The increasing importance of satellite observations to assess the ocean carbon sink and ocean acidification

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Abstract

The strong control that the emissions of carbon dioxide (CO_2) have over Earth's climate identifies the need for accurate quantification of the emitted CO_2 and its redistribution within the Earth system. The ocean annually absorbs more than a quarter of all CO_2 emissions and this absorption is fundamentally altering the ocean chemistry. The ocean thus provides a fundamental component and powerful constraint within global carbon assessments used to guide policy action for reducing emissions. These carbon assessments rely heavily on satellite observations, but their inclusion is often invisible or opaque to policy. One reason is that satellite observations are rarely used exclusively, but often in conjunction with other types of observations, thereby complementing and expanding their usability yet losing their visibility. This exploitation of satellite observations led by the satellite and ocean carbon scientific communities is based on exciting developments in satellite science that have broadened the suite of environmental data that can now reliably be observed from space. However, the full potential of satellite observations to expand the scientific knowledge on critical processes such as the atmosphere-ocean exchange of CO_2 and ocean acidification, including its impact on ocean health, remains largely unexplored. There is clear potential to begin using these observation-based approaches for directly guiding ocean management and conservation decisions, in particular in regions

where *in situ* data collection is more difficult, and interest in them is growing within the environmental policy communities. We review these developments, identify new opportunities and scientific priorities, and identify that the formation of an international advisory group could accelerate policy relevant advancements within both the ocean carbon and satellite communities. Some barriers to understanding exist but these should not stop the exploitation and the full visibility of satellite observations to policy makers and users, so these observations can fulfil their full potential and recognition for supporting society.

1. Introduction

The latest assessment by the Intergovernmental Panel on Climate Change (IPCC) on the state of our climate identified that warming of 1.5°C appears unavoidable (IPCC, 2022) and that rapid emissions reductions are urgently needed to reduce further warming and stabilise climate. These recommendations are guided by annual assessments of the carbon budget (e.g. by the Global Carbon Project, GCP) which attempt to quantify annual emissions (fossil fuel, cement production, land use change), their redistribution within the atmosphere and their uptake by the land biosphere and the ocean (e.g. Friedlingstein *et al.,* 2019, 2020, 2022). The relatively well-mixed nature of the atmosphere allows the quantification of the long-term CO_2 accumulation using a small number of observing stations (e.g. Keeling, 1978). Observation-based estimates of the annual ocean carbon uptake (sink) have now become a key component within these assessments, complementing the ocean model-based estimates. In contrast, the land sink continues to be estimated via models (Friedlingstein *et al.,* 2022) due to its highly heterogeneous nature. Thus, ocean and atmosphere observations form the key observational pillars and constraints within these annual carbon budget assessments, with their uncertainties directly impacting the closure of the total budget. The policy relevance of these annual carbon assessments cannot be underestimated; they provide information about the impact of mitigation policies and they also enable updates on the so called “remaining carbon budget”, which identifies how much CO_2 can be emitted in the coming decades without overshooting specific climate targets (e.g. as determined using models within IPCC, 2022 and Friedlingstein *et al.,* 2022). Thus, efforts to increase understanding of, as well as improve the quantification of the ocean carbon sink, will strengthen its constraint on the remaining components of the budget within annual assessments, and increase the strength of any resulting policy guidance.

Models and the analyses of ocean interior observations show that more than a quarter of the total anthropogenic emissions have been taken up by the ocean (Sabine *et al.,* 2004; Gruber *et al.,* 2019b) with the proportion absorbed remaining near constant over the last five decades (Friedlingstein *et al.,* 2022; Gruber *et al.,* 2023). This uptake occurs predominantly through gas exchange across the atmosphere-ocean interface and penetrates into the subsurface layers, changing the marine carbonate chemistry. The net effect is often called “Ocean Acidification” and is detrimental to marine life and the ocean’s ability to function as a carbon sink. This ocean acidification encompasses the anthropogenic CO_2 driven increase in acidity ([H+], decreasing in pH), the increase in the concentration of dissolved CO_2, the decrease in the concentration of the carbonate ion and the resulting decrease in the saturation state of seawater with regard to solid forms of calcium carbonate such as aragonite and calcite (e.g. Feely *et al.,* 2009). Ocean acidification is decreasing the ocean’s capacity to absorb further CO_2 (Orr *et al.,* 2005) and its impact on marine organisms and ecosystems varies substantially across taxa and systems, but tends to be especially detrimental for calcifying organisms, including those with significant economic or ecological importance such as corals,

mussels, and pelagic calcifiers (e.g. Dixon *et al.,* 2022; Doney *et al.* 2020). The changes induced by ocean acidification percolate up entire food webs, populations and ecosystems, threatening essential marine ecosystem services (Sunday *et al.,* 2017; Fabry *et al*., 2019) such as coastal or flood protection and fisheries (e.g. Doney *et al.,* 2020) and degrading their related socio-economical values.

Historically, most knowledge about global ocean carbon was derived from models (Gruber *et al.,*2023) but since the 1990s ocean observations are providing an increasing number of constraints. Within this *in situ* observations are critical, but given the ocean's size and its often inhospitable nature, their coverage remains limited. The unique capability of space-based observations for providing large spatial scale (figure 1a), and increasingly regional-scale, observations means that they are now heavily used alongside *in situ* observations. Beyond the differences in spatial coverage, this combination is needed as some key properties cannot be observed from space but can be *in situ* (e.g. gaseous CO_2 within the ocean), whilst some observations require specialist *in situ* capability not routinely available, but which is routinely deployed in space (e.g. near-infrared sensed temperature at 1 mm depth, or microwave evaluation of ice coverage). Just as *in situ* instruments require regular laboratory calibrations, satellite instruments require regular monitoring and calibration via *in situ* data. Consequently, the ability to use satellite observations relies upon *in situ* data campaigns, and global and regional observation-based assessments of ocean carbon rely heavily upon the integration of satellite observations with extensive *in situ* data and model re-analyses (Shutler *et al.,* 2020).

Clearly the only way to slow the rate of ocean acidification is to drastically reduce the rate of the human-made emissions of CO_2, in order to, at least stabilize the atmospheric CO_2 concentration, and satellite and *in situ* observation-based ocean carbon assessments will be critical to identify any stabilisation. Even when stabilisation occurs, we will need mitigation and adaption strategies and satellite observations are well placed to support these. Similarly, a plethora of outstanding, and critical, science questions that carbon-cycle communities are now focussing on, such as identifying the strength and role of the Southern Ocean carbon sink (e.g. Gruber *et al*., 2019), or the importance of ocean biology in modulating carbon exchange and how this will change (e.g. Arico *et al.,* 2020) will all require the use of satellite observations.

This paper, supported with new primary data, first reviews how and why satellite observations are critical to ocean carbon science and assessments. It then identifies new scientific opportunities and key areas where satellite observations will provide greatest benefit to the carbon community, and identifies how to strengthen the important link between these satellite observation-based approaches and potential end users, a link that is currently weak. This includes mapping how the satellite capabilities could be used to support mitigation and adaption at regional and international levels. This map has been co-designed with early adopters whose communities are already grappling with the decreasing pH of their seas. This paper forms part of a special issue and accompanies the work of Brewin *et al.,* (2023) which identifies the capabilities for studying inorganic and organic ocean carbon from space, and a large range of scientific needs. This paper expands upon this by focussing solely on the ocean carbon sink and ocean acidification, identifying scientific and policy priorities and opportunities for quantifying surface water inorganic carbon.

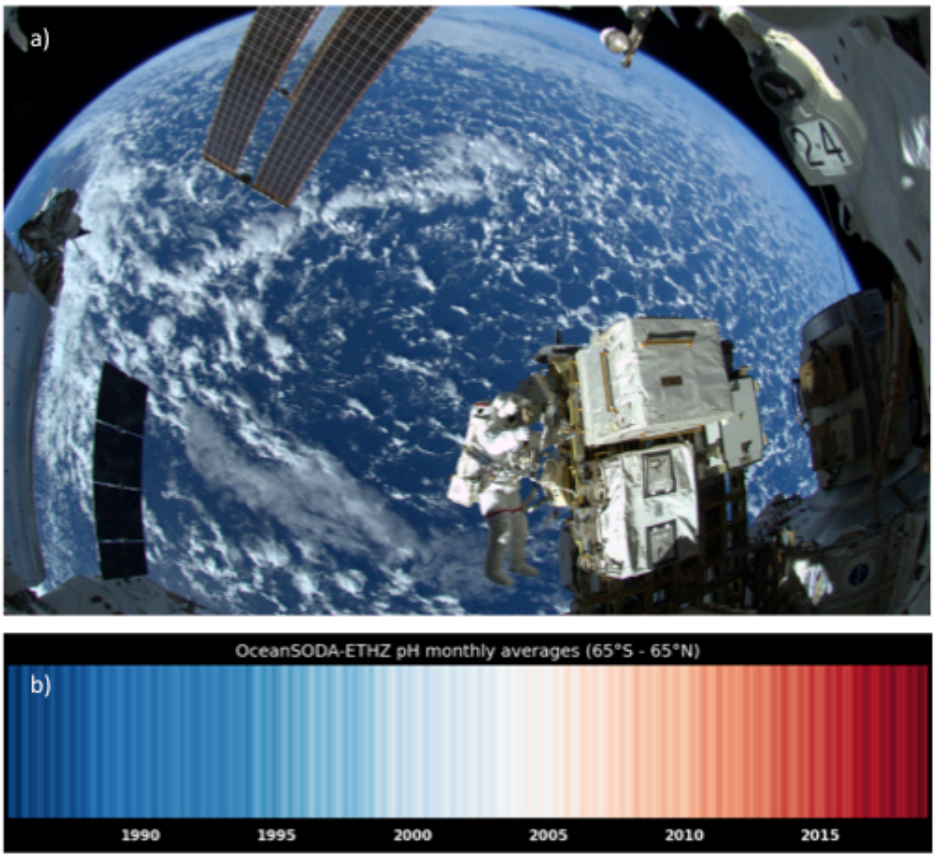

Figure 1: Satellite Earth observations are already used extensively to study ocean health and increasingly ocean acidification. a) This view of the Pacific Ocean from the largest satellite ever built, the International Space Station, illustrates the synoptic-scale view uniquely provided by satellite observations – everything in this view is the Pacific Ocean (credit, European Space Agency). This platform has hosted >30 different experimental satellite sensors which have yet to be explored by the ocean carbon community; b) The 'pH stripe' highlighting the long-term change in ocean pH since the 1980s, as determined using satellite observation-based data illustrates how satellite observations can help highlight the impact that carbon emissions are having on ocean health (generated using data from Gregor and Gruber, 2021).

2. Satellite data are extensively used for ocean carbon assessments

The relationships between the different carbonate system parameters are fundamentally driven by thermodynamics. Salinity directly affects the coefficients of the carbonate system equations (Land *et al.*, 2015) and covaries with alkalinity across the globe (Millero *et al.,* 1998; Lee *et al.,* 2006). Temperature is a strong controller of CO_2 solubility (Woolf *et al.,* 2016); so temperature and salinity are highly related to changes in dissolved inorganic carbon (e.g. Bakker *et al.,* 1999). Hence, temperature and salinity are important diagnostic variables and are needed to assess the surface water carbonate system (Dickson *et al.,* 2007). This has led to satellite temperature data now routinely being used to identify the causes of wider spatial scale variability in the surface carbonate system (e.g. Lefevre *et al.,* 2021; Olivier *et al.,* 2022). The relatively recent capability for satellite salinity observations has unlocked the ability for space-based carbonate system monitoring (Land *et al.,* 2015; Salisbury *et al.,* 2015) of surface waters via empirically derived salinity-alkalinity relationships. Early work demonstrated its credibility enabling the first observations of synoptic scale alkalinity in the Atlantic (Fine *et al.,* 2016), and alkalinity and dissolved carbon temporal

mixing in the Amazon plume (Land *et al.,* 2019). The use of machine learning has produced observation-driven decadal-scale assessments of a single carbon parameter (partial pressure of CO_2, e.g. Watson *et al.,* 2020; Chau *et al.,* 2022; Friedlingstein *et al.,* 2021; figure 2) and even the complete carbonate system (Gregor and Gruber, 2021; figure 2) through combining the satellite observations with large *in situ* databases (Global Ocean Data Analysis Project, GLODAP, Lauvset *et al.,* (2021) or the Surface Ocean CO_2 Atlas, SOCAT, Bakker *et al.*, 2016). Such methods extensively rely on satellite temperature, wind speed, sea surface height and ocean colour, in conjunction with *in situ* re-analyses or climatologies, to identify the underlying processes controlling in-water concentrations. For ocean sink assessments, the direction of exchange with the atmosphere is determined by the CO_2 concentration above and below the atmosphere-ocean interface, whereas the turbulent exchange itself is primarily water-side controlled so it is routinely characterised using sea surface temperature and wind speed data (e.g. Ho *et al.,* 2016). An array of methods combine elements of all of these satellite approaches to determine the CO_2 concentrations along with satellite observed ice coverage and re-analysis data (e.g. for atmospheric conditions) to calculate atmosphere-ocean CO_2 exchange and the net carbon sink (e.g. the eight methods presented within Friedlingstein *et al* (2021) and its annual updates used to guide policy; the six methods within Fay *et al.,* 2021). This use of satellite remote sensing has enabled the ocean carbon community to reconstruct multi-decadal ocean carbon assessments. These efforts have been encouraged and supported by international carbon observing strategies (e.g. CEOS, 2014; GOA-ON 2019; Tilbrook *et al.,* 2019) and individual scientific community efforts (e.g. the international Surface Ocean and Lower Atmosphere Study, SOLAS). Collectively this exploitation means that satellite observations have become critical for assessing marine carbon and the impact that carbon absorption is having on ocean ecosystems and health (Shutler *et al.,* 2020; Arico *et al.,* 2021). They are therefore being used to guide policy and have now been identified as important for supporting delivery of the UN Ocean Decade outcomes (Dobson *et al.,* in-press; Arico *et al.,* 2021). Despite these advances in understanding and capability, the critical importance of satellite observations for such assessments, along with the fragile nature of any underlying *in situ* networks (e.g. SOCAT) on which they also rely, is often opaque to, or overlooked by, policy makers. Clearly, the routine integration of all forms of observations, combining satellite and *in situ* observations from ships, moorings, and robotic platforms is now possible. And sustained funding and international prioritization mechanisms would enable an integrated global carbon observing network (Shutler *et al.,* 2020) to better inform and support policy decisions and outcomes.

