

VARIATIONS

A joint US CLIVAR & OCB Newsletter



Fall 2015 • Vol. 13, No. 4

The Southern Ocean's role in climate

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Vertical exchange in the Southern Ocean between the atmosphere and the surface and deep ocean has a profound influence on the oceanic uptake of anthropogenic carbon and heat, as well as nutrient resupply from the abyss to the surface. Despite this importance, the Southern Ocean, defined here as the stretch of ocean between Antarctica and approximately 30°S, remains the most poorly observed and understood part of the global ocean. Reduced uncertainties in global climate projections will be difficult to achieve without significant progress toward understanding the Southern Ocean's response to climate forcings.

Recent advances in observational and modeling capabilities have the capability to transform our understanding of the Southern Ocean and its role in climate. The global array of profiling Argo floats, combined with satellite data, has produced temperature, salinity, and pressure data with unprecedented spatial coverage. Floats equipped with biogeochemical sensors are

Anthropogenic carbon and heat uptake by the ocean: Will the Southern Ocean remain a major sink?

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The global ocean has taken up more than a quarter of the carbon emitted from human activities (since 1750; e.g., Sabine et al. 2004) and more than 90% of the excess heat that has accumulated in the Earth system as a result of these emissions (since 1971; e.g., Church et al. 2011). Hence, the ocean is greatly mitigating the rise of global mean surface temperatures. Among all the oceanic basins, the Southern Ocean, which we define here as the vast area south of 30°S that surrounds Antarctica, is thought to play a dominant role in the uptake of anthropogenic carbon and heat (e.g., Frölicher et al. 2015, Roemmich et al. 2015). Over recent decades, the Southern Ocean has experienced significant changes such as increases in air temperature, precipitation, glacial melting and westerly winds. These changes are expected to intensify over the 21st century and have the potential to greatly impact the uptake of carbon and heat. Careful monitoring of key properties and processes in the Southern Ocean and an improved understanding of their effects on heat and carbon uptake are thus needed to assess the present and project the future of the climate system.

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beginning to provide the scientific community with measurements essential for studies of the carbon cycle. Numerical models are beginning to resolve spatial scales of 10-20 km, which is adequate for capturing the mesoscale dynamics that are thought to be significant in the mixing and circulation of the Southern Ocean. Finally, the development of state estimates provides us with realistic model solutions that are compatible with modern observational datasets.

Despite this progress, many challenges remain. The spatial and temporal sampling coverage in the Southern Ocean remains inadequate. Earth system models continue to have incomplete physics and biogeochemistry and thus rely on parameterizations of several important processes. Interactions between the main components of the climate system—the atmosphere, land, ocean and sea ice—tend to be poorly understood relative to processes in each of these individual components. This joint edition of the US CLIVAR and OCB newsletters includes a series of articles that highlight recent progress and identify the scientific gaps in our knowledge of the Southern Ocean's role in climate and the ocean's response to climate forcings.

US CLIVAR VARIATIONS

Editors: Mike Patterson and Kristan Uhlenbrock
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The Southern Ocean is one of the most remote, inhospitable places on Earth, making *in situ* observations extremely difficult to obtain. In addition, temperature and carbon concentration measured at the ocean surface are not easily linked to heat and carbon uptake. For instance, an increase in surface temperature or carbon concentration is not necessarily due to an increase in ocean uptake, but could instead be driven by an increased upward flux of heat or carbon from deep waters. Anomalies of heat and carbon due to natural climate system variability are usually referred to as *natural*. In contrast, *anthropogenic* refers to anomalies linked to human-induced climate change, either through a circulation change or a surface flux change driven by the atmosphere. The sum of natural and anthropogenic signals forms the *total* heat and carbon, which is what we measure. It is generally quite difficult to determine whether observed changes arise from the natural or the anthropogenic component. This fact together with the lack of observational data, especially in winter, leads to large uncertainties in how much anthropogenic heat and carbon the Southern Ocean is currently absorbing and how this uptake may evolve in the future.

In this article, we provide an overview of recent breakthroughs and ongoing work in understanding Southern Ocean heat and carbon uptake. We highlight remaining gaps and uncertainties, and discuss opportunities that will help address the challenges these present.

Southern Ocean dominance of global anthropogenic carbon and heat uptake

Observational analyses and numerical models both indicate that the Southern Ocean currently accounts for about 40 to 50% of the cumulative global oceanic uptake of anthropogenic carbon (Figure 1a; Sabine et al. 2004; Mikaloff-Fletcher et al. 2006; Frölicher et al. 2015). According to models, the Southern Ocean is responsible for around 75% of the global oceanic uptake of anthropogenic heat (Figure 1b; Frölicher et al. 2015). This result is consistent with recent observational estimates that show that 67 to 98% of the global ocean heat gain over the 2006–2013 period occurred in the Southern Ocean (Roemmich et al. 2015). Nonetheless, comparison to observations of heat uptake remains difficult, as observation-based air-sea heat flux estimates are problematic due to difficulties in adequately characterizing the many complex processes involved in ocean-atmosphere heat exchange (e.g., radiation, conduction, and convection). Consequently, air-sea heat flux products primarily depend on models and parameterizations. In the Southern Ocean, different products disagree on both the sign and magnitude of the climatological net heat flux (e.g., Cerovečki et al. 2011).

The storage of anthropogenic carbon and heat is better constrained by observations than the uptake. Furthermore, storage can offer insight into the uptake, as it directly depends on how much anthropogenic heat and carbon the ocean has taken up since the preindustrial era. The spatial pattern of storage also

