dissipation of wind waves. Modeling of physical and statistical properties of breakers still remains poorly described.

In this work, we present an new analysis of statistical properties of video-detected breaking waves. More precisely, the analysis is based on the use of a near-Gaussian statistical assumption applied to the filtered wave field within a given velocity interval



and a given propagation direction. Whitecaps, as associated to regions of the field exceeding some critical threshold, can be described with high-level statistics (e.g. Adler, 1981). For a Gaussian field, high excursions shall be well approximated with elliptical paraboloid whose centers follow a Poisson process. Accordingly, individual foam patches are also approximated with ellipses with a mean eccentricity connected to the directional mean square slopes of the filtered waves. Within a given velocity range, whitecap surface sizes are also randomly distributed to closely obey an exponential distribution. Individual breaking crest lengths must thus be Rayleigh distributed.

These theoretical predictions were validated with a massive experimental data set. Field video observations of wavebreaking statistics were obtained during filed campaign at the Black sea platform in Katsiveli, Ukraine. Validation was performed for wide range of wave and wind conditions.

The present results can be used to provide realistic statistical properties of wavebreaking field, as well as to provide some improved means to efficiently model the whitecap coverage and thickness for different wind and wave conditions.

Status: Presented at the scientific workshop.





8. Annex of abstracts from the draft papers

The contemporary air-sea flux of carbon dioxide I: Sources and types of uncertainty in the OceanFlux Climatology

David K. Woolf; Lonneke M. Goddijn-Murphy; Jamie D. Shutler; Peter E. Land, Craig J. Donlon, John Prytherch; Margaret J. Yelland; Phil D. Nightingale, Ricardo Torres, Bertrand Chapron, Jean-Francois Piolle, Sylvain Herledan, Jenny Hanafin, Fanny Girard-Ardhuin, Fabrice Ardhuin and Ben Moat

We consider the problem of producing air-sea gas flux climatologies with a complete and traceable description of uncertainties. We start with a consideration of the generic problem of calculating the uncertainties inherent in a system and then focus on the particular sources of error for calculating air-sea gas fluxes from a flux equation. The approach to the generic problem starts with the identification of errors, each of which is categorised according to location, level, nature and randomness. The first three categories follow the definitions proposed by *Warmink et al.* (2010). "Randomness" separates errors into a consistent bias and a wholly random error. Having identified and classified the errors we make a preliminary assessment of their significance, first to the error in individual estimates of flux and secondly, to the bias uncertainty in averaged air-sea gas fluxes. While the limited number of measurements of dissolved gas concentration is certainly an issue for all gases, the dispute over gas transfer velocities may be a greater issue for averaged fluxes of carbon dioxide, especially in basins such as the North Atlantic where observations of dissolved concentration are relatively common.

The contemporary air-sea flux of carbon dioxide, II Scenario and ensemble estimates of global fluxes in the OceanFlux climatology

David K. Woolf; Jamie D. Shutler, Lonneke Goddijn-Murphy, Craig J. Donlon, Phil D. Nightingale, Peter E. Land, Ricardo Torres, Bertrand Chapron, Jean-Francois Piolle, Sylvain Herledan, Jenny Hanafin, Fanny Girard-Ardhuin, Fabrice Ardhuin, John Prytherch, Ben Moat and Margaret Yelland

A global flux of CO₂ of ~80 Pg C yr⁻¹ is exchanged between atmosphere and ocean annually with a net flux in recent years of ~2 Pg C yr⁻¹ into the oceans. While other methods are available to estimate global and basin-scale fluxes, regional and subseasonal estimates are only practical through application of an air-sea flux equation that requires concentrations in atmosphere and ocean and estimates of transfer velocity. Uncertainties arise throughout the calculation and the propagation of these errors through to a final flux estimate of flux. Various data sets (in situ, Earth Observation and modelling) and algorithms are used to compute air-sea gas flux. Fluxes are calculated at monthly and one-degree resolution for a reference year of 2010, but the analysis presented here focusses on annual fluxes for the global oceans. A large number of calculations are presented representing different scenarios and formal ensembles. The results suggest relatively high uncertainty in global and regional carbon dioxide flux.