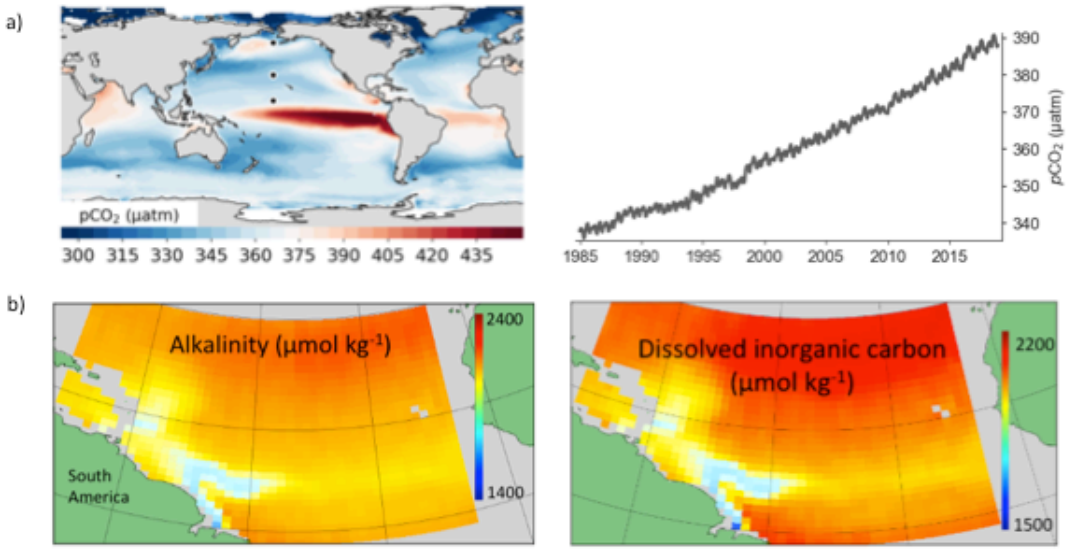

Figure 2: Recent advances in satellite observation-based data for studying the surface water marine carbonate system. a) Global assessments of the amount of gaseous CO_2 (pCO_2) can be mapped using satellite observations in conjunction with *in situ* databases to provide decadal-scale monthly data inputs to annual carbon assessments (i.e. Friedlingstein *et al.,* 2021) (data from Gregor and Gruber, 2021); b) Regional assessments using satellite observation-based methods can quantify alkalinity and dissolved carbon flowing from the Amazon into the Atlantic (data from Land *et al.*, 2019).

3. Achievable advances needed within the next 2 to 5 years

The following sections identify how remote sensing advances in ocean carbon research can help further constrain the global carbon budget and benefit the wider carbon community increasing the ability to guide, advise and manage mitigation, adaptation and conservation efforts.

3.1 Scientific advances in understanding or capability

Six areas of scientific importance where satellite observations can play a critical role are discussed in the following sections. Satellite approaches hold the potential for: reducing major sources of uncertainties in global ocean carbon assessments (section 3.1.1); addressing inconsistencies between observed and re-analysis assessments of upper ocean mixing (section 3.1.2); quantifying the variability and trends in land to ocean carbon exchange (section 3.1.3); resolving meso-scale features and variability for supporting regional and local-scale assessments of ocean acidification (section 3.1.4); identifying those regions and times where compound events are occurring (section 3.1.5), and for understanding the role of biology in the evolution of the long-term ocean carbon sink (section 3.1.6).

3.1.1 Exploring the air-sea interface

Despite the focus on global-scale assessments, the actual exchange of CO_2 occurs across a sub-millimetre depth of the mass boundary layer where the atmosphere and ocean interact. Small gradients in concentration either side of this interface are considered significant when scaled globally (Bellenger *et al.,* 2023; Goddijn-murphy *et al.,* 2015; Dong *et al.,* 2022; Watson *et al.,* 2020; Woolf *et al.,* 2016; Shutler *et al.,* 2020), and the water-side control of CO_2 exchange implies that the water-side gradients are particularly important. Improved understanding of the impact of near-surface temperature gradients (Woolf *et al.,* 2016)

has helped to advance satellite observation-based assessments of the ocean carbon sink (e.g. Dong *et al.,* 2022; Shutler *et al.*, 2020; Woolf *et al.,* 2019; Watson *et al.,* 2020;), but debate continues over their significance as field evidence of the impact of these gradients is lacking (Friedlingstein *et al.,* 2022). Microwave penetration depth in water is within the mass boundary layer and therefore microwave observed temperatures can be considered a sub-skin temperature (Minnett *et al.,* 2019), whereas infra-red observations are close to the atmosphere-ocean interface. Coincident ship-mounted remotely sensed infra-red and passive microwave temperature observations could therefore enable the temperature across the mass boundary layer to be experimentally evaluated in the field; measurements that could then constrain a high-resolution turbulence model (e.g. as used within Merchant *et al.,* 2019) or be compared with boundary layer imaging from advanced air-sea interaction facilities (e.g. Nagal *et al.,* 2015) to provide the missing evidence sought by the wider carbon community. Similarly, passive microwave satellite salinity retrievals originating from within the mass boundary layer could help further refine our understanding of near-surface salinity gradients (as haline gradients can also occur; e.g. Woolf *et al.,* 2016).

The parameterisation and understanding of the atmosphere-ocean exchange of gases is considered the major source of uncertainty within global scale ocean carbon sink assessments (e.g., Woolf *et al.,* 2019). Passive microwave measurements across multiple wavelengths contain the signature of key processes controlling this surface exchange and offer a unique and largely untapped resource for direct observations of multiple exchange processes, which could reduce the reliance on wind-speed based proxies of air-sea gas exchange (Shutler *et al.,* 2020). Whilst future passive microwave satellite concepts will provide significant opportunities for simultaneously studying multiple ocean-atmosphere processes to enable more advanced understanding of these interactions (e.g., Ciani *et al.,* 2019; Gentemann *et al.,* 2020). It may also be possible to observe or parameterise alkalinity directly from passive microwave emissivity data, in contrast to current methods (e.g., Land *et al.,* 2019) which rely on the emissivity derived salinity to then derive alkalinity. Such efforts could focus on long-standing microwave sensors designed for salinity (e.g., the soil moisture and ocean salinity satellite mission, SMOS) through exploiting large alkalinity datasets (e.g., Lauvset *et al.,* 2021) and regions of high data densities like the Atlantic. Whereas the potential and advantages of using satellite backscatter to parameterize gas exchange has been previously highlighted (Shutler *et al.,* 2020) but no new advances have so far appeared despite a plethora of suitable satellite sensors already in orbit, and the development of ship mounted synthetic aperture radar instruments means that radar focused gas exchange experiments are now feasible.

3.1.2 Connecting the interface with the sub-surface and upper ocean dynamics and mixing

The conditions below the surface can enhance or diminish the surface carbon absorption and alter the carbonate system state, and surface observed conditions can provide insights into the processes or conditions occurring at depth. Dependent upon the sensing technology the relevant depth of satellite observations can range from sub-millimeter (e.g. thermal infrared) down to tens of meters (e.g., ocean colour in an oligotrophic gyre) or below (e.g. altimetry). These depth-specific, or depth-relevant, analyses are now possible using satellite data, which combined with knowledge of physical oceanography may allow the sub-surface carbonate system conditions, internal ocean transport and the mixing of water from the interface into the upper ocean to be determined. For example, the evaluation of the impact of near-surface gradients (discussed in section 3.1.1) relies upon the depth specific nature of satellite thermal infrared observations

and surface to depth export fluxes have been estimated based on ocean colour satellite observations (Stukel *et al*., 2023). A thorough understanding of atmosphere-ocean interactions combined with satellite measurements of surface winds has enabled the vertical and horizontal water flow in the Californian upwelling and its influence on the carbonate system to be determined (Quilfen *et al.,* 2021). Similarly, the analysis of altimeter observed eddies analysed alongside *in situ* data and knowledge of their rotation characteristics has allowed the regional significance of eddy-driven vertical mixing to be quantified (Ford *et al.,* 2023), which could easily be applied globally.

Upper ocean turbulence and mixing of all ocean constituents including carbon is predominantly driven by atmospheric winds at the ocean-atmosphere interface. However, there are clear disparities between existing wind re-analysis data products which are critical for quantifying ocean carbon and the observed storm tracks from polar lows and tropical cylones (e.g., Verezemskaya *et al.,* 2017). The significance of this disparity is likely to grow as the intensity and frequency of storms changes with the changing climate (e.g., Bhatia *et al.,* 2019) and these inconsistencies are likely impacting more than just surface turbulence estimates, as storms are known to alter upper ocean mixing and vertical motions which influence temperature, salinity and biology (e.g., Reul *et al.,* 2020) and they can interact with the barrier layer in the upper ocean to inhibit vertical mixing (Balaguru *et al.,* 2012). Different satellite technologies offer a selection of complementary capabilities to address these issues. Satellite scatterometers can provide high spatial resolution observations of low to medium wind speed and direction, but their sensitivity is reduced at higher speeds (e.g., Polverari *et al.,* 2021), whereas new advances in polarised synthetic aperture radar have enabled the wind speeds (but not direction) within the eyes of storms to be resolved (e.g., Mouche *et al.,* 2019), although the coverage of the storm within the satellite view can be limited. New passive microwave approaches show high sensitivity to cyclone wind speed and direction, but at relatively low spatial resolutions (e.g., Reul *et al.,* 2017). Intelligently and consistently combining data from all satellite approaches would enable an observation-based wind-speed and direction dataset relevant for all wind conditions with more consistent wind distributions, and work has begun in this area (e.g., the MAXSS project, https://www.maxss.org/). Consistency between observation-based wind and wave climate data records will be needed to enable the creation of an upper turbulence climate data record, as extreme waves do not always occur coincident with extreme winds (Hell *et al.*, 2021). These approaches would be suitable for addressing disparities in wind re-analysis data products, leading to a better quantification and understanding of upper ocean turbulence and mixing through time (and would benefit advances in air-sea exchange, by providing consistent wind and wave data for use in gas exchange parameterisations, as discussed in section 3.1.1). Existing satellites networks could enable these advancements, and coverage and understanding will improve further with new proposed satellite wind missions (e.g., Kilic *et al.,* 2018) and proposed active microwave satellite sensors hold the potential to further increase knowledge of surface ocean mixing by directly observing atmosphere and ocean surface velocities and ocean current interactions (e.g., Ardhuin *et al.,* 2019; Gommenginger *et al.,* 2019; Morrow *et al.,* 2019).

3.1.3 Constraining land to ocean carbon flow

Various methods are used to characterise land to ocean flow of inorganic carbon by rivers including *in situ* upscaling methods (e.g. Regnier *et al.,* 2013), ocean inverse model estimates (Jacobson *et al.,* 2007) and ocean sink estimates (Watson *et al.,* 2020), or atmosphere inversion based approaches (Rödenbeck *et al.,*

2018). Despite the plethora of approaches there is lively debate over the river transport value, and its temporal variability, any potential long-term trends, and how these relate to human activity are all poorly constrained (e.g. Regnier *et al.,* 2013b; Lacroix *et al.,* 2020 and Regnier *et al.,* 2022). Hence annual carbon assessments conducted by the global carbon budget rely on long-term static values. Satellite observations are well placed to characterise this flow and an example method presented in Panel 1 suggests that the Amazon inter-annual variation in dissolved inorganic carbon outflow is ±10%. Combining high-quality data from existing satellites (e.g., Sentinels 2 and 3) with data from commercial CubeSats (that have higher spatial resolution and observation frequency, but lower spectral quality) and gauging stations could enable satellite observation-based methods to characterise global land-to-ocean flow of carbon for inclusion within global assessments. This characterisation could include its magnitude, variability, any long-term trends and causal factors, the latter of which is likely to change with time. Such combined use of agency and commercial satellite sensors is already used for monitoring global coral health (Li *et al.,* 2019).