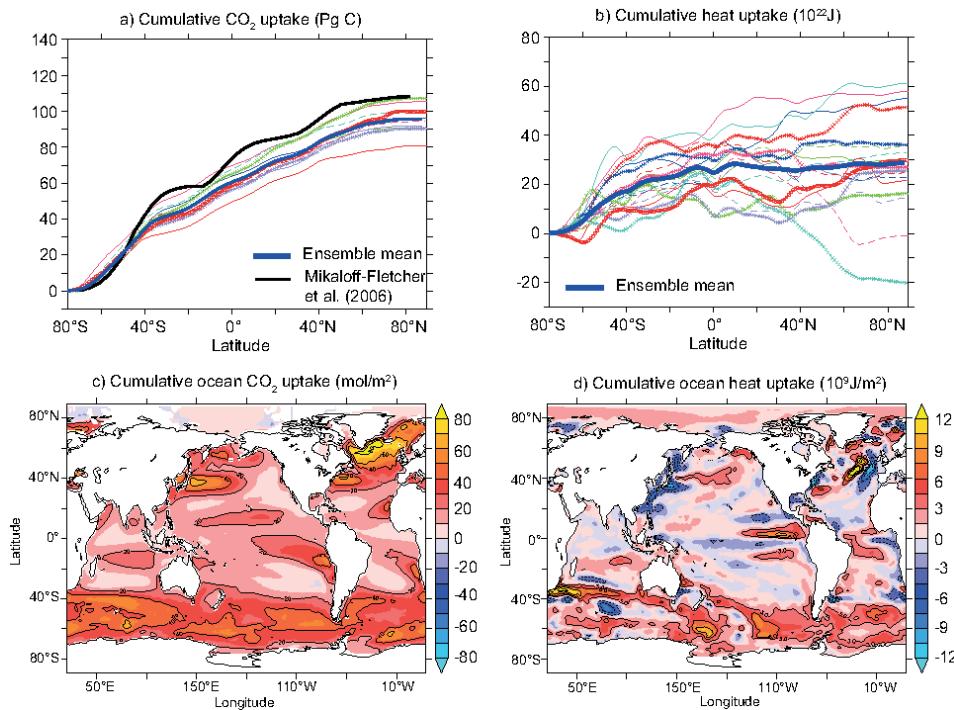


Figure 1. Oceanic uptake of anthropogenic CO₂ and heat between 1870 and 1995 simulated by a subset of CMIP5 models. (a,b) Zonal integrated cumulative ocean CO₂ and heat uptake integrated from 80°S to 90°N such that the vertical scale goes from 0 at 80°S to the total uptake at 90°N for each model. The anthropogenic carbon flux estimates from atmospheric inversions of Mikaloff-Fletcher et al. (2006) are indicated in black. (c,d) Multimodel mean in cumulative anthropogenic carbon and heat uptake. Adapted from Frölicher et al. (2015).

reflects the penetration of anthropogenic anomalies into the ocean interior and hence determines if anomalies are sequestered or are likely to reemerge at the surface on short timescales. In the Southern Ocean, the patterns of anthropogenic carbon and heat storage show significant differences, indicating that the redistribution of carbon in the ocean interior is driven by different processes than those governing the redistribution of heat. Several studies indicate that while anthropogenic carbon is transported much like a passive tracer, anthropogenic heat feeds back on the circulation with direct implications for heat transport into the ocean interior (Bryan and Spelman 1985; also Winton et al. 2012; Morrison et al. 2015a). In addition to dominating the global oceanic uptake of anthropogenic heat and carbon, the Southern Ocean is the

region where the most significant uncertainties are found. CMIP5 (Coupled Model Intercomparison Project Phase 5) models show the largest spread for both cumulative anthropogenic carbon and heat uptake in the Southern Ocean (Figure 1a-b; Frölicher et al. 2015), with a much greater intermodel spread for heat ($\pm 71\%$) than for carbon ($\pm 8\%$; Frölicher et al. 2015). A large portion of the differences between models can be attributed to the large internal variability in the Southern Ocean, stemming from the chaotic nature of the Earth system, which explains about half of the inter-model spread for anthropogenic carbon and of order three-quarters for anthropogenic heat in CMIP5 models (Frölicher et al. 2015). A better grasp on ocean internal variability should thus help characterizing the anthropogenic carbon and heat uptake in the Southern Ocean from climate models.

Mechanisms for the Southern Ocean dominance

The important role of the Southern Ocean in the global uptake of anthropogenic carbon and heat is due to its unique circulation. To maintain a high rate of oceanic uptake, ancient deep waters that are cold and uncontaminated with carbon from anthropogenic emissions need to be continuously exposed to the

relatively warmer and carbon-richer atmosphere. Once anthropogenic carbon and heat have been absorbed, these waters must then be efficiently isolated from the atmosphere. In the Southern Ocean, these conditions are met through several mechanisms (see Figure 2). The vigorous wind-driven overturning circulation brings ancient deep waters to the surface at the Antarctic Divergence ($\sim 60^{\circ}\text{S}$; e.g., Marshall and Speer 2012; Morrison et al. 2015b). Once at the surface, these waters absorb large amounts of anthropogenic carbon and heat while being transported across the intense fronts of the Antarctic Circumpolar Current by the northward Ekman transport (e.g., Dufour et al. 2015). The subduction eventually transfers these waters into the ocean interior through the deep winter mixed layers that form around 45°S . In models, regions of strongest anthropogenic heat and carbon uptake in the Southern

Ocean are generally found within two latitudinal bands around 60°S and 45°S (Figure 1c-d) suggesting that the locations of deep water upwelling and deep winter mixed layers dominate the pattern of uptake.

This chain of mechanisms reflects the traditional zonal-mean view of the Southern Ocean circulation that has gained wide acceptance over the past two decades. However, this paradigm has been recently questioned by studies that highlight important zonal asymmetries in the circulation (e.g., Tamsitt et al. 2015; Talley 2013; Sallée et al. 2010), impacting the pattern of uptake and subduction of anthropogenic carbon and heat. Namely, patterns of anthropogenic heat and carbon uptake