For a reference year of 2000, we estimate a net global flux from air to sea of 2.0 Pg C yr⁻¹, but with a high bias uncertainty. An optimistic interpretation of existing uncertainty in gas transfer velocities leads to a bias uncertainty of ~0.5 Pg C yr⁻¹, while a more pessimistic interpretation implies a bias uncertainty > 1 Pg C yr⁻¹. Similarly, a set of simulated upper ocean CO₂ fields created by a bootstrap method are also used to study the uncertainty in flux. Some ensemble members suggest a very large uncertainty in global net flux. Some of the scenarios and ensemble members may be contradicted by global and regional estimates by other methods, but they cannot be easily dismissed directly.

FluxEngine: A flexible processing system for calculating air-sea carbon dioxide gas fluxes and climatologies

Jamie D. Shutler, Jean-Francois Piolle, Peter Land, David K. Woolf, Lonneke Goddijn-Murphy, Frederic Paul, Fanny Girard-Ardhuin, Bertrand Chapron, Craig J. Donlon

The air-sea flux of Greenhouse gases (e.g. carbon dioxide, CO₂) is a critical part of the climate system and a major factor in the biogeochemical development of the oceans. More accurate and higher resolution calculations of these gas fluxes are required if we are to fully understand and predict our future climate. Satellite Earth observation is able to provide large spatial scale datasets that can be used to study gas fluxes. However, the large storage requirements needed to host such data can restrict its use by the scientific community. Fortunately, the development of cloud-computing can provide a solution. Here we describe a cloud-computing based air-sea CO_2 flux processing toolbox called the 'FluxEngine'. The toolbox allows users to easily generate global and regional airsea CO₂ flux data from model, in situ and Earth observation data. The air-sea gas flux calculation is user configurable and the toolbox allows users to easily exploit more than 8 terabytes of climate quality Earth observation data for the derivation of gas fluxes. The resultant NetCDF data output can be easily downloaded and each file contains >20 data layers containing the various stages of the flux calculation along with process indicator layers to aid interpretation of the data. The toolbox exploits a cloudcomputing platform that provides efficient and fast data processing. This paper describes the toolbox design, the verification of the air-sea CO₂ flux calculations, demonstrates the use of the tools for studying global and shelf sea air-sea fluxes and discusses future developments.

Characterising the impact of rain on global and regional air-sea fluxes of CO₂: a 20 year global sensitivity analysis

J. D. Shutler, P. E. Land, D. K. Woolf, G. Quartly, C. J. Zappa and W. R. McGillis

The global oceans are considered a major sink of atmospheric carbon dioxide (CO₂). Rain is known to alter the physical and chemical conditions at the sea surface, and thus influences the transfer of CO_2 between the ocean and atmosphere. However, to date no quantification of these effects on global net air-sea fluxes exists. Rain can influence gas exchange through surface layer dilution, enhanced gas transfer velocity, altering the sea skin temperature and through the direct export of carbon from the atmosphere to the



ocean. We investigate the impact of all of these processes using a 20+ year archive of monthly global climate quality satellite Earth observation (EO) data. Globally rain can increase the annual oceanic integrated net sink of CO₂ by up to 6 %. Regionally, the annual variations can be larger, the largest of which is in the Southern Ocean where rain can increase the net sink by up to 13%. The regional monthly variations can be much higher. The Pacific and Southern ocean monthly net fluxes can be significantly modulated by rain with regular variations of $> \pm 15\%$. Instances of very large modulation of $> \pm 50\%$ are also possible. The impacts of rain should be included in the uncertainty analysis of studies that estimate net air-sea fluxes of CO2 as the rain can have a considerable impact on the fluxes, dependent upon the region and timescale.