3.1.4 Towards the study of meso-scale phenomena

Current satellite observation-based datasets for individual carbon system parameters (e.g. alkalinity, Land *et al.,* 2019) and the complete marine carbonate system (Gregor and Gruber, 2021) are monthly data at 1° resolution (~110 km at the equator). Whilst these demonstrate the potential of such methods and are useful for seasonal-scale or global analyses, they are clearly less useful for regional or local assessments and understanding, particularly when some conditions and interactions can be high frequency or short lived (e.g., Desmet *et al.,* 2021). These existing methods could be further developed to provide close to weekly and ~25 km resolutions, as the key underlying observations important for higher-frequency changes in the carbonate system are available at these scales (e.g. temperature at ~25 km as the first order controller of the gaseous quantity of CO_2), whilst those observations only available at lower resolutions due to sensing constraints (e.g. salinity at >50 km spatial resolution useful for alkalinity) are characterising aspects that change more slowly. At a basic level using these higher resolution inputs would enable the extension or re-training of existing published algorithms to become near-coastal in regions where a high density of near-coast *in situ* data already exist (e.g., California Current upwelling region). The focus on only deriving higher resolution versions of those parameters needed to isolate the higher-frequency (rather than doing so for all parameters) means that this approach could be applied to global analyses. These higher resolution data are likely to be more useful for regional and local users wishing to identify the extent to which their regional waters are already being impacted by ocean acidification. The increasing amount of globally available higher resolution optical and microwave satellite observations (e.g., daily at <60 m from Sentinel 1, Sentinel 2, Landsat, Planet Labs) mean it is now possible to view or resolve sub-mesoscale features and these could support investigations into any errors within ocean carbon sink assessments (e.g. as studied by Gloege et al., 2021).

3.1.5 Identifying regional compound events

Of special concern are the interactions of the changes in ocean chemistry with other concurrent changes, especially warming, but also deoxygenation, pollution, and fishing pressures often termed compound events (e.g. Gruber *et al.*, 2021). These compound events often occur in the aftermath of marine heatwaves (e.g., Frölicher and Laufkötter, 2020) and tend to add an additional dimension of stress to the already stressed ecosystems (Gruber *et al.*, 2021) which can impact all tropic levels. The ability to use satellite-observation data to derive heat wave duration and extent (e.g., Oliver *et al.,* 2020), surface ocean carbonate data

(Gregor and Gruber, 2021) and atmosphere-ocean carbon flux data (e.g. Watson *et al.,* 2020) offers the potential to identify where and when these compound events are occurring (figure 3) and to probe the impact of heat waves on the surface ocean carbon system. Increasing the temporal and spatial resolution of existing datasets (section 3.1.4) and exploiting experimental or operational higher frequency satellite approaches (e.g., Planet Labs dove network, or those mentioned in figure 1a) could enable the detection and analysis of shorter and more intense individual extreme conditions and any resulting compound events. They may also enable precursor events or conditions to be identified as indicators of future change towards short-term forecasting (e.g., 6 monthly). Machine learning (e.g., time-series forecasting) could then likely enable observation (satellite and *in situ*) driven short-term forecasting aligned with the needs of policy makers and marine users (Arico *et al.,* 2021).

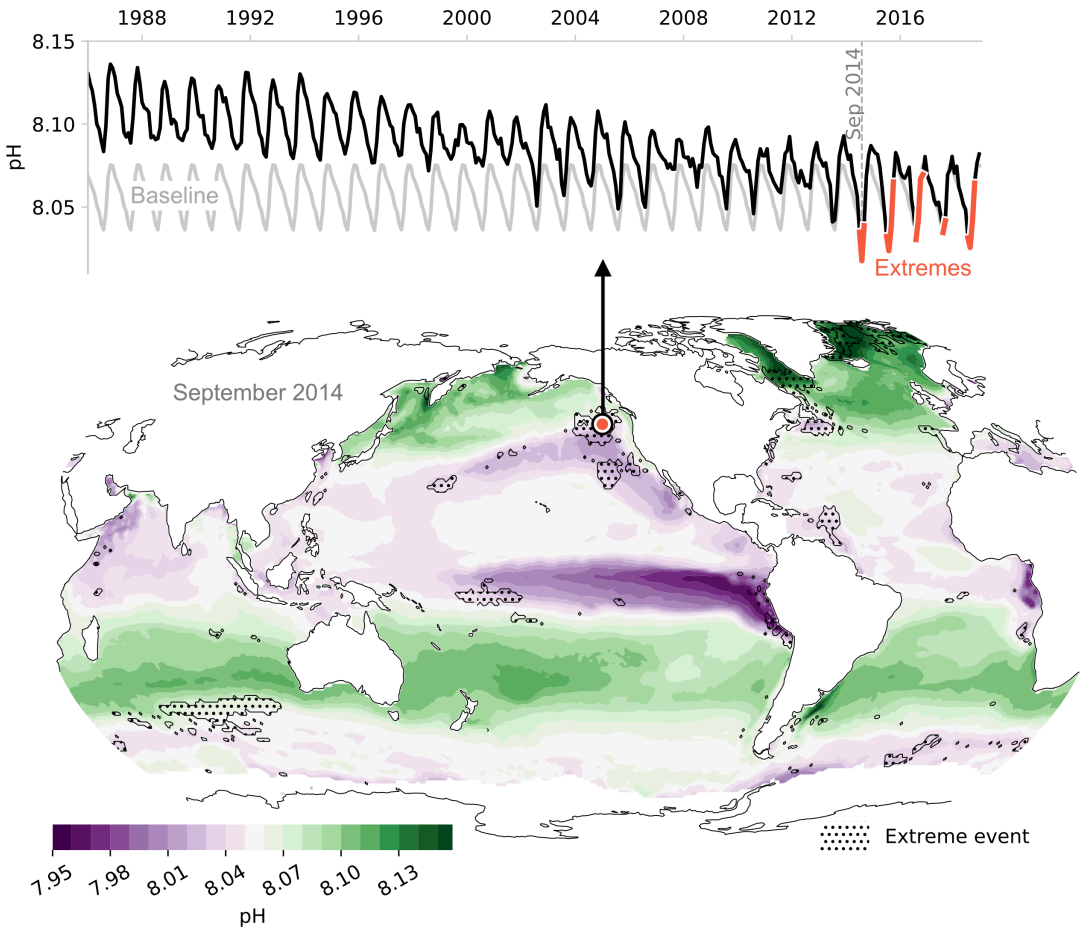

Figure 3: The ability to identify global and regional conditions and variability across all marine carbonate system parameters means that we can now study regional changes in pH to identify where and when ecosystems are experiencing extreme conditions (determined using data from Gregor and Gruber, 2021).

3.1.6 Identifying and capturing the role of biology

Phytoplankton biological growth can modulate surface water CO_2 concentrations as CO_2 in the water is used during photosynthesis, but is also respired, and CO_2 is the net output from calcification (e.g. Ford *et al.,* 2022; and as reviewed by Brewin *et al.,* 2021). This biological control, how future changes in biology may alter the oceanic sink of CO_2 and how changes in biological growth can indicate ocean health and stress have all been identified as important areas of research (e.g., Arico *et al.,* 2021). Satellite-observations are

already extensively used to study biological carbon (Brewin *et al.,* 2021). But currently the majority of observation-based ocean carbon sink data used within carbon assessments (e.g. within Friedlingstein *et al.,* 2021) focus on observations of ocean physics to intelligently interpolate the sparse surface *in situ* gaseous CO_2 data, so these are likely to overlook biological control mechanisms. Climate-quality satellite ocean colour observations (e.g., Sathyendranath *et al.,* 2019) offer the opportunity to include biology within these interpolation schemes. Assessments have been attempted using satellite observed chlorophyll-a estimates (as an indicator of photosynthetic processes) which is a good first step (e.g. Gregor *et al.,* 2021). But evaluations should also focus on satellite-based primary production or net community production data (as reviewed by Brewin *et al.,* 2021) that are more likely to capture the fuller impact of biology on surface water gaseous CO_2 (Ford *et al.,* 2022) and the inclusion of calcification processes that is likely to be important in some regions (Shutler *et al.,* 2013). More work is needed to extend some methods and datasets to achieve global coverage and to build more complete uncertainty budgets (e.g., for net community production). Ocean colour observations, upon which these biological data partly rely, are not retrievable during low light periods, polar winters or below clouds (but biology may still exist), and these data also contain integrated contributions across multiple optical depths within the water and so may not be purely near surface. So methods exploiting these satellite data for surface assessments will need to be able to handle missing or masked data and avoid making assumptions about the underlying biological state when observations are missing, and should consider optical depth. As a first step, a hierarchical approach could be used for regions of missing data, where the method progressively moves through a list of ranked datasets until data coverage is found (e.g., satellite observations, then re-analysis data with the last option being a long-term observational mean). Addressing the issue of missing data is an aspect that should be considered by the satellite observation community to increase the usability of their data, as example machine learning and statistical methods exist (e.g., Liu and Wang, 2022). But these now need to be used within climate data records following the example of the sea surface temperature community who provide gap filled daily data records (Merchant *et al.,* 2019).

3.2 Overcoming barriers to the utility and full exploitation of satellite observations

Most remote sensing data and approaches are unlikely to achieve the same precision and accuracy as laboratory measurements, whilst satellite sensor performance can also change over time as the sensor and optics age. Similarly, all field-deployed *in situ* instrumentation, such as buoys or floats, can have instrument performance lower than their laboratory equivalent and their performance can degrade over time (e.g., due to biofouling, calibration drift, damage, or battery degradation). This means that both space-based and *in situ* observations have their own unique capabilities, advantages, and individual characteristics to consider. Therefore the evaluation of the utility of satellite observation approaches should focus on what they can they provide that is complementary to other observations or measurements, such as providing higher frequency sampling in space and time (e.g., to enable global assessments, for studying river outflows or episodic events) and sampling where other types of observations are sparse, impractical, or impossible (e.g., polar regions or regions that experience piracy). Then the accuracy and precision of these satellite observations with respect to reference measurements defines how to interpret these data and their potential applicability to a given scientific question. For example, identifying the existence of long-term change or short-lived episodic events versus attempting to precisely identify the rate or range of change of a specific carbonate parameter have very different needs in terms of uncertainties. Consequently, assessing the utility of satellite

observations solely by comparing their precision and accuracy to that possible from laboratory analyses is a mistake. Along with the intended application, such assessments should also consider differences in sampling in time and space between different observation techniques (laboratory analyses, *in situ* instrumentation and satellites) as ignoring them can introduce artificial errors (e.g., Land *et al.,* 2023). Overlooking the uncertainties associated with the reference data (e.g., laboratory or *in situ*) being used can also lead to misleading performances (e.g., Ford *et al.,* 2021). Furthermore, for some applications (e.g., identifying the existence of long-term change and its direction) it will be more important to use temporally stable (long-term) data sources to minimise bias and maximise the precision, rather than concentrating purely on the accuracy of the approach (e.g., using a climate data record; see Taylor, 1967 for an explanation of the underlying statistics). Assessing the utility and potential applications of satellite observations requires consideration of all of these points.

3.3 The need for aligned scientific communities

As discussed, it is clear that marine carbon assessments are heavily reliant on satellite observations, and there are a large amount of observations available, each with individual nuances; however, the reasons for specific data choices that are used within these assessments are not always clear. For example, the majority of the satellite observation datasets chosen within data submissions to the global carbon budget (Friedlingstein *et al.,* 2022) focus on operational datasets (e.g. Donlon *et al.,* 2012), designed for short-term forecasting systems, whereas climate-quality data would be more appropriate (e.g. Boutin *et al.*, 2021; Dodet *et al*, 2021; Merchant *et al.,* 2019; Sathyendranath *et al.,* 2019). These non-optimal dataset choices may be driven by the specific time period being studied, the spatial extent, the visibility of the dataset, uncertainties, a lack of confidence in the data or a misunderstanding of the nuances and intricacies of these satellite observations (e.g. see the extensive content within Robinson 2010) and the potential impact of different choices. Similarly, key studies that are guiding community methods and priorities contain misunderstanding of the use and interpretation of satellite data. For example, Fay, Gregor *et al.,* (2021) misinterpret what satellite chlorophyll-a data represent (referring to them as surface biological activity) potentially leading to incorrect conclusions about their efficacy. Gloege *et al.,* (2021) use satellite observations extensively but omit the data sources or versions, and Gloege *et al.,* (2021) and Lefèvre *et al.,* (2021) overlook the associated data uncertainties (e.g., river plume contamination causing increased chlorophyll-a uncertainties). Irrespective of the reasons for these errors - poor or inconsistent dataset choice and reporting, misunderstandings in capabilities, and overlooking uncertainties are all likely to limit the quality of these carbon assessments and community guidance with implications for policy development.