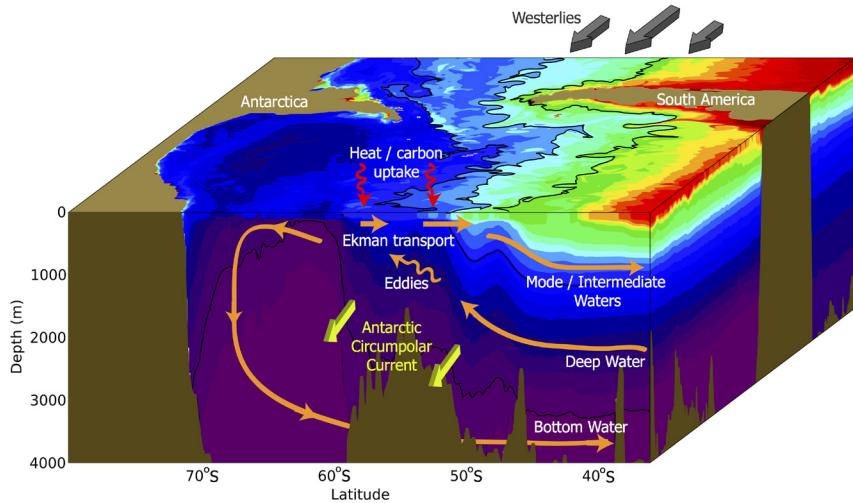


Figure 2. Schematic of the Southern Ocean circulation. A vigorous upwelling driven by powerful Westerlies brings ancient deep water that is relatively cold and rich in carbon to the ocean's surface in a region called the Antarctic Divergence. Once at the surface, much of this water is transported to the north by an intense Ekman transport across the eastward Antarctic Circumpolar Current (ACC). En route to the north, the water takes up large amounts of anthropogenic carbon and heat. At the northern boundary of the ACC, the water is subducted into the ocean interior, thus transferring anthropogenic carbon and heat to the deep ocean. Mesoscale eddies oppose the wind-driven circulation at the surface and below topographic ridges (i.e., oppose the northward Ekman flow and southward geostrophic flow, respectively) and form the main driver of the upwelling of deep waters above topographic ridges. Due to the difficulty in measuring the eddy effects in observations and in resolving them in models, the magnitude and pattern of the eddy-induced transport is still under debate, as is their resulting effect on the anthropogenic carbon and heat uptake. Adapted from Morrison et al. (2015b).

show spatial structure both at the inter- and intra-basin scale, with the heat uptake being much more localized than the carbon uptake (Figure 1c-d). Sallée et al. (2012) also demonstrated that subduction of anthropogenic carbon is occurring in specific locations corresponding to formation regions of SubAntarctic Mode and Antarctic Intermediate waters. These studies explore how the complex interplay between ocean and atmosphere circulation and their interactions with continents and topography sets the inter-basin differences.

Upwelling, Ekman transport, and subduction are known to be key drivers in the uptake of anthropogenic carbon and heat in the Southern Ocean (e.g., Russell et al.

2006; Mignone et al. 2006), but additional processes, like mesoscale eddies, may also play a role in regulating the uptake. Over the last decade, many studies have highlighted the importance of mesoscale eddies in the Southern Ocean circulation (e.g., Hallberg and Gnanadesikan 2006). Transport induced by eddies opposes the wind-driven circulation (Figure 2), thus reducing the rate at which deep waters are exposed to the surface (e.g., Dufour et al. 2012; Morrison and Hogg 2013). Eddies also restratify the upper ocean, reducing the subduction of light waters (Lachkar et al. 2009). Mesoscale eddy processes are thus expected to cause a reduction of Southern Ocean carbon uptake due to anthropogenic emissions. Consistent with this, models show that as mesoscale eddies are better resolved, the Southern Ocean anthropogenic carbon uptake decreases (Lachkar et al. 2007).

Contemporary trends and projected changes

Despite current limitations, models and observations have been used extensively to estimate the trends in anthropogenic heat and carbon uptake over recent decades and to project uptake over the next century. One of the key questions that needs to be addressed is whether the oceanic sink of anthropogenic carbon and heat has kept pace with atmospheric increases and how this will evolve in the future.

In the Southern Ocean, observation-based estimates and models suggest a weakening in the rate of the total carbon uptake from the 1980s to 2000s (Figure 3; e.g., Le Quéré et al. 2007; Lovenduski et al. 2007). This weakening is attributed to

the intensification of westerly winds associated with positive phases of the Southern Annular Mode, which strengthens upwelling and thus brings old waters rich in carbon to the surface at a higher rate. This exposure of carbon-rich waters results in enhanced outgassing of carbon, provided that the biological pump only partially compensates the physical pump. This enhanced outgassing opposes the increasing uptake of carbon from anthropogenic emissions, hence reducing the rate of uptake of total carbon. Recent studies postulate that the rate of uptake has been reinvigorated since 2002 (Figure 3; Fay et al. 2014) possibly due to changes in the atmospheric pressure systems (Landschützer et al. 2015). The magnitude of the trend in uptake is, however, highly uncertain since it is very sensitive to the method used (Fay et al. 2014). Moreover, a robust detection of the trend in carbon uptake would require roughly two decades of continuous monthly observations with 200 biogeochemical profiling floats (Majkut et al. 2014) because of the high temporal variability (Lovenduski et al. 2015). The trend in heat uptake is even harder to

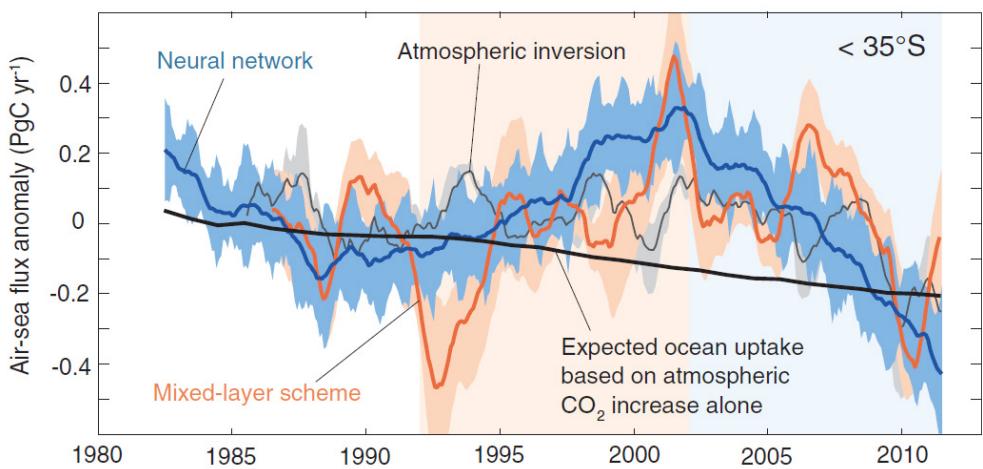


Figure 3. Evolution of total air-sea CO_2 flux integrated south of 35°S and computed as an anomaly relative to the 1980s. Negative values indicate anomalous uptake by the ocean. The flux is computed from (blue) a two-step neural network technique, (orange) a mixed-layer scheme, and (gray) an atmospheric inversion based on measurements of atmospheric CO_2 . The thick black line corresponds to the expected uptake based on the growth of atmospheric CO_2 alone. Observation-based estimates show that the rate of the total carbon uptake weakened from the 1980s to 2000s but has strengthened since 2002. From Landschützer et al. (2015). Reprinted with permission from AAAS. See Landschützer et al. (2015) for more details on the methods and associated references.

estimate, with various products strongly disagreeing on the strength and pattern of the net climatological heat flux.