Deriving a sea surface climatology of CO₂ fugacity in support of air-sea gas flux studies

L. M. Goddijn-Murphy, D. K. Woolf, P. E. Land, J. D. Shutler, and C. Donlon

Climatologies, or long-term averages, of essential climate variables are useful for evaluating models and providing a baseline for studying anomalies. The Surface Ocean Carbon Dioxide (CO2) Atlas (SOCAT) has made millions of global underway sea surface measurements of CO2 publicly available, all in a uniform format and presented as fugacity, fco₂. fco₂ is highly sensitive to temperature and the measurements are only valid for the instantaneous sea surface temperature (SST) that is measured concurrent with the in-water CO₂ measurement. To create a climatology of fco₂ data suitable for calculating air-sea CO₂ fluxes it is therefore desirable to calculate f_{CO2} valid for climate quality SST. This paper presents a method for creating such a climatology. We recomputed SOCAT's fco2 values for their respective measurement month and year using climate quality SST data from satellite Earth observation and then extrapolated the resulting f_{CO_2} values to reference year 2010. The data were then spatially interpolated onto a $1 \times 1^{\circ}$ grid of the global oceans to produce 12 monthly fco₂ distributions for 2010. The partial pressure of CO_2 (pcO₂) is also provided for those who prefer to use pcO₂. The CO₂ concentration difference between ocean and atmosphere is the thermodynamic driving force of the air-sea CO₂ flux, and hence the presented f_{CO₂} distributions can be used in air–sea gas flux calculations together with climatologies of other climate variables.

Sensitivity of modelled CO₂ air-sea flux in a coastal environment using a complex ecosystem model

Ricardo Torres, Yuri Artioli, V. Kitidis, Stefano Ciavatta, Manuel Villareal, Jamie Shutler, Luca Polimene, Victor Martinez, Claire Widdicombe, E. Malcolm S. Woodward, Timothy Smyth, James Fishwick, Gavin Tilstone, and Diane Knappett

This work evaluates the sensitivity of CO₂ air-sea gas exchange in a coastal site to four different model system configurations of the 1D coupled hydrodynamic-ecosystem model GOTM-ERSEM. The European Sea Regional Ecosystem Model (ERSEM) is a biomass and functional group based biogeochemical model that includes a comprehensive carbonate system and explicitly simulates the production of dissolved organic carbon, dissolved inorganic carbon and organic matter.

The model was implemented at the coastal station L4 (4 nm south of Plymouth, 50°15.00'N, 4°13.02'W, depth of 51 m). The model performance was evaluated using more than 1500 hydrological and biochemical observations routinely collected at L4 through the Western Coastal Observatory activities of 2008-2009. In addition to a reference simulation (A), we ran three distinct experiments to investigate the



sensitivity of the carbonate system and modelled air-sea fluxes to B) the sea surface temperature (SST) diurnal cycle, C) biological suppression of gas exchange and D) data assimilation using satellite Earth observation data.

The reference simulation captures well the physical environment (simulated SST has a correlation with observations equal to 0.94 with a p> 0.95). Overall, the model captures the seasonal signal in most biogeochemical variables including the air-sea flux of CO₂ and primary production and can capture some of the intra-seasonal variability and short-lived blooms. The model correctly reproduces the seasonality of nutrients (correlation > 0.80 for all three macronutrients silicate, nitrate and phosphate), surface chlorophyll-a (correlation > 0.43) and total biomass (correlation > 0.7) in a two year run for 2008-2009. The model simulates well the concentration of DIC, pH and in water partial pressure of CO₂ (pCO₂) with correlations between 0.4-0.5. The model results suggest that L4 is a weak net source of CO₂ (0.3-1.8 molC m⁻² year⁻¹).

The results of the three sensitivity experiments indicate that resolving the temperature profile near to the surface appears the most important feature for a skilled simulation of the biogeochemistry at L4. This result indicates that this finer vertical scale should be included in future shelf sea models used in air-sea flux modelling studies.



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