Given the high reliance on satellite data for supporting policy, and its potential role in mitigation, adaptation and conservation approaches, the formation of an international expert advisory group to support optimal use of satellite observation datasets and novel sensors or products within carbon assessments and relevant policy is now needed. This would also enable the carbon community to guide the satellite observation community in identifying and providing the most appropriate data for key scientific questions, and enable the exchange of knowledge on uncertainty assessments, data standards and metadata. This would support the goals of the Observing Air-Sea Interactions Strategy (OASIS, Cronin *et al.,* 2022) and the carbon aims and interests of the Committee of Earth Observation Satellites (CEOS) (and more widely the Global Ocean Observing System, GOOS, and Global Climate Observing System, GCOS), and it could also support and

guide efforts by the *in situ* communities to develop a network of reference observations (Wanninkhof *et al.*, 2019); with mutual benefits as reference observations are needed to assess satellite data-based products. This advisory group would need to consist of multi-sensor satellite and *in situ* experts and could be led by the International Ocean Colour Coordinating Group (IOCCG) or the Group for High Resolution Sea Surface Temperature (GHRSST) as both have experience of developing cross-disciplinary groups. These efforts would greatly benefit from support and input from the International Ocean Carbon Coordination project (IOCCP), with key input from climate teams (e.g. the various ESA Climate Change Initiative teams) and individual experts where coordinating groups or climate teams do not exist (e.g. for satellite observed atmospheric column integrated gases). Advances will only be possible through collaboration and co-developed work to guide and identify the advantages of linking expert knowledge across the communities. Collectively, this could lead to aligned communities in terms of data knowledge, availability, visibility, accessibility and standards. This exchange of knowledge could also help support ocean acidification groups by accelerating the integration of different sources of marine carbon data for supporting decision making (e.g., towards holistic representations of current and future ocean acidification conditions and short-term monitoring).

3.4 Informing climate adaptation and mitigation measures

Local and regional approaches to minimize the effects of ocean acidification are emerging with a much stronger focus on adaptation and local mitigation (Gattuso *et al.,* 2015). These approaches often work towards effective legislative and governance mechanisms that incorporate ocean acidification data to underpin adaptation and mitigation strategies (Dobson *et al.,* 2022). This includes i) measures to better protect the organisms and ecosystems under stress from ocean acidification against other compound threats (e.g. from overfishing or physical destruction); ii) measures that aim to repair the system (e.g., by building artificial reefs, restoring blue carbon ecosystems or by adding alkaline substances to offset the effect of ocean acidification) and iii) measures to combat the more local or regional drivers of high acidity and low pH conditions, (e.g., by reducing local eutrophication, pollution, and coastal erosion, Kelly *et al.,* 2011). Common to all three approaches is the need for high quality observations, both to assess the level of threat and exposure to the local organisms and ecosystems, as well as to measure the potential success or co-benefit of any action. While *in-situ* based systems are developing and expanding rapidly in some areas of the world, satellite-based observations are now of a sufficient quality to provide a global perspective and constraints for many regions that are only marginally observed. Importantly, satellite observation-based data can be used to call attention to the plight of the oceans in the context of climate change by highlighting regions already under stress and taking on risk (figure 1b; figure 3). There is potential to link satellite observations with the conditions being experienced by some species, the need to support increased understanding of satellite methods within some communities (particularly climate policy leads and marine managers), and the opportunity to co-develop interpretation or indicator methods with key users (Panel 2). The need to increase ocean acidification awareness and literacy more widely has been identified by the UN Decade endorsed Ocean Acidification Research for Sustainability programme OARS (Dobson *et al.,* 2022) and imagery based on satellite observational-based data could support this (e.g., figure 1b). In this way, satellite observation-based data could now be used to aid bottom-up initiatives, to support communities in planning adaptation, management, and monitoring strategies and top-down initiatives to allow policy makers to identify those regions most at risk, highlight their plight and identify necessary mitigation and adaptation

needs (Wible, 2021; e.g., figure 3). These same approaches could be applied to support action on, and understanding of, other compounding issues of ocean health (e.g., eutrophication in the coastal zone),

A satellite and *in situ* based observing system for climate adaption and mitigation that is now possible (Shutler *et al.,* 2020) is needed to support these actions by providing targeted and useful data to a broad user base. To do so, the observing system would need the following characteristics: (i) access to data in marginally observed regions, or regions where little *in situ* data are collected to enable 'new users', (ii) data must be retrieved with high resolution in time and space, especially in regions of concern, (iii) data must be easily and quickly available after their retrieval, and (iv) any ocean carbon data need to be well integrated within other data streams addressing marine stressors, and (v) to ensure uptake and use of these data, it is likely that efforts need to be co-designed with end users (including climate policy leads and marine managers) and undertaken in such a way as to provide suitable data visualization or analysis tools (e.g. Kain and Covi, 2013) and to train early adopters, stakeholders and users in how to use these tools and interpret any data.

3.5 Actively demonstrating the value of advances in estimating the ocean carbon sink

The concept of a digital twin component or that of observing system simulation experiment could now be used to illustrate the powerful constraint that ocean carbon sink estimates have on global carbon assessments. This would be a digital representation of the global carbon cycle, with a focus on ocean carbon assessments along with representation of all major sources, pools and sinks of carbon and its redistribution within the Earth system (figure 4). By assuming fossil fuel combustion is well known (box 7; figure 4) this approach can be used to identify closure of the budget, and how improvements in ocean carbon sink estimates impact that closure. All components of this approach are already being routinely used by international groups in a pre-operational, ad-hoc, or distributed manner (e.g., a similar approach is used to assess budget closure within annual assessments, Friedlingstein *et al.,* 2022) so efforts for the implementation would focus purely on addressing technical aspects (e.g., data storage, timely data access, computing requirements, consistency of implementations, full and consistent documentation, testing frameworks etc). Such an approach would allow the importance of the advances made through satellite observation-based methods to be evaluated and highlighted (i.e., the developments identified in section 3.1 of this paper). It could also be used to identify where scientific community effort is best focussed to improve assessments, used to assess the scientific and policy advice impact of major national funding decisions to infrastructure, whilst also being used to automate routine assessments to simplify the monitoring of the present state of the ocean to support conservation, mitigation and global carbon assessments; and in doing so, support the aims of sections 3.2, 3.3 and 3.4 of this paper.

These capabilities could be demonstrated and evaluated under a range of scientific and policy focussed 'what if' scenarios including: what happens to the ocean carbon sink estimate and global budget closure if we include ocean eddies, ocean biology, or novel *in situ* data types within the analyses (e.g., Argo floats, gliders, autonomous vessels)? And what happens to the budget closure if the uncertainties within the ocean observational constraint or the river to ocean carbon flow are reduced? Or what happens to the strength of any resultant policy advice if key in situ ocean observation networks are funded, versus not funded?

This approach would help address the needs in the UNESCO and IOC decadal roadmap for ocean carbon (Arico et al., 2021) by i) highlighting, clarifying, elevating and promoting the use of satellite observations within ocean carbon analyses and understanding, ii) being used to help evaluate the importance of biology within ocean carbon assessments, iii) helping identify beneficial approaches for long-term support of the *in situ* ocean carbon observing system and iv) demonstrating how a satellite observation-based system in conjunction with *in situ* networks, and model re-analyses can be constructed to support policy.

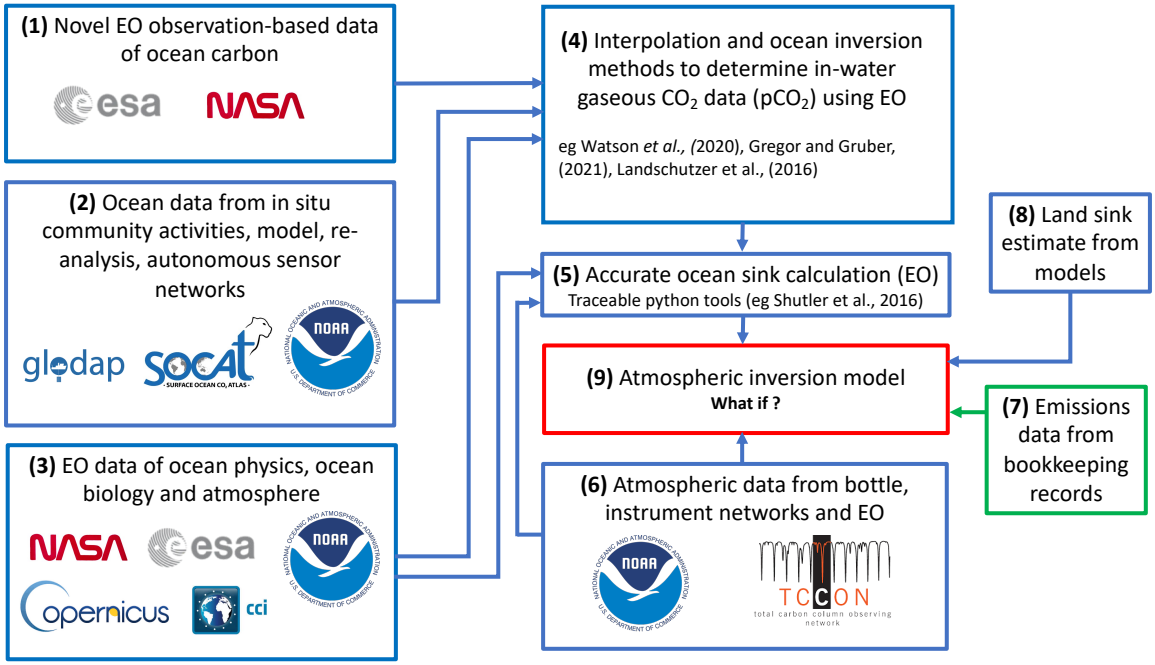

Figure 4: The digital twin component structure or an observing system simulation experiment approach to identify the strength of the observation-based carbon sink estimates. The logos within each module element give typical agency and community data providers. Boxes in blue are where satellite Earth observation data are exploited within global assessments (e.g., Friedlingstein *et al.,* 2022). Techniques typically used for the boxes in green and red are beginning to use satellite observations through new carbon emissions focussed satellite missions, and this exploitation is expected to continue increasing.

4.0 Conclusions

The urgency of providing the most accurate and precise ocean carbon assessments within the next 5 years, and to continue refining them is highlighted by the latest IPCC reports where they warn of the need to drastically reduce carbon emissions. Whilst the performance of any ocean assessments will govern, or limit, the ability to clearly identify the ocean and carbon budget response to ongoing emissions. Such data will continue to be needed following any emissions reduction to help track the response of the Earth system. The heavy reliance and necessity of satellite Earth observation data to enable global ocean carbon assessments is now scientifically clear and this importance has been recognised by the United Nations Education Scientific and Cultural Organisation (UNESCO) and the International Oceanographic Commission (IOC). Combined with the powerful constraint that ocean carbon data have on global carbon assessments, this importance demonstrates the need to focus efforts on further advancing the use of satellite observations. The importance of space-based salinity, temperature and wind speed data within assessments and for

enabling new scientific capabilities and insight continues to grow, and despite large advances remains relatively under exploited. Alongside this, it is likely that satellite retrieved ocean colour in particular will become increasingly important for these assessments, along with satellite sea-state, ocean currents and atmospheric column integrated gas observations. Greater community cohesion and co-design between satellite, *in situ*, and modelling researchers/users focussing on the carbon system will increase the potential for greater scientific advances, further increase the strength of the ocean constraint within carbon assessments, and enable the advances to actively guide ocean mitigation and conservation efforts. There is a need for sustained effort and funding to provide expert guidance on the use of satellite observations within carbon studies and assessments, to provide support for the key ocean *in situ* measurements that underpin the satellite approaches, and to underpin these efforts within annual carbon assessments used to guide policy, marine management and behavioural change. This policy advice would be considerably strengthened by the formation of an integrated multi-platform observing system with satellite data at the heart; an approach that is now scientifically and physically possible.

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6.0 References

Ardhuin F, Brandt P, Gaultier L, Donlon C, Battaglia A, Boy F, Casal T, Chapron B, Collard F, Cravette S, *et al.,* (2019) SKIM, a Candidate Satellite Mission Exploring Global Ocean Currents and Waves. *Frontiers in Marine Science,* doi: 10.3389/fmars.2019.00209

Arico S, Arietta JM, Bakker DCE, Boyd PW, Cotrim da Cunha L, Chai L, Dai F, Gruber N, Isensee K, Ishii N, *et al***.,** *Integrated ocean carbon research: a summary of ocean carbon research, and vision of coordinated ocean carbon research and observations for the next decade.* UNESCO and the IOC, online, UNESCO, Paris, 45 pages, (2021).