Over recent decades, the Southern Ocean has been experiencing significant changes that are expected to persist over the 21st century. Among those changes are increases in air temperature, precipitation, and glacial melting that strengthen the stratification of the upper ocean, and an intensification of westerly winds that strengthens the wind-driven circulation. These changes drive competing effects on anthropogenic carbon and heat uptake (e.g., Sarmiento et al. 1998, Matear and Lenton 2008), but the net effect remains unclear. Increased stratification would reduce both the flux of old waters to the surface and the subduction of newly formed waters into the ocean interior. On the other hand, increased wind-driven circulation would enhance the flux of old waters to the surface hence opposing the effect of increased stratification on carbon (e.g., Lovenduski and Ito 2009). Increased stratification and wind-driven circulation also tend to produce opposite effects on the biological drawdown of surface carbon as they both control the supply of nutrients to the surface (Matear and Lenton 2008, Hauck et al. 2015). However, to date, the anthropogenic carbon uptake does not seem to be strongly affected by the change in circulation; rather it is primarily driven by the surface flux change due to the increase in atmospheric carbon concentration (Frölicher et al. 2015). In contrast, changes in ocean circulation increase the efficacy of the ocean in taking up heat by shifting locations of the heat uptake to high-latitudes where the air-sea temperature contrast is greater (Winton et al. 2013).

Perspectives and challenges

In the past decade, we entered a new era of observations of the Southern Ocean, which will help reduce uncertainties in heat and carbon uptake and better constrain simulations. The use of autonomous profiling floats has

dramatically increased the number of temperature and salinity observations in the Southern Ocean since 2000 (Argo program, <http://www.argo.ucsd.edu/>). Substantially more biogeochemical observations are on the horizon with the release over the next five years of roughly 200 Argo-equivalent floats equipped with oxygen, nitrate, and pH sensors (SOCCOM, <http://soccom.princeton.edu/>). Efforts are underway to extend the Argo array to the deep ocean below 2000 m (Johnson et al. 2015), which will provide better constraints on heat storage and abyssal circulation and, in turn, on heat and carbon uptake. On the modeling side, recent development of high-resolution climate models that are able to resolve a large portion of the ocean mesoscale eddy spectrum allows us to investigate the impact of eddies on heat and carbon uptake (e.g., Griffies et al. 2015).

Opportunities arising from new data and tools will hopefully enable the scientific community to tackle the numerous challenges that come with estimating contemporary and predicting future heat and carbon uptake in the Southern Ocean. Overall, the biggest challenges remain the improvement of data coverage and the representation of physical processes in models (Heinze et al. 2015).

Acknowledgments

C. O. Dufour and I. Frenger are supported by NASA under award NNX14AL40G. A. R. Gray is supported by NOAA through a Climate and Global Change Postdoctoral Fellowship. A. K. Morrison is supported by DOE under award DE-SC0012457. J. L. Sarmiento is supported by the Southern Ocean Carbon and Climate Observations and Modeling (SOCCOM) project under NSF award PLR-1425989. T. L. Frölicher acknowledges financial support from the Swiss National Science Foundation (Ambizione grant PZ00P2_142573).

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Estimating Southern Ocean air-sea fluxes from models and observations

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Air-sea fluxes determine the transfer of heat, momentum, and gas between the atmosphere and the ocean, and the Southern Ocean is at the nexus of these exchanges. Winds are critical to air-sea exchanges, and the Southern Ocean experiences some of the strongest winds in the world. Water within the oceanic mixed layer readily comes into contact with the atmosphere, and the low stratification of the Southern Ocean gives it some of the deepest mixed layers found anywhere, often extending to several hundred meters in depth (e.g., Dong et al. 2008). And cold water holds higher quantities of dissolved gas, meaning that the Southern Ocean has the potential to take up large quantities of CO₂ or O₂ from the atmosphere. Despite the central role of the Southern Ocean in the climate system, quantifying air-sea fluxes with an accuracy that is meaningful for climate studies has proved challenging.

The goal of this article is not only to highlight the main sources of uncertainties in current flux estimates but also to show what information we can learn from existing flux products for the open ocean regions of the Southern

Ocean.¹ Our focus is on heat fluxes and, to a lesser extent, freshwater and gas fluxes, all of which are less well defined than momentum fluxes and arguably more critical to understanding long-term climate processes.

Consider, for example, the challenges in determining Southern Ocean air-sea heat fluxes. The Southern Ocean is the most rapidly warming sector of the global ocean, as evidenced in Argo profiling float data from the last decade (Roemmich et al. 2015). Comparisons between historic data and modern Argo observations suggest that this warming has been persistent since early in the 20th century (e.g., Böning et al. 2008; Gille 2008). Regions of the ocean can warm either because of horizontal advection of heat within the ocean or because of air-sea exchange, but growing evidence suggests that air-sea fluxes are likely to be a major player in the net increases in ocean heat content (Fyfe and Swart, personal communication). Existing data are too sparse to distinguish these processes

¹ We do not consider marginal ice zones, which introduce additional physical processes.

with any real confidence. Although warming patterns extend through the water column in the Southern Ocean (e.g., Purkey and Johnson 2010), warming trends are nonetheless surface-intensified and could be explained by a net heat input to the Southern Ocean of about 0.6 W m^{-2} , roughly consistent with estimates of the global ocean energy imbalance (e.g., Abraham et al. 2013). This net heat input to the ocean sets an air-sea flux accuracy requirement that is more than an order of magnitude smaller than what we can achieve with current observational capabilities.

Challenges of measuring and modeling air-sea fluxes

Surface fluxes are difficult to measure, because they are associated with the time derivatives of upper-ocean heat content, upper-ocean kinetic energy, or upper-ocean dissolved gas concentrations. Since derivatives are inherently noisier than their time integrals, fluxes are inherently plagued by large statistical uncertainties.

In situ observation of high-latitude air-sea fluxes has proved particularly difficult for a number of reasons (e.g., Bourassa et al. 2013). The Southern Ocean is remote, with high winds, high sea states, and icing conditions. The environment makes mooring deployment difficult and leads to logistical challenges for ship and aircraft operations. Air-sea fluxes are typically computed from bulk formulae. In high-wind conditions with evolving wave conditions, even when basic meteorological variables are measured, the direct flux covariance measurements that would be needed to calibrate bulk formulae are not readily available. However, there is some promise for the future as a result of recent technological developments.

These developments include wave gliders, unmanned aerial vehicles, the deployment of flux moorings in the Southern Ocean, and new concepts for obtaining high quality ship measurements, along with evolving algorithms for retrieving air-sea flux-related parameters from satellite observations and advances toward coupled data assimilation.