Balaguru, K., Chang, P., Saravanan, R., Leung, L.R., Xu, Z., Li, M., Hsieh, J.S., (2012) Ocean barrier layers' effect on tropical cyclone intensification. *Proceedings of the National Academy of Sciences*, *109*(36), pp.14343-14347

Bakker, D. C. E., Pfeil, B. Landa, C. S., Metzl, N., O'Brien, K. M., Olsen, A., Smith, K., Cosca, C., Harasawa, S., Jones, S. D., Nakaoka, S., Nojiri, Y., Schuster, U., Steinhoff, T., Sweeney, C., Takahashi, T., Tilbrook, B., Wada, C., Wanninkhof, R., Alin, S. R., Balestrini, C. F., Barbero, L., Bates, N. R., Bianchi, A. A., Bonou, F., Boutin, J., Bozec, Y., Burger, E. F., Cai, W.-J., Castle, R. D., Chen, L., Chierici, M., Currie, K., Evans, W., Featherstone, C., Feely, R. A., Fransson, A., Goyet, C., Greenwood, N., Gregor, L., Hankin, S., Hardman-Mountford, N. J., Harlay, J., Hauck, J., Hoppema, M., Humphreys, M. P., Hunt, C. W., Huss, B., Ibánhez, J. S. P., Johannessen, T., Keeling, R., Kitidis, V., Körtzinger, A., Kozyr, A., Krasakopoulou, E., Kuwata, A., Landschützer, P., Lauvset, S. K., Lefèvre, N., Lo Monaco, C., Manke, A., Mathis, J. T., Merlivat, L., Millero, F. J., Monteiro, P. M. S., Munro, D. R., Murata, A., Newberger, T., Omar, A. M., Ono, T., Paterson, K., Pearce, D., Pierrot, D., Robbins, L. L., Saito, S., Salisbury, J., Schlitzer, R., Schneider, B., Schweitzer, R.,

Sieger, R., Skjelvan, I., Sullivan, K. F., Sutherland, S. C., Sutton, A. J., Tadokoro, K., Telszewski, M., Tuma, M., Van Heuven, S. M. A. C., Vandemark, D., Ward, B., Watson, A. J., Xu, S. (2016) A multi-decade record of high quality fCO_2 data in version 3 of the Surface Ocean CO_2 Atlas (SOCAT). *Earth System Science Data*, 8, 383-413. doi:10.5194/essd-8-383-2016.

Bakker, D. C.E, De Baar, H. J.W, De Jong, E., (1999) The dependence on temperature and salinity of dissolved inorganic carbon in East Atlantic surface waters, *Marine Chemistry*, 65 (3-4), doi: 10.1016/S0304-4203(99)00017-1

Bellenger, H., Bopp, L., Ethé, C., Ho, D., Duvel, J.P., Flavoni, S., Guez, L., Kataoka, T., Perrot, X., Parc, L., Watanabe, M., (2023). Sensitivity of the global ocean carbon sink to the ocean skin in a climate model. *Journal of Geophysical Research: Oceans*, *128*(7), p.e2022JC019479.

Bhatia, K. T., Gabriel A. Vecchi, Thomas R. Knutson , Hiroyuki Murakami, James Kossin, Keith W. Dixon, Carolyn E. Whitlock (2019) Recent increases in tropical cyclone intensification Rates. *Nature Communications*, 10:635

Boutin, J., Reul, N., Koehler, J., Martin, A., Catany, R., Guimbard, S., Rouffi, F., Vergely, J.L., Arias, M., Chakroun, M., *et al.* (2021) Satellite-Based Sea Surface Salinity Designed for Ocean and Climate Studies. *Journal of Geophysical Research Oceans*, 126, e2021JC017676.

Brewin RJW, Sathyendranath, S., Kulk, G., *et al.,* (2023) Ocean carbon from space: current status and priorities for the next decade, *Earth-Science Reviews, doi:1* 0.1016/j.earscirev.2023.104386

Brewin RJW, Sathyendranath S, Platt T, Bouman H, Ciavatta S, Dall'Olmo G, Dingle J, Groom S, Jönsson B, Kostadinov TS, *et al.,* (2021) Sensing the ocean biological carbon pump from space: a review of capabilities, concepts, research gaps and future developments. *Earth-Science Reviews*, *217*, 103604-103604

CEOS (2014) CEOS strategy for carbon observations from space, The Committee on Earth Observation Satellites (CEOS) Response to the Group on Earth Observations (GEO) Carbon Strategy, September 30 2014.

Chau, T. T. T., Gehlen, M., Chevallier, F. (2022) A seamless ensemble-based reconstruction of surface ocean pCO_2 and air–sea CO_2 fluxes over the global coastal and open oceans, *Biogeosciences*, 19, 1087–1109, https://doi.org/10.5194/bg-19-1087-2022.

Ciani *et al.,* (2019) Copernicus Imaging Microwave Radiometer (CIMR) Benefits for the Copernicus Level 4 Sea-Surface Salinity Processing Chain, *Remote Sensing*, doi: 10.3390/rs11151818

Cronin *et al.,* (2022) Developing an Observing Air-Sea Interactions Strategy (OASIS) for the global ocean, *ICES Journal of Marine Science*, doi: 10.1093/icesjms/fsac149

611 Desmet, F., Gruber, N., Köhn, E. E., Münnich, M., Vogt, M. (2022) Tracking the Space-Time Evolution of
612 Ocean Acidification Extremes in the California Current System and Northeast Pacific. *Journal of Geophysical*
613 *Research: Oceans*, 127(5), e2021JC018159. Doi: 10.1029/2021JC018159
614
615 Dickson, A.G., Sabine, C.L., Christian, J.R. (2007) Guide to Best Practices for Ocean CO 2 Measurements,
616 *PICES Special Publication 3*, 191 pp.
617
618 Dixon AM, Forster PM, Heron SF, Stoner AMK, Beger M (2022) Future loss of local-scale thermal refugia in
619 coral reef ecosystems. *PLOS Climate* 1(2): doi: 10.1371/journal.pclm.0000004
620
621 Dobson KL, Newton JA, Widdicombe S, Schoo KL, Acquafredda MP, Kitch G, Bantelman A, Lowder K,
622 Valauri-Orton A, Soapi K, Azetsu-Scott K, Isensee K (2022) Ocean Acidification Research for Sustainability:
623 Co-designing global action on local scales. *ICES Journal of Marine Science*, doi:
624 doi.org/10.1093/icesjms/fsac158
625
626 Dodet, G., Piolle, J.-F., Quilfen, Y., Abdalla, S., Accensi, M., Ardhuin, F., Ash, E., Bidlot, J.-R.,
627 Gommenginger, C., Marechal, G., Passaro, M., Quartly, G., Stopa, J., Timmermans, B., Young, I., Cipollini,
628 P., and Donlon, C. (2020) The Sea State CCI dataset v1: towards a sea state climate data record based on
629 satellite observations, *Earth System Science Data*, 12, 1929–1951, doi: 10.5194/essd-12-1929-2020.
630
631 Doney, Scott C, Busch, D. S., Cooley, S. R., Kroeker, K. J., (2020) The Impacts of Ocean Acidification on
632 Marine Ecosystems and Reliant Human Communities. *Annual Review of Environment and Resources* 45 (1):
633 83–112, doi:10.1146/annurev-environ-012320-083019.
634
635 Donlon, C. J., *et al.,* (2012) The Operational Sea Surface Temperature and Sea Ice Analysis (OSTIA)
636 system, *Remote Sensing of Environment*, 116, pp. 140-158 (DOI: 10.1016/j.rse.2010.10.017).
637
638 Fabry, V. J., Seibel, B. A., Feely, R. A., Orr, J. C. (2019) Impacts of ocean acidification on marine fauna and
639 ecosystem processes. *ICES Journal of Marine Science*, 65, 185–195. Doi: 10.2307/j.ctv8jnzw1.25
640
641 Fay, A. R., Gregor, L., Landschützer, P., McKinley, G. A., Gruber, N., Gehlen, M., Iida, Y., Laruelle, G. G.,
642 Rödenbeck, C., Roobaert, A., Zeng, J. (2021) SeaFlux: harmonization of air-sea CO_2 fluxes from surface
643 pCO2 data products using a standardized approach. *Earth System Science Data*, 13(10), 4693–4710.
644 https://doi.org/
645
646 Feely, R A, Doney, S C, Cooley, S. C., (2009) Ocean Acidification: Present Conditions and Future Changes
647 in a High-CO_2 World. *Oceanography* 22 (4): 36–47. doi: 10.5670/oceanog.2009.106.
648
649 Fine R., Willey, D. A, Millero, F. J., (2016) Global variability and changes in ocean total alkalinity from
650 Aquarius satellite data, *Geophysical Research Letters*, doi: 10.1002/2016GL071712
651

Friedlingstein *et al.*, (2019) Global Carbon Budget 2019, *Earth System Science Data*, 11, 1783–1838, doi:10.5194/essd-11-1783-2019

Friedlingstein *et al.*, (2020) Global Carbon Budget 2020, *Earth System Science Data*, 12, 3269–3340, doi: 10.5194/essd-12-3269-2020.

Friedlingstein *et al.*, (2021) Global Carbon Budget 2021, *Earth System Science Data, doi:* 10.5194/essd-14-1917-2022

Ford D, Tilstone GH, Shutler JD, Kitidis V, Lobanova P, Schwarz J, Poulton AJ, Serret P, Lamont T, Chuqui M, *et al.,* (2021) Wind speed and mesoscale features drive net autotrophy in the South Atlantic Ocean. *Remote Sensing of Environment*, *260*, 112435-112435

Ford, D. J., Tilstone, G. H., Shutler, J. D., Kitidis, V. (2022) Derivation of seawater pCO_2 from net community production identifies the South Atlantic Ocean as a CO_2 source, *Biogeosciences*, 19, 93–115, doi: 10.5194/bg-19-93-2022

Ford DJ, Tilstone GH, Shutler JD, Kitidis V, Sheen KL, Dall'Olmo G, Orselli IBM (2023). Mesoscale Eddies Enhance the Air-Sea CO_2 Sink in the South Atlantic Ocean. *Geophysical Research Letters*, *50*(9)

Gentemann *et al.,* (2019) FluxSat: Measuring the Ocean–Atmosphere Turbulent Exchange of Heat and Moisture from Space, *Remote Sensing*, doi: 10.3390/rs12111796

Gloege, L., McKinley, G. A., Landschützer, P., Fay, A. R., Frölicher, T. L., Fyfe, J. C., *et al.* (2021). Quantifying Errors in Observationally Based Estimates of Ocean Carbon Sink Variability. Global Biogeochemical Cycles, 35(4), e2020GB006788

Goddijn-Murphy, L. M., Woolf, D. K., Land, P. E., Shutler, J. D., and Donlon, C. (2015) The OceanFlux Greenhouse Gases methodology for deriving a sea surface climatology of CO_2 fugacity in support of air–sea gas flux studies, *Ocean Science*, 11, 519–541, doi: 10.5194/os-11-519-2015

Gommenginger *et al.,* (2019) SEASTAR: A Mission to Study Ocean Submesoscale Dynamics and Small-Scale Atmosphere-Ocean Processes in Coastal, Shelf and Polar Seas, *Frontiers in Marine Science*, doi: 10.3389/fmars.2019.00457

GOA-ON (2019) GOA-ON (Global Ocean Acidification Observing Network), 2019. "Global Ocean Acidification Observing Network (GOA-ON) Implementation Strategy, 2019." http://www.goa-on.org/documents/general/GOA-ON_Implementation_Strategy.pdf

Green, H., Findlay, H., Shutler, J. D., Land, P. E., Bellerby, R. G. J., (2021), Satellite Observations Are Needed to Understand Ocean Acidification and Multi-Stressor Impacts on Fish Stocks in a Changing Arctic Ocean, *Frontiers in Marine Science*, 8, p692, https://doi.org/10.3389/fmars.2021.635797

Gregor, L., Gruber, N. (2021) OceanSODA-ETHZ: a global gridded data set of the surface ocean carbonate system for seasonal to decadal studies of ocean acidification, *Earth System Science Data*, 13, 777–808, https://doi.org/10.5194/essd-13-777-202

Gruber, N., Landschützer, P., Lovenduski, N. S. (2019) The variable southern ocean carbon sink, *Annual Review of Marine Science,* 2019 11:1, 159-186

Gruber, N., Clement, D., Carter, B. R., Feely, R. A., van Heuven, S., Hoppema, M., *et al.* (2019b). The oceanic sink for anthropogenic CO_2 from 1994 to 2007. *Science*, *363*(6432), 1193–1199. https://doi.org/10.1126/science.aau5153

Gruber, N., Boyd, P.W., Frölicher, T.L. *et al.* (2021) Biogeochemical extremes and compound events in the ocean. *Nature* 600**,** 395–407. doi: 10.1038/s41586-021-03981-7

Gruber, N., Bakker, D. C. E. , DeVries, T., Gregor, L., Hauck, J., Landschützer, P., McKinley, G. A., Müller, J. D., (2023) Trends and variability of the ocean carbon sink, *Nature Reviews Earth and Environment*, **4**, pages 119–134

Gattuso, J.- P., Magnan, A., Bille, R., Cheung, W. W. L., Howes, E. L. ., Joos, F., Allemand, D., *et al.* (2015) Contrasting Futures for Ocean and Society from Different Anthropogenic CO_2 Emissions Scenarios. *Science* 349 (6243): aac4722–aac4722, doi:10.1126/science.aac4722.

Hell, M.C., Ayet, A., Chapron, B., (2021) Swell generation under extra-tropical storms. *Journal of Geophysical Research: Oceans*, *126*(9), p.e2021JC017637.

Ho, D., *et al.,* (2006) Measurements of air-sea gas exchange at high wind speeds in the Southern Ocean: Implications for global parameterizations, *Geophysical Research Letters*, doi: 10.1029/2006GL026817

Jacobson, A. R., Fletcher, S. E. M., Gruber, N., Sarmiento, J. L., Gloor, M. (2007) A joint atmosphere-ocean inversion for surface fluxes of carbon dioxide: 1. Methods and global-scale fluxes. *Global Biogeochemical Cycles*, doi:10.1029/2005gb002556

Keeling (1978) Atmospheric carbon dioxide in the 19th century, *Science*, doi: 10.1126/science.202.4372.1109

Kain, D., Covi, M (2013) Visualizing complexity and uncertainty about climate change and sea level rise, *Communication Design Quarterly*, doi: 10.1145/2466489.2466499

Keil, K. E., Feifel, K. M., Russell, N. B., (2021) Understanding and Advancing Natural Resource Management in the Context of Changing Ocean Conditions, *Coastal Management*, 49:5, 458-486, doi: 10.1080/08920753.2021.1947127

Kelly, R P, M M Foley, W S Fisher, R A Feely, B S Halpern, G G Waldbusser, M R Caldwell (2011) Mitigating Local Causes of Ocean Acidification with Existing Laws. *Science* 332 (6033): 1036–37. https://doi.org/10.1126/science.1203815.

Kilic, L., Prigent, C., Aires, F., Boutin, J., Heygster, G., Tonboe, R. T., Roquet, H., Jimenez, C., Donlon, C. (2018), Expected performances of the Copernicus Imaging Microwave Radiometer (CIMR) for an all-weather and high spatial resolution estimation of ocean and sea ice parameters. J*ournal of Geophysical Research: Oceans*, 123, doi: 10.1029/2018JC014408

Lacroix, F., Ilyina, T., & Hartmann, J. (2020) Oceanic CO_2 outgassing and biological production hotspots induced by pre-industrial river loads of nutrients and carbon in a global modeling approach. *Biogeosciences*, 17(1), 55–88. https://doi.org/10.5194/bg-17-55-2020

Land P.E., Shutler J.D., Findlay H., Girard-Ardhuin F., Sabia R., Reul N., Piolle J., Chapron B., Quilfen Y., Salisbury J.E., *et al* (2015) Salinity from space unlocks satellite-based assessment of ocean acidification, *Environmental Science & Technology*, 49 (4), pp 1987–1994, doi: 10.1021/es504849s

Land P.E., Findlay H.S., Shutler J.D., Ashton I.G., Holding T., Grouazel A., Girard-Ardhuin F., Reul N., Piolle J.F., Chapron B., Quilfen Y., (2019) Optimum satellite remote sensing of the marine carbonate system using empirical algorithms in the global ocean, the Greater Caribbean, the Amazon Plume and the Bay of Bengal, *Remote Sensing of Environment*, *235*, p.111469, doi: 10.1016/j.rse.2019.111469

Lauvset, S. K., Lange, N., Tanhua, T., Bittig, H. C., Olsen, A., Kozyr, A., Álvarez, M., Becker, S., Brown, P. J., Carter, B. R., Cotrim da Cunha, L., Feely, R. A., van Heuven, S., Hoppema, M., Ishii, M., Jeansson, E., Jutterström, S., Jones, S. D., Karlsen, M. K., Lo Monaco, C., Michaelis, P., Murata, A., Pérez, F. F., Pfeil, B., Schirnick, C., Steinfeldt, R., Suzuki, T., Tilbrook, B., Velo, A., Wanninkhof, R., Woosley, R. J., and Key, R. M. (2021) An updated version of the global interior ocean biogeochemical data product, GLODAPv2.2021, *Earth System Science Data*, 13, 5565–5589, doi:10.5194/essd-13-5565-2021,

Lee, K., Tong, L. T., Millero, F. J., Sabine, C. L., Dickson, A. G., Goyet, C., Park, G. -H. , Wanninkhof, R. Feely, R. A., Key, R. M. (2006), Global relationships of total alkalinity with salinity and temperature in surface waters of the world's ocean. *Geophysical Research Letter.*, 33, L19605,

Lefèvre N., Mejia, C., Khvorostyanov D., Beaumont, L., Koffi U., (2021) Ocean Circulation Drives the Variability of the Carbon System in the Eastern Tropical Atlantic. *Oceans*, 2(1), 126-148

Li *et al.,* (2019) Object-Based Mapping of Coral Reef Habitats Using Planet Dove Satellites *Remote Sensing*, 11, doi: 10.3390/rs11121445

Liu, X., Wang, M., (2022) Global daily gap-free ocean color products from multi-satellite measurements, *International Journal of applied Earth observation and geoinformation*, 108, 102714, doi :10.1016/j.jag.2022.102714

Merchant, C.J., Embury, O., Bulgin, C.E. *et al.* (2019) Satellite-based time-series of sea-surface temperature since 1981 for climate applications. *Scientific Data* **6,** 223. https://doi.org/10.1038/s41597-019-0236-x

Millero, F. J., Lee, L., Roche, M. P. (1998), Distribution of alkalinity in the surface waters of the major oceans, *Marine Chemistry*, 60, 111– 130.

Minnett *et al.,* (2019) Half a century of satellite remote sensing of sea-surface temperature, *Remote Sensing of Environment*, doi: 10.1016/j.rse.2019.111366

Morrow, R., Fu, L-L., Ardhuin, F., Benkiran, M., Chapron, B., Cosme, E., d'Ovidio, F., Farrar, J.T., Gille, S.T., Lapeyre, G., Le Traon, P-Y., Pascual, A., Ponte, A., Qiu, B., Rascle, N., Ubelmann, C., Wang, J., and Zaron, E.D. (2019), Global Observations of Fine-Scale Ocean Surface Topography with the Surface Water and Ocean Topography (SWOT) Mission, *Frontiers in Marine Science*, 6, doi: 10.3389/fmars.2019.00232

Mouche, A., B. Chapron, J. Knaff, Y. Zhao, B. Zhang, and C. Combot, (2019) Copolarized and cross-polarized SAR measurements for high-resolution description of major hurricane wind structures: Application to Irma category 5 hurricane, *Journal of Geophysical Research*, 124, 3905-3922.

Nagel, L., Krall, K. E., and Jähne, B.: Comparative heat and gas exchange measurements in the Heidelberg Aeolotron, a large annular wind-wave tank, *Ocean Science*, 11, 111–120, https://doi.org/10.5194/os-11-111-2015, 2015

Land, P. E., Findlay, H. S., Shutler, J. D., Piolle, J.-F., Sims, R., Green, H., Kitidis, V., Polukhin, A., and Pipko, I. I., (2023) OceanSODA-MDB: a standardised surface ocean carbonate system dataset for model–data intercomparisons, *Earth System Science Data*, 15, 921–947, doi: 10.5194/essd-15-921-2023.

Oliver, E. C. J. J., Benthuysen, J. A., Darmaraki, S., Donat, M. G., Hobday, A. J., Holbrook, N. J., Schlegel, R. W., Gupta, A. Sen, & Sen Gupta, A. (2021) Marine Heatwaves. *Annual Review of Marine Science*, 13(1), 1–30. Doi: 10.1146/annurev-marine-032720-095144

Olivier, L., Boutin, J. ,Reverdin, G., Lefèvre, N., Landschützer, P., Speich, S., Karstensen, J., Labaste, M., Noisel, C., Ritschel, M. *et al.* (2022) Wintertime process study of the North Brazil Current rings reveals the region as a larger sink for CO2 than expected. *Biogeosciences*, 19, 2969-2988, doi:10.5194/bg-19-2969-2022.

Orr JC, Fabry VJ, Aumont O, *et al*., (2005) Anthropogenic ocean acidification over the twenty-first century and its impact on calcifying organisms. *Nature,* 437: 681– 86

816 Phillips *et al.,* (2006) Maximum entropy modelling of species geographic distributions, *Ecological Modeling*,
817 190, doi: 10.1016/j.ecolmodel.2005.03.026
818
819 Polverari, F., Portabellow, M., Lin, W., *et al.* (2021) On High and Extreme Wind Calibration Using ASCAT,
820 *IEEE Transactions on Geoscience and Remote Sensing*, doi:10.1109/TGRS.2021.3079898
821
822 Quilfen Y, Shutler J, Piolle J-F, Autret E (2021) Recent trends in the wind-driven California current upwelling
823 system, *Remote Sensing of Environment*, *261*, 112486-112486.
824
825 Reul, N., B. Chapron, E. Zabolotskikh, C. Donlon, A. Mouche, J. Tenerelli, F. Collard, J.F. Piolle, A. Fore, S.
826 Yueh, J. Cotton, P. Francis, Y. Quilfen, and V. Kudryavtsev, (2017) A new generation of tropical cyclone size
827 measurements from space. *Bulletin of the American Meteorology Society*, 98, 2367-2385,
828 doi:10.1175/BAMS-D-15-00291.1
829
830 Reul, N., Chapron, B., Grodsky, S.A., Guimbard, S., Kudryavtsev, V., Foltz, G.R. and Balaguru, K., (2021)
831 Satellite observations of the sea surface salinity response to tropical cyclones. *Geophysical Research*
832 *Letters*, *48*(1), p.e2020GL091478
833
834 Robinson (2010) Discovering the ocean from space, the unique applications of satellite oceanography,
835 Springer, ISBN: 978-3-540-68322-3
836
837 Rödenbeck, C., Zaehle, S., Keeling, R., Heimann, M. (2018) How does the terrestrial carbon exchange
838 respond to inter-annual climatic variations? A quantification based on atmospheric CO 2 data,
839 *Biogeosciences*, 15, 2481-2498.
840
841 Regnier, P., Friedlingstein, P., Ciais, P., Mackenzie, F. T., Gruber, N., Janssens, I. a., *et al.* (2013)
842 Anthropogenic perturbation of the carbon fluxes from land to ocean. *Nature Geoscience*, *6*(8), 597–607.
843 https://doi.org/10.1038/ngeo1830

844 Regnier, P., Friedlingstein, P., Ciais, P., Mackenzie, F. T., Gruber, N., Janssens, I. a., *et al.* (2013b)
845 Anthropogenic perturbation of the carbon fluxes from land to ocean. *Nature Geoscience*, *6*(8), 597–607.
846 https://doi.org/10.1038/ngeo1830

847 Regnier, P. A. G., Resplandy, L., Najjar, R. G., Ciais, P. (2022). The land-to-ocean loops of the global carbon
848 cycle. *Nature*, 2022 603:7901, 603(7901), 401–410. doi: 10.1038/s41586-021-04339-9
849
850 Sabine *et al.,* (2004) The oceanic sink for anthropogenic CO_2, *Science*, doi: 10.1126/science.109740
851
852 Salisbury, J., Vandemark, D., Jönsson, B., Balch, W., Chakraborty, S., Lohrenz, S., *et al.* (2015) How can
853 present and future satellite missions support scientific studies that address ocean acidification?
854 *Oceanography* 28, 108–121. doi: 10.5670/oceanog.2015.35
855

Sathyendranath, S, Brewin, RJW, Brockmann, C, Brotas, V, Calton, B, Chuprin, A, Cipollini, P, Couto, AB, Dingle, J, Doerffer, R, Donlon, C, Dowell, M, Farman, A, Grant, M, Groom, S, Horseman, A, Jackson, T, Krasemann, H, Lavender, S, Martinez-Vicente, V, Mazeran, C, Mélin, F, Moore, TS, Müller, D, Regner, P, Roy, S, Steele, CJ, Steinmetz, F, Swinton, J, Taberner, M, Thompson, A, Valente, A, Zühlke, M, Brando, VE, Feng, H, Feldman, G, Franz, BA, Frouin, R, Gould, Jr., RW, Hooker, SB, Kahru, M, Kratzer, S, Mitchell, BG, Muller-Karger, F, Sosik, HM, Voss, KJ, Werdell, J, and Platt, T (2019) An ocean-colour time series for use in climate studies: the experience of the Ocean-Colour Climate Change Initiative (OC-CCI). *Sensors*, 19, 4285. doi:10.3390/s19194285

Shutler J.D., Land P.E., Brown C.W., Findlay H.S., Donlon C.J., Medland M., Snooke R., Blackford J.C., (2013) Coccolithophore surface distributions in the North Atlantic and their modulation of the air-sea flux of CO_2 from 10 years of satellite Earth observation data. *Biogeosciences*, *10*(4), 2699-2709.