Model-based assessment of air-sea fluxes has also proved difficult. In Figure 1, we show the time-mean differences between three air-sea heat flux products

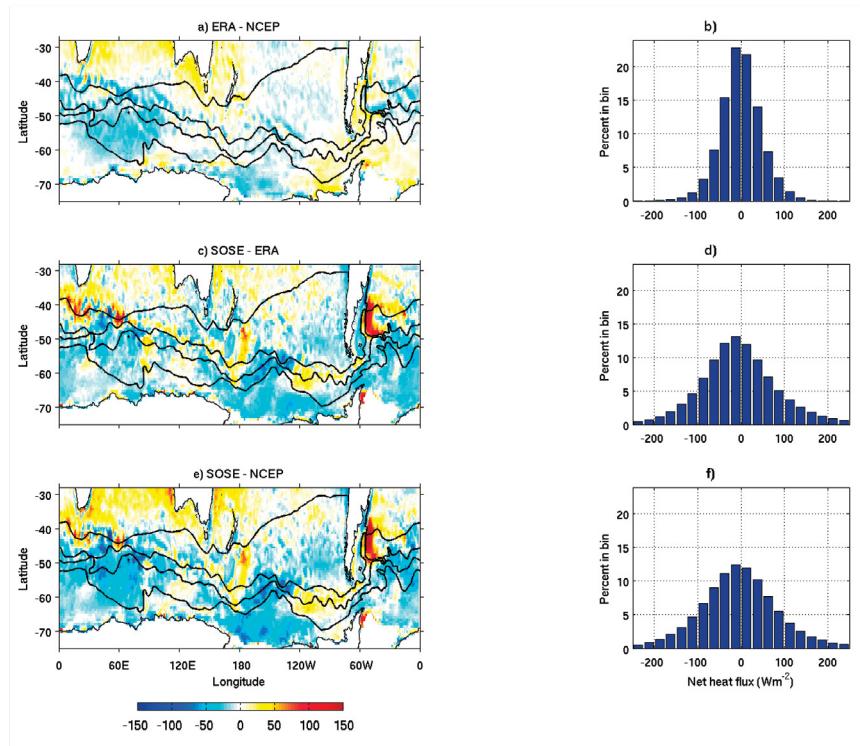


Figure 1. The difference between daily estimates of net air-sea heat flux (W m^{-2}), time averaged over years 2005 – 2010, considering only ice-free time periods, obtained from: (a) ERA-Interim (ERA) reanalysis minus NCEP-NCAR Research Reanalysis 1 (NCEP), (c) the Southern Ocean State Estimate (SOSE) from SOSE iteration 100 minus ERA and (e) the SOSE minus NCEP. Positive values indicate more ocean heat loss (less ocean heat gain) by the first product relative to the second. Right-column panels show corresponding normalized histogram of daily net air-sea heat flux differences (W m^{-2}). All flux estimates have been interpolated on ERA grid. The differences are in 25 W m^{-2} wide bins, normalized to show percent of the net air-sea heat differences in each bin, where the sum over all the bins is 100%. They thus indicate the probability that the net air-sea heat difference will be in the range $12 \pm 12.5 \text{ W m}^{-2}$. Averaged over the Southern Ocean domain shown in the figure, mean differences are: SOSE – ERA $-3.4 \pm 96.2 \text{ W m}^{-2}$; SOSE – NCEP $-4.1 \pm 97.7 \text{ W m}^{-2}$; and ERA-NCEP $-0.6 \pm 48.1 \text{ W m}^{-2}$. The black contours in panels a, c, e show the climatological positions of the fronts given by Orsi et al. (1995), from north to south: Subtropical Front, Subantarctic Front, Polar Front, and Southern ACC Front.

over the six-year interval from 2005 to 2010. Two flux products are derived from numerical weather prediction atmospheric reanalyses that are produced by the European Centre for Medium-Range Weather Forecasts Reanalysis (ERA-Interim) and by the National Center for Environmental Prediction (NCEP). The third comes from iteration 100 of the Southern Ocean State Estimate (SOSE, available from sose.ucsd.edu), which is an oceanic counterpart to the atmospheric reanalyses. SOSE uses a 4-dimensional variational assimilation approach, analogous to the methods used for numerical weather prediction and atmospheric reanalysis, and it determines air-sea fluxes that are most consistent with the constraints imposed by available ocean observations and ocean dynamics (Mazloff et al. 2010). In their time means, the three sets of fluxes differ substantially, with large-scale offsets visible in Figure 1. The atmospheric reanalyses differ from each other and SOSE shows significant departures from the atmospheric reanalyses, particularly in the Agulhas Retroflection region south of Africa, in the Brazil-Malvinas Confluence region to the east of South America, and in the region extending from Campbell Plateau south of New Zealand to the Eltanin-Udintsev Fracture Zones in the central Pacific. The standard deviations of the differences (Figure 2) are also pronounced in the same three regions, all of which are marked by strong topographically influenced oceanic currents with topographically generated eddy energy. In contrast to the differences illustrated in Figures 1 and 2, the amplitude and phasing of their annual cycles largely agree, as illustrated in Figure 3.

The differences suggest two major challenges to determining fluxes: one challenge is properly calibrating large-scale local mean air-sea fluxes (e.g., minimizing the