Shutler J.D., Quartly G.D., Donlon C.J., Sathyendranath S., Platt T., Chapron B., Johannessen J.A., Girard-Ardhuin F., Nightingale P.D., Woolf D.K., *et al.,* (2016) Progress in satellite remote sensing for studying physical processes at the ocean surface and its borders with the atmosphere and sea-ice. *Progress in Physical Geography*, *40*, 215-246.

Shutler J.D., Wanninkhof R., Nightingale P.D., Woolf D.K., Bakker D.C., Watson A., Ashton I.G., Holding T., Chapron B., Quilfen Y., Fairall C., (2020). Satellites will address critical science priorities for quantifying ocean carbon, *Frontiers in Ecology and the Environment*, doi: 10.1002/fee.2129

Sunday, J., Fabricius, K., Kroeker, K. *et al.,* (2017) Ocean acidification can mediate biodiversity shifts by changing biogenic habitat. *Nature Climate Change,* **7,** 81–85. https://doi.org/10.1038/nclimate3161

Stukel, M.R., Irving, J.P., Kelly, T.B. *et al.* (2023) Carbon sequestration by multiple biological pump pathways in a coastal upwelling biome. *Nature Communications,* **14**. doi: 10.1038/s41467-023-37771-8

Takahashi *et al.,* (1997) Global air-sea flux of CO_2: An estimate based on measurements of air-sea pCO2 difference, *Proceedings of the National Academy of Sciences*, doi: 10.1073/pnas.94.16.829

Taylor, J. R., (1976) An introduction to error analysis, the study of uncertainties in physical measurements, Second edition, University Science Books, ISBN-13: 978-0-935702-75-0

Tilbrook B, Jewett EB, DeGrandpre MD, Hernandez-Ayon JM, Feely RA, Gledhill DK, Hansson L, Isensee K, Kurz ML, Newton JA, Siedlecki SA, Chai F, Dupont S, Graco M, Calvo E, Greeley D, Kapsenberg L, Lebrec M, Pelejero C, Schoo KL and Telszewski M (2019) An Enhanced Ocean Acidification Observing Network: From People to Technology to Data Synthesis and Information Exchange. *Frontiers in Marine Science,* 6:337. doi: 10.3389/fmars.2019.00337

Verezemskaya, P., Tilinina, N., Gulev, S., Renfrew, I. A., Lazzara, M. (2017). Southern Ocean mesocyclones and polar lows from manually tracked satellite mosaics. *Geophysical Research Letters*, *44*(15), 7985–7993.

Wanninkhof, R., Pickers, P.A., Omar, A.M., Sutton, A., Murata, A., Olsen, A., Stephens, B.B., Tilbrook, B., Munro, D., Pierrot, D., Rehder, G., (2019) A surface ocean CO_2 reference network, SOCONET and associated marine boundary layer CO_2 measurements. *Frontiers in Marine Science*, *6*, p.400.

Watson, A.J., Schuster, U., Shutler, J.D. *et al.,* (2020) Revised estimates of ocean-atmosphere CO_2 flux are consistent with ocean carbon inventory. *Nature Communications.* 11**,** 4422.

Wibble, B., (2021), Out of harms way, *Science*, 372, 6548, pp. 1274-1275, doi: 10.1126/science.abi9209.

Woolf D.K., Land P.E., Shutler J.D., Goddijn-Murphy L.M., Donlon C.J., (2016) On the calculation of air-sea fluxes of CO_2 in the presence of temperature and salinity gradients. *Journal of Geophysical Research: Oceans*, *121*(2), 1229-1248.

Woolf DK, Shutler JD, Goddijn‐Murphy L, Watson AJ, Chapron B, Nightingale PD, Donlon CJ, Piskozub J, Yelland MJ, Ashton I, *et al* (2019). Key Uncertainties in the Recent Air‐Sea Flux of CO_2. *Global Biogeochemical Cycles*, *33*(12), 1548-1563.

Widdicombe, S., Isensee, K., Artioli, Y., Gaitán-Espitia, J.D., Hauri, C., Newton, J.A. , Wells, M., Dupont, S., (2023) Unifying biological field observations to detect and compare ocean acidification impacts across marine species and ecosystems: What to monitor and why, *Ocean Sciences*, doi: 10.5194/os-19-101-2023

7.0 Appendix

The following sections detail the methods for the example land to ocean carbon flow estimate**.**

7.1 Integrated carbon mass across the depth of the Amazon river plume

Ocean surface total dissolved inorganic carbon (CT) concentration data were obtained for the period 2010 to 2020 from a publically available monthly gridded CT time series (Sims *et al.,* 2022). This dataset encompasses the whole Amazon outflow region including regions that mainly contain oceanic water masses from the South Atlantic, so it is necessary to first distinguish between the oceanic waters and those relating to the river plume. The Amazon river plume was identified using sea surface salinity (SSS) specified as any grid cells with SSS < 35 (as used by Coles *et al.,* 2013; Hu *et al.,* 2004). The monthly gridded time series data are a surface dataset and so do not include subsurface values through the total plume depth, so plume depth is needed to quantify the total riverine CT. To account for changes in SSS and likely CT concentration with depth, the mean SSS throughout the plume, S_{plume}, was calculated from surface SSS using the relationship described by Hu *et al.,* (2004):

$$S_{plume} = 4.352 + SSS * 0.881 \quad (1)$$

The depth integrated CT concentration of each plume grid cell (CT_{plume}) was then calculated using S_{plume} and by assuming CT is conservative with salinity using:

$$CT_{plume} = CT_{surf} \frac{S_{plume}}{SSS} \quad (2)$$

where CT_{surf} is the monthly mean surface CT concentration. Total plume CT (CT_{total}) for a given month can then be calculated by summing CT_{plume} for each grid cell within the plume (as identified by regions SSS < 35). In an effort to separate out the riverine CT from the oceanic originating CT, the proportion of CT in each plume grid cell which originates from the river, κ, was estimated by assuming conservative mixing with ocean water, and linearly interpolating between 0 and 35 (such that a salinity of 0 indicates 100% riverine source, and 35 indicates 100% oceanic source). The gridded riverine CT ($CT_{riverine}$) is then calculated as:

$$CT_{riverine} = \kappa CT_{plume} \quad (3)$$

where κ is the mixing factor. The total carbon mass resulting from $CT_{riverine}$ is then calculated for each grid cell by multiplying $CT_{riverine}$ by plume volume and molecular mass of carbon, m_c, to give:

$$M_{CT} = V_{plume} CT_{riverine} m_c \quad (4)$$

where V_{plume} is the volume of the plume for the respective grid cell, calculated by multiplying the grid cell surface area by S_{plume}. Collectively equations 1 to 4 enable a spatial dataset of carbon mass integrated across the depth of the plume to be calculated.

7.2 Quantifying Amazon river discharge

Calculating the flux of carbon originating from the river requires a measure of river flow and the need to identify a region or location across which the river plume flow is measured or quantified. Along a river this measurement location would be a river gauging station where the flow is channelled, but here the data give the plume as it extends into the ocean. So to quantify the CT discharge as it flows into the ocean a family of 24 radii transects were drawn across the plume, centred on the mouth of the Amazon (figure A1). For each portion of each radii that intersects with the plume M_{CT} was summed and the monthly riverine CT flow estimate for each radii transect (i.e. the resultant sum of carbon passing through, or intersecting, each individual radii) was calculated by dividing the sum of M_{CT} by the monthly Amazon river discharge:

$$CT_{outflow,r} = \frac{\sum^{i \in G} M_{CT,i}}{Q} \quad (5)$$

where G is the set of all plume grid cells intersecting with the radii transect with radius r, $M_{CT,i}$ is the mass of CT in grid cell i, and Q is the monthly volume of water discharged by the Obidos gauging station. This calculation is repeated for all radii and months, producing 24 different estimates of $CT_{outflow}$. Note, that outflow estimates of zero (i.e. where G = ⌀) were excluded, since this indicated that no plume cells were intersected by the radii perimeter. This could occur, for example, if there is a break in the plume, or if the plume does not extend as far as the radii.

Choosing an optimal radii is not straightforward, since small radii are more likely to include near-coastal data where uncertainties in the CT data are likely greater (eg due to land-sea adjacency effects for the satellite Earth observation inputs), while larger radii will increase the time lag in the calculation because it will intersect water that is temporally older. This time lag is not expected to always follow a linear relationship with distance due to temporal and/or spatial variation in plume direction, discharge rate, wind speed and ocean current interactions. Larger radii, which have larger time lags, are likely to result in larger uncertainties in the calculations, as the water will have likely experienced more interactions (mixing, chemical alteration or losses due to gas exchange), and so the grid cells selected by larger radii are less likely to solely contain water of a similar age.

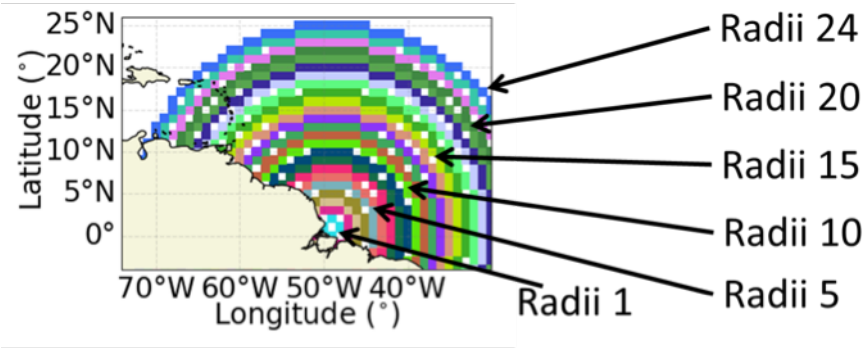

Figure A1 Radii centred on the mouth of the Amazon that were used to quantify the flow of carbon originating from the river plume.

Using the mean CT outflow calculated from multiple radii will reduce the uncertainty associated with coastal cell inaccuracies and variations in plume shape. Conversely, including larger radii increases the time-lag between the mean of river flow variations and the mean identified CT outflow. To mitigate this, CT outflow is calculated from a set of radii, R = {1, 2, … n_r}, where n_r is chosen to minimise this time-lag. This is done by selecting the n_r that maximises the correlation coefficient between mean seasonal CT outflow and mean seasonal river discharge. The aim is to maximise the number of radii used to estimate the mean, while keeping the size of radii small enough to ensure that the temporal lag is inconsequential at the monthly temporal resolution used. It is expected that this maximum correlation method will be robust to variation in the calculated mean seasonal (monthly) CT outflow, but it does not always guarantee alignment to the peak value. For the Amazon dataset the radii 5 gave the highest correlation between the mean seasonal CT outflow and mean seasonal discharge (r=0.99).

7.3 Uncertainty analysis

Uncertainties were propagated at each step of equations 1 to 5 and an analysis was conducted to identify the main sources of uncertainty in CT. The resulting uncertainty in CT outflow combines uncertainties from the surface CT gridded time series data, discharge data, plume depth relationship (Coles *et al.,* 2013) and the mean plume salinity (Hu *et al.,* 2004). Standard analytical error propagation methods were used where possible (see Taylor, 1997). The uncertainty in monthly discharge was estimated as the standard deviation of the mean monthly discharge (ie assuming that sub-monthly measurements were independent repeated samples of the monthly mean). Uncertainties in the plume depth were estimated from the 95% confidence limits shown in figure 13 of Coles *et al.,* (2013). No uncertainties are reported for the relationship between mean plume salinity and surface salinity in Hu *et al.,* (2004), (which is equation 1) so an estimate of ±10% uncertainty in the coefficients has been used for both intercept and slope.

An analytical approach was not appropriate for determining the uncertainty in the plume mask from SSS (and therefore plume surface area), and so an ensemble approach was used instead. For this, a set of 100 ensembles were calculated using the SSS dataset with added noise (i.e. sampling 100 times from a grid of normally distributed random numbers) with a mean equal to the original SSS data set value and standard deviation equal to the uncertainty in that value for each grid cell:

$$S_{ensemble,i,j} = N\left(S_{mean,j}, S_{uncertainty,j}\right) \quad (6)$$

where $S_{ensemble,i,j}$ is the ensemble SSS for the sample *i* at grid cell *j*, and $S_{mean,j}$ and $S_{uncertainty,j}$ are the mean and uncertainty from the SSS data set for grid cell *j*. The plume masks for each ensemble SSS were calculated by applying the SSS < 35 threshold, leading to an ensemble of 100 separate plume masks.

Uncertainties arising from SSS, including from the plume mask, were propagated using these 100 ensemble data sets. The calculation was repeated for each ensemble SSS at each stage (equations 1 to 5). This results in 100 ensemble outputs for each step in the calculation, from which the standard deviation was calculated to estimate uncertainty at that stage. For example, to calculate uncertainty in the plume surface area, the surface area of each ensemble plume mask was calculated, and the standard deviation of these

100 surface areas calculated. Similarly, to calculate the uncertainty in mean plume salinity (equation 1) arising from the SSS input data, equation 1 was applied to each ensemble, resulting in 100 S_{plume} values from which the standard deviation was calculated. In calculating the uncertainty of the CT content of the plume (CT_{plume}, from equation 2) the full ensemble of 100 ensemble S_{plume} data sets were used in conjunction with the 100 SSS ensembles to propagate this uncertainty forward. Note that the uncertainty propagated from SSS data is combined with any other source of uncertainty at each step (e.g. the ±10% on the Hu *et al.,* (2004) relationship) resulting in a combined uncertainty estimate for all input data and models, from which the standard deviation is calculated to estimate the combined uncertainty of the complete approach.

7.4 Results

The mean annual CT outflow of the Amazon was calculated as 43.7 ± 3.0 Tg C yr^{-1} (table 4) with a standard deviation of 4.3 Tg C yr^{-1} and a coefficient of variation of 0.10. Therefore the Amazon to Atlantic flow of inorganic carbon is estimated to be 44 Tg Cyr^{-1} with an annual variation of ~10%. Current estimates of land to ocean carbon flow are 0.45, 0.60 and 0.78 GtC yr^{-1} (Jacobson *et al.,* 2007; Watson *et al.,* 2020; Resplandy *et al.,* 2018; Sarmiento & Sundquist, 1992) and there is much debate over which value to use, hence the latest global carbon assessment used the mean value of 0.61 GtC yr^{-1} (Freidlingstein *et al.,* 2020). Therefore using 0.61 GtC yr^{-1} as the reference suggests that the Amazon could be responsible for ~7 % of global land to ocean flow of inorganic carbon and the first estimate of the inter-annual variation in this Amazon land to ocean flow is ±10%.

Annual results	**Mean ± uncertainty**
Amazon discharge	$5.56\times10^{12} \pm 5.15\times10^{8}$ m^3
Plume surface area	$1.38\times10^{12} \pm 3.42\times10^{9}$ m^2
Plume thickness	13.2 m
Plume volume	$1.87\times10^{13} \pm 7.18\times10^{10}$ m^3
Plume CT	$3.64\times10^{13} \pm 4.39\times10^{11}$ g C
CT outflow (r_n = 5)	43.71 ± 3.00 Tg C

Table A1: Annual mean results and standard deviations for each component of the CT outflow calculation for the Amazon river based on r_n = 5.

References

Coles, V. J., Brooks, M. T., Hopkins, J., Stukel, M. R., Yager, P. L., Hood, R. R. (2013) The pathways and properties of the Amazon River Plume in the tropical North Atlantic Ocean, *Journal of Geophysical Research Ocean*, 118(12), 6894–6913, doi:10.1002/2013JC008981.

Druffel, E. R. M., Bauer, J. E., Griffin, S. (2005) Input of particulate organic and dissolved inorganic carbon from the Amazon to the Atlantic Ocean, Geochemistry, *Geophysics, Geosystems*, 6(3), doi:10.1029/2004GC000842.

Friedlingstein, P. *et al.,* (2020) Global Carbon Budget 2020, Earth Syst. Sci. Data, 12, 3269–3340, https://doi.org/10.5194/essd-12-3269-2020

Hu, C., Montgomery, E. T., Schmitt, R. W., Muller-Karger, F. E. (2004) The dispersal of the Amazon and Orinoco River water in the tropical Atlantic and Caribbean Sea: Observation from space and S-PALACE floats, *Deep Sea Research Part II Tropical Studies in Oceanography,* 51(10-11 SPEC. ISS.), 1151–1171, doi:10.1016/j.dsr2.2004.04.001.

Jacobson, A. R., Fletcher, S. E. M., Gruber, N., Sarmiento, J. L., Gloor, M. (2007) A joint atmosphere-ocean inversion for surface fluxes of carbon dioxide: 1. Methods and global-scale fluxes, *Global Biogeochemical Cycles*, 21(1), doi:10.1029/2005GB002556.

Richey, J. E., Hedges, J. I., Devol, A. H., Quay, P. D., Victoria, R., Martinelli, L., Forsberg, B. R. (1990) Biogeochemistry of carbon in the Amazon River, *Limnology and Oceanography*, 35(2), 352–371, doi:10.4319/lo.1990.35.2.0352.

Sarmiento, J. L., Sundquist, E. T. (1992) Revised budget for the oceanic uptake of anthropogenic carbon dioxide, *Nature*, 356(6370), 589–593, doi:10.1038/356589a0.

Sims, R. P., Holding, T. M., Land, P. E., Piolle, J.-F., Green, H. L., Shutler, J. D. (2022) OceanSODA-UNEXE: A multi-year gridded Amazon and Congo River outflow surface ocean carbonate system dataset, *Earth System Science Data Discussions*, doi: 10.5194/essd-2022-294

Taylor, J. R. (1997) An introduction to error analysis : the study of uncertainties in physical measurements, *University Science Books*.

Resplandy, L., Keeling, R. F., Rödenbeck, C., Stephens, B. B., Khatiwala, S., Rodgers, K. B., Long, M. C., Bopp, L., Tans, P. P. (2018) Revision of global carbon fluxes based on a reassessment of oceanic and riverine carbon transport, *Nature Geoscience,* 11, 504–509, https://doi.org/10.1038/s41561-018-0151-3.

Watson, A. J., Schuster, U., Shutler, J. D., Holding, T., Ashton, I. G. C., Landschützer, P., Woolf, D. K., and Goddijn-Murphy, L. (2020) Revised estimates of ocean-atmosphere CO_2 flux are consistent with ocean carbon inventory, *Nature Communicaions,* 11, 1–6, https://doi.org/10.1038/s41467-020-18203-3.

Panel 1: *The potential for quantifying land to ocean flow of inorganic carbon*

Quantifying extent, magnitude and variability

Land to ocean flow of inorganic carbon by rivers is included within the annual carbon assessments, with an equivalent annual size of 20% to 35% of the contemporary oceanic carbon sink (range taken from Friedlingstein *et al.,* 2022). However, the complexity of these systems, their distribution throughout the world combined with their high heterogeneity means that current assessments assume static values. Given the size of this carbon exchange, improving our ability to monitor them and characterise their flows would help improve closure of the global carbon assessments.

Combining satellite, *in situ* and empirical approaches and data sources

Surface extent and monthly variability of large river flows can be viewed and accurately quantified using satellite data (Land *et al.,* 2019; Sims *et al.,* 2022; Figure P1). These satellite data provide spatially resolved observations, but are limited in their temporal resolution and they are unable to determine the plume depth. Combining empirical understanding from *in situ* analyses with river gauging information and satellite data can enable the depth, flow and spatial extent to be characterised.

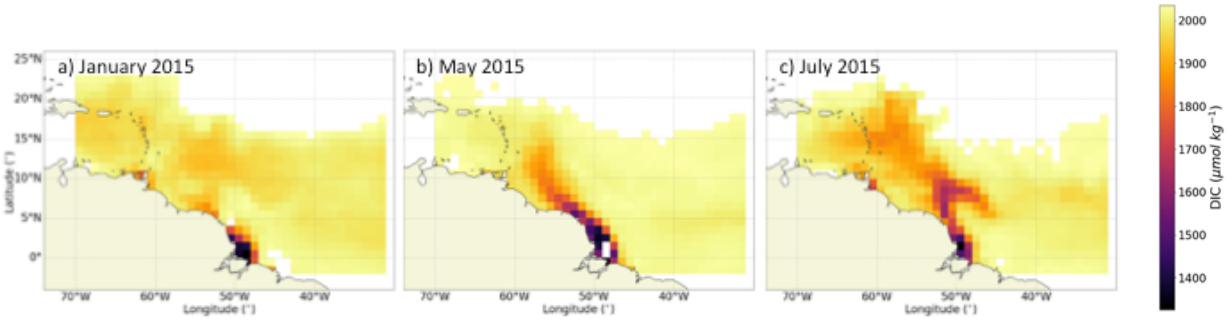

Figure P1: Satellite observation-based estimates of the surface dissolved inorganic carbon within the Amazon plume during three different months in 2015 showing high spatial and temporal variability

Example method

Ocean surface total dissolved inorganic carbon concentration data were obtained from a publicly available Amazon region monthly gridded time series (Sims *et al.,* 2022) and regions where salinity <35 was used to identify the river plume (as used by Hu *et al.,* 2004). The mean salinity and carbon within the plume were calculated from the surface salinity using the relationship described by Hu *et al.,* (2004), from which the depth integrated carbon concentration was calculated, assuming the carbon is conservative with salinity. The riverine carbon estimate was further refined by assuming conservative mixing with ocean water through linearly interpolating between salinity of 0 and 35 (i.e. 0 is 100% riverine, 35 is 100% oceanic). River flow gauging data then allows the carbon flow through an arc that bisects the plume (e.g. equivalent to an offshore gauging station) to be calculated giving a total riverine land to ocean carbon flow with respect to time. Please see the appendix of this paper for the full methods.

This analysis identifies a net flow of 44 terra grams of carbon per year (Tg C yr^{-1}) for the Amazon with an inter-annual variation of ±10%. This total flow is equivalent to ~7% of the total annual global riverine flux currently used in global assessments (e.g. as used in Friedlingstein *et al.,* 2021).

Panel 2: *The potential to use satellite observations to guide management and mitigation*

Linking satellite observations with species

Space observations will be key for understanding the impact of acidification on economically important marine resources to identify the baseline conditions and variability, and to map life histories of key species against changing conditions (as proposed by Green *et al.*, 2021) towards underpinning management decisions, and where and when to focus remedial efforts. This could be applied to any marine species, but potential foci could be key sentinel species of ecosystem health (e.g., tuna, marine turtles or birdlife), economically, or socially, important fisheries, such as oysters, or artisanal fish species and key plankton species that form the base of the food chain (e.g., pteropods). This could identify regions of interest such as those that are already experiencing high variability in marine carbon conditions, indicate when conditions cross experimentally-derived thresholds of tolerance for particular species, guide where efforts should be focussed to support communities and marine life, or identify highly-variable but healthy ecosystems towards identifying populations with phenotypes more resistant to change. It may be possible to use satellite observations in conjunction with niche modelling approaches (e.g., Phillips *et al.,* 2006) to understand how the existing conditions are impacting the different life stages of each species. And matching satellite observations of carbon, with key biological processes or indicator data could provide quantitative evaluation of the impacts of acidification through time at an ecosystem level (e.g., Widdicombe *et al.,* 2023)

The co-development of indicators and easy access alongside other observations

Many user groups are unlikely to require a deep understanding of the ocean conditions and instead will require the data to be translated into simple indicators. For example, to identify regions that are under-stress, particularly vulnerable, hot spots of activity, or pre-cursor indicators of a potential detrimental change in conditions. To be of most use, ocean acidification data and its complete metadata needs to be assessed in the context of other stressors, especially that of ocean warming, but also coastal eutrophication, coastal habitat destruction and pollution (Gruber *et al.,* 2011). The co-development of these simple indicators, using satellite observation-based data and constructed in ways that are understandable for non-experts, could be used to identify regions or societies that require protection, remedial action or support. For most users, local to regional monitoring information that is available in a timely and easily-accessible manner will be of most relevance, although for major stakeholders (e.g. governments or international assessments) global information is likely to be crucial (e.g., the Inter-governmental Panel on Climate Change, IPCC).

Supporting community understanding and uptake of satellite observations

Training in data interpretation and capacity building are likely to be the main limitations on uptake of satellite-derived information, along with making data easily available to those without reliable internet connectivity. Potential user groups, including policy makers (e.g., country-wide or regional politicians), to regional resource managers (e.g., who determine regional monitoring), to end users (e.g., shellfish growers), will have different needs and understanding. Direct engagement with marine and coastal resource managers who are uniquely working on improving ocean acidification and hypoxia management responses, interventions, and resilience building strategies is essential. For addressing climate change, successful coastal and marine management depends upon an improved understanding of regional ocean and coastal

change and enhanced communication between resource managers and other stakeholder groups (Keil *et al.,* 2021).