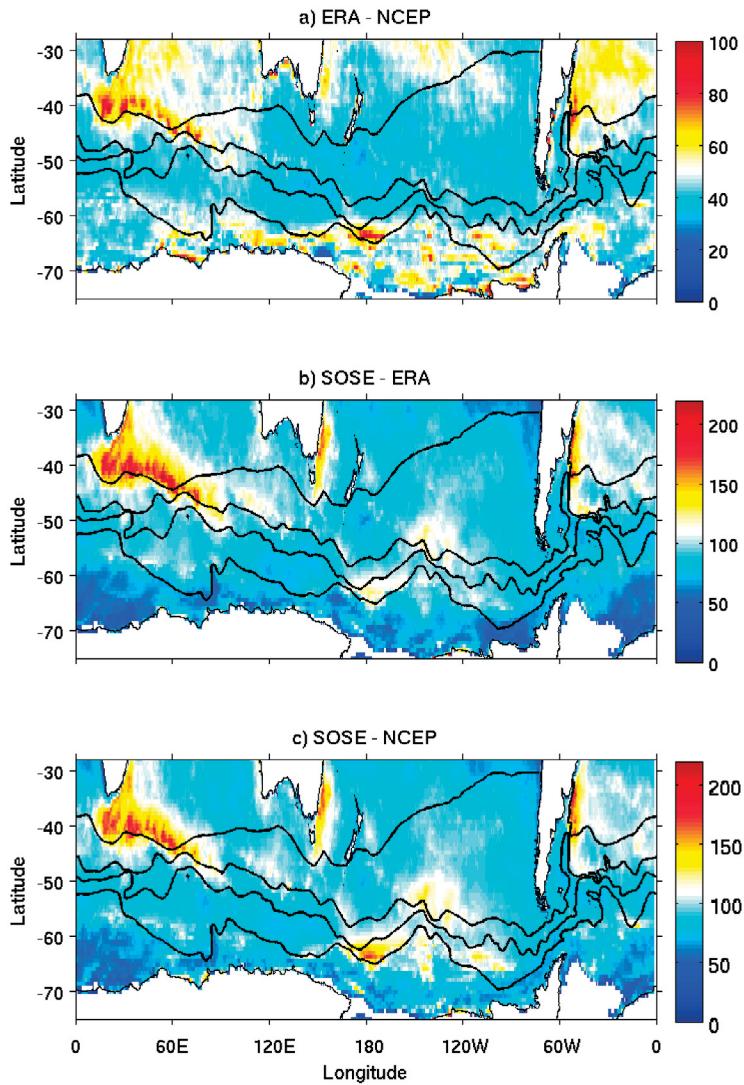


Figure 2. As in Figure 1 a, c, e, except for the standard deviation.

large-scale patterns in Figure 1), and the second challenge is understanding the detailed physics that governs air-sea fluxes at mesoscale gradients associated with eddies and fronts (e.g., the frontal or eddy-scale differences in Figure 2).

Ongoing and future efforts

Despite inaccuracies in flux estimates, they nevertheless provide valuable information about the specific processes that drive air-sea exchange and show the physics that modulate seasonal to interannual variations in exchanges between the ocean and atmosphere. Flux

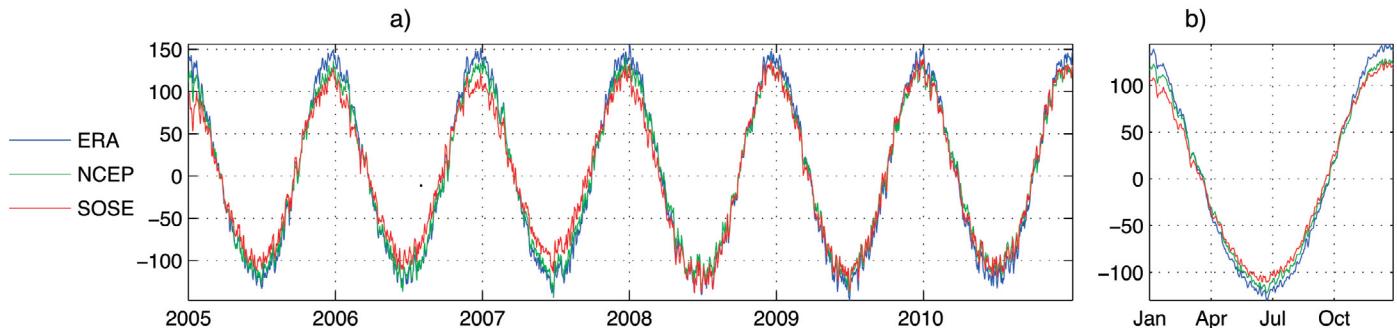


Figure 3. (a) Time series of net air-sea heat flux for the latitude range 30°-60°S, with area and time means removed. This domain is chosen to avoid the marginal ice zones close to Antarctica and the SOSE northern boundary. (b) Net air-sea heat flux climatology obtained from time series shown in panel (a). The time-mean RMS differences are 7.8 W m⁻² for the ERA-NCEP difference, 6.7 W m⁻² for the SOSE-NCEP difference, and 13.3 W m⁻² for the SOSE-ERA difference.

estimates enable us to evaluate how water properties are transformed at the ocean surface, for example to form SubAntarctic Mode Water. Upper ocean budgets for heat and freshwater are determined by surface fluxes, working in tandem with diapycnal mixing, advection, and storage (Cerovečki and Mazloff 2015). Close analysis of air-sea heat fluxes suggests that in the time mean, net air-sea fluxes into the ocean are balanced by advection. In SOSE, on seasonal scales, the Indian and Atlantic Oceans appear to be governed by Ekman divergence, while the Pacific Ocean heat fluxes are balanced both by Ekman divergence and geostrophic advection (Tamsitt et al. 2015). Reduced uncertainties in surface flux estimates would allow us to refine our evaluations of upper-ocean water mass transformation processes.

A September 2015 workshop entitled “[Air-Sea Fluxes for the Southern Ocean: Strategies and Requirements for Detecting Physical and Biogeochemical Exchanges](#)” revisited the challenges associated with improving Southern Ocean air-sea fluxes. Participants identified a number of impediments to progress. Not only are air-sea fluxes difficult to measure, but they are also not currently part of the coordinated observing system, in part because the difficulty in measuring them has prevented them from being classified as Essential Climate Variables.

While Southern Ocean flux observations have historically been nearly non-existent, there are good prospects for improvements in the future. As an outcome of the September 2015 workshop, a Southern Ocean Observing System (SOOS) Capability Working Group on Southern Ocean air-sea fluxes is being established. The priorities have been fine-tuned with input from the earlier US CLIVAR High-Latitude Surface Flux and the US CLIVAR/OCB Southern Ocean Working Groups. The SOOS Capability Working Group envisions a two-pronged effort that will develop a pilot project to move towards a Southern Ocean air-sea flux observing system and at the same time to evaluate the feasibility of defining fluxes or flux-related variables as Essential Climate Variables. While we do not expect to measure fluxes with sufficient accuracy to close the upper ocean heat budgets at the 0.6 W m⁻² level, nor do we expect equivalent levels of accuracy for CO₂ fluxes, we do think that we can unravel the processes that contribute to spatial and temporal variations in air-sea fluxes of heat, as well as freshwater, gas, and momentum.

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Observed and projected trends in Antarctic sea ice

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Antarctic sea ice extent has increased over the ~36-year satellite record, in striking contrast to the observed decline of the Arctic sea ice cover over this period (e.g., Parkinson and Cavalieri 2012). Concurrent with Antarctic sea ice expansion has been an overall cooling of the Southern Ocean surface. These trends may seem at odds with greenhouse gas-induced warming over recent decades and, disconcertingly, are not reproduced by the historical simulations of comprehensive global climate models (e.g., Turner et al. 2013; Hobbs et al. 2015). Here,

we review the recent progress toward understanding the response of the Southern Ocean to climate forcing, and argue that the community's results are converging on a solution to the apparent conundrum of Antarctic sea ice expansion. We propose that while a variety of different factors may have contributed to Southern Ocean changes over recent decades, it is large-scale atmospheric circulation changes—and the changes in ocean circulation they induce—that have emerged as the most likely cause of the observed Antarctic sea ice trends.

Observations of recent Southern Ocean change

Before we delve into the possible mechanisms driving recent Southern Ocean changes, we want to describe the observations in more detail to establish a baseline that any such mechanisms must explain. Figure 1 shows sea ice concentration and sea-surface temperature (SST) trends over the era of continuous satellite observations (1979-present). While both fields show regions of increasing and decreasing trends over this period, the total sea ice extent has increased, and SSTs have largely cooled, south of the Antarctic Circumpolar Current (ACC). Notable exceptions are the regions of decreasing sea ice concentration in the Amundsen and Bellingshausen Seas, which overlie increasing SSTs—though we note that the sign of the trends in these regions has changed after about year 2000 (not shown). Although the patterns of trends in sea ice concentration and SST vary with season, the association between sea ice and SST generally prevails in every season and region (we show only the annual means here for brevity and because the signal to noise is greater than in the seasonal means). Further, we see that the spatial patterns of sea ice trends are closely mirrored by trends in SSTs that extend beyond the sea ice edge over a much larger area of the ocean—typically out to the southern flank of the ACC.

Taking a cue from Fan et al. (2014), we see that this tight relationship between total sea ice extent and Southern Ocean SSTs (south of 50°S, the approximate latitude of the ACC) appears to hold over a much longer observational period as well (Figure 2). The sea ice cover in September of 1964 (recently recovered from the Nimbus I satellite by Meier et al. 2013) was more expansive than at any

time since the start of the continuous record from passive microwave satellites—consistent with Southern Ocean SSTs that were at or near their coldest levels. In the early 1970s, an early microwave satellite and the Navy-NOAA ice charts indicated the sea ice was in between the extent in 1964 and post 1979 (see e.g., Kukla and Gavin 198; Zwally et al. 1983). Overall, the Southern Ocean has warmed slowly (by ~0.02 per decade south of 50°S) relative to the global ocean (~0.08 per decade) since 1950. The spatial

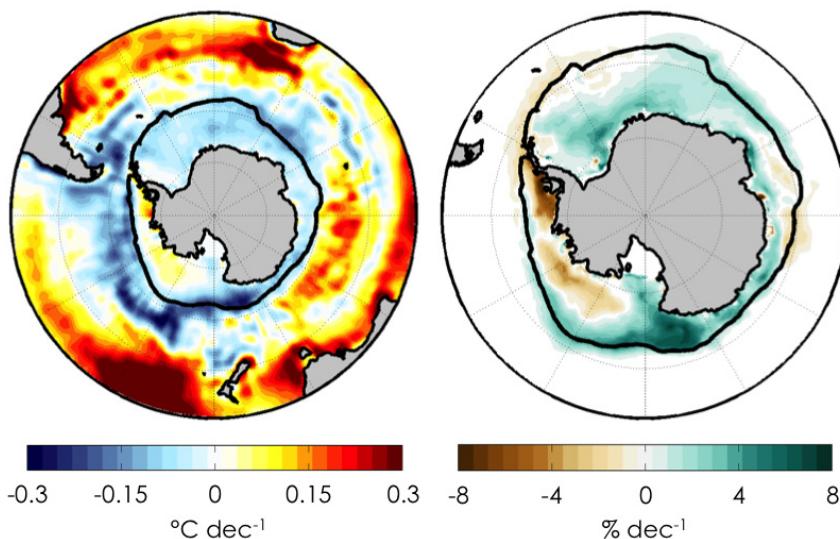


Figure 1. Linear trends of annual-mean SST (left) and annual-mean sea ice concentration (right) over 1980-2014. Sea-surface temperature is from NOAA's Optimum Interpolation Sea Surface Temperature dataset (version 2; Reynolds et al. 2002). Sea ice concentration is from passive microwave observations using the NASA Team algorithm (https://nsidc.org/data/seacie_index/archives.html).

and temporal relationships in Figures 1 and 2 imply that Antarctic sea ice trends should be viewed in the broader context of trends over the whole of the Southern Ocean, and that trends in sea ice and SSTs likely share some common driving mechanisms. That is, a key constraint on any mechanism proposed to drive the observed Southern Ocean changes is that it must allow for both the characteristics of sea ice trends and the coincident patterns of large-scale SST trends, simultaneously.

In light of the above observations, we organize the rest of our discussion around several guiding questions, which we see as relating to distinct physical mechanisms that have, together, acted to produce the observed Southern Ocean trends.

Mechanisms of delayed Southern Ocean warming

Why has the Southern Ocean been so slow to warm over the 20th century (Figure 2), relative to the global ocean and the Arctic? Recent work suggests that the primary cause of delayed surface warming is the mean divergence of seawater at the Southern Ocean surface, which is then refreshed (or buffered) by the upwelling of unmodified water from depth (Marshall et al. 2014a,b; Armour et al. submitted); hence the majority of heat taken up at the Southern Ocean surface is diverged with the mean circulation to the north, and, to a lesser extent, downward along the Antarctic continental shelf. A secondary source of delayed warming is reduced surface buoyancy loss owing to a combination of increased downward heat flux, increased precipitation minus evaporation, and reduced sea ice growth near Antarctica—each acting to increase upper ocean stratification and inhibit convection and vertical mixing, in turn reducing the upward flux of heat from warmer waters at depth (Manabe et al. 1991; Russell and Rind 1999; Gregory 2000; Kirkman and Bitz 2011).

Global climate models (GCMs) robustly simulate much slower warming and less sea ice loss over the Southern Ocean than in the Arctic under global warming (e.g., Manabe et al. 1991; Stouffer 2004; Kirkman and Bitz 2011; Li et al. 2012; Marshall et al. 2014a,b). Within GCM

simulations, delayed warming of the Southern Ocean surface is seen to be a fundamental response of the ocean to anomalous surface heat and freshwater fluxes induced by greenhouse forcing. We argue that because this response is broadly consistent with observations (Armour et al. submitted), climate models seem to be adequately representing the above mechanisms of delayed Southern Ocean warming. Importantly, it is against this background of very gradual warming—rather than the rapid warming seen in the Arctic—that the mechanisms of Southern Ocean surface cooling and sea ice expansion must be understood and evaluated.

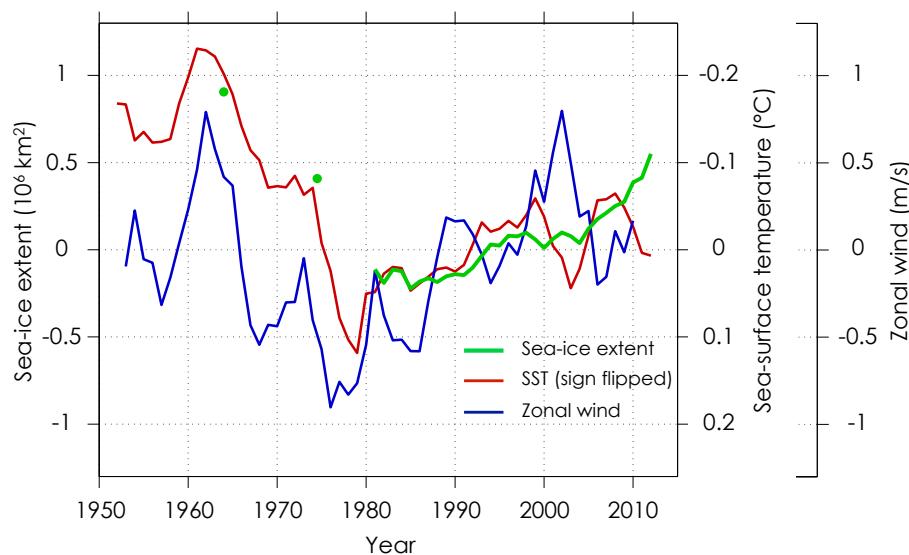


Figure 2. Time-series of anomalies in the total annual-mean Antarctic sea ice extent, annual-mean Southern Ocean SST (averaged south of 50°S), and DJF (December-January-February) zonal-mean zonal wind over 50-70°S. The sea ice extent in 1964 is the September 1964 anomaly from the Nimbus 1 satellite (Meier et al. 2013). The sea ice extent in 1974 is an average of 1973-1976 from the electrically scanning microwave radiometer (https://nsidc.org/data/smmr_ssmi_ancillary/area_extent.html) and the Navy-NOAA Joint Ice Charts (Ropelewski, 1983). The sea ice extent from 1979 and onward is from passive microwave observations using the NASA Team algorithm (https://nsidc.org/data/seoice_index/archives.html); SST is from NOAA's Extended Reconstruction Sea-Surface Temperature dataset (version 3b; Smith et al. 2008); and zonal wind data was provided by D. Schneider from the study of Fan et al. (2014). All anomalies are taken with respect to their 1980-2010 means.

Mechanisms of Southern Ocean surface cooling and sea ice expansion

What has driven the apparent variation in Southern Ocean conditions about this gradual warming trend (Figure 2), and what has driven the recent period of surface cooling and sea ice expansion (Figure 1) in particular? One possible cause of sea ice expansion is increased freshwater input to the ocean from Antarctic ice loss (Bintanja et al. 2013)—primarily from basal melt of ice shelves—which could act to cool the sea surface via increased stratification and decreased deep ocean convection as described above. However, Pauling et al. (submitted) point out that best estimates of the current mass imbalance of Antarctica's ice sheet and shelves is at most about one-fifth the magnitude of the present-day anomaly in precipitation minus evaporation south of 50°S, relative to preindustrial, as simulated by climate models. Indeed, Liu and Curry (2010) argue that this increase in precipitation is responsible for sea ice expansion, but the question remains as to why climate models do not reproduce the observations given that they do robustly simulate increased precipitation over the Southern Ocean.

Moreover, both Swart and Fyfe (2013) and Pauling et al. (submitted) find that enhanced freshwater input to the Southern Ocean does not cause significant sea ice expansion within their simulations—even when the magnitude of freshwater flux far exceeds that applied by Bintanja et al. (2013). One important factor in the sea ice response to freshwater forcing may be the degree to which the Southern Ocean is deeply convecting. Based on the findings of Swart and Fyfe (2013) and Pauling et al. (submitted), we speculate that models that show little deep Southern Ocean convection over recent decades—consistent with observations (e.g., de Lavergne et al. 2014)—would also show little sensitivity to increased freshwater input from Antarctica. Altogether, these studies suggest that freshwater forcing is not the primary cause of the observed sea ice expansion.

Perhaps the most substantial Southern Hemispheric climate signal has been the strengthening and poleward

shift of westerly winds since the late 1970s (Figure 2). This trend—often characterized as a strengthening of the Southern Annular Mode (SAM)—is thought to be primarily driven by stratospheric ozone depletion (Polvani et al. 2011a), but may also reflect natural variability (Deser et al. 2012; Thomas et al. 2015). As noted by Thompson et al. (2011), the observed correlation between SAM and SSTs on interannual timescales—wherein a strongly positive SAM is correlated with Southern Ocean surface cooling—suggests that the trend in SAM may be responsible for the observed SST and sea ice trends.

Yet, GCMs have thus far been unable to reproduce this proposed connection—perhaps, in part, due to the fact that their historical westerly wind trends are typically too weak, lack the correct seasonality, or lack the correct spatial patterns compared to the observed (Swart and Fyfe 2012; Haumann et al. 2014). This discrepancy between observed and simulated wind trends is plausibly due to a combination of (i) errors in the prescribed (or simulated) magnitude, spatial pattern (Waugh et al. 2009), or temporal resolution (Neely et al. 2014) of stratospheric ozone depletion and (ii) natural variability in SAM (Deser et al. 2012; Thomas et al. 2015).

Further complicating matters, climate models tend to show *enhanced* Southern Ocean surface warming and sea ice loss in response to ozone depletion (Sigmond and Fyfe 2010; Bitz and Polvani 2012; Smith et al. 2012; Sigmond and Fyfe 2014; Haumann et al. 2014). Clarification on this front can be gleaned from the results of Ferreira et al. (2015), who showed that two opposing sea ice trends should be expected in response to a strengthening of westerly winds: the immediate response is enhanced Ekman advection of surface waters, which transports colder waters northward and drives surface cooling south of the ACC; the longer-term response is upwelling of relative warm waters to the surface from depth, induced by anomalous wind-driven divergence of surface waters south of the maximum wind anomaly, as shown in Figure 3. Thus, while the initial response to a strengthening of westerly winds is that of surface cooling and sea ice expansion, the long-term response is that of surface warming and sea ice loss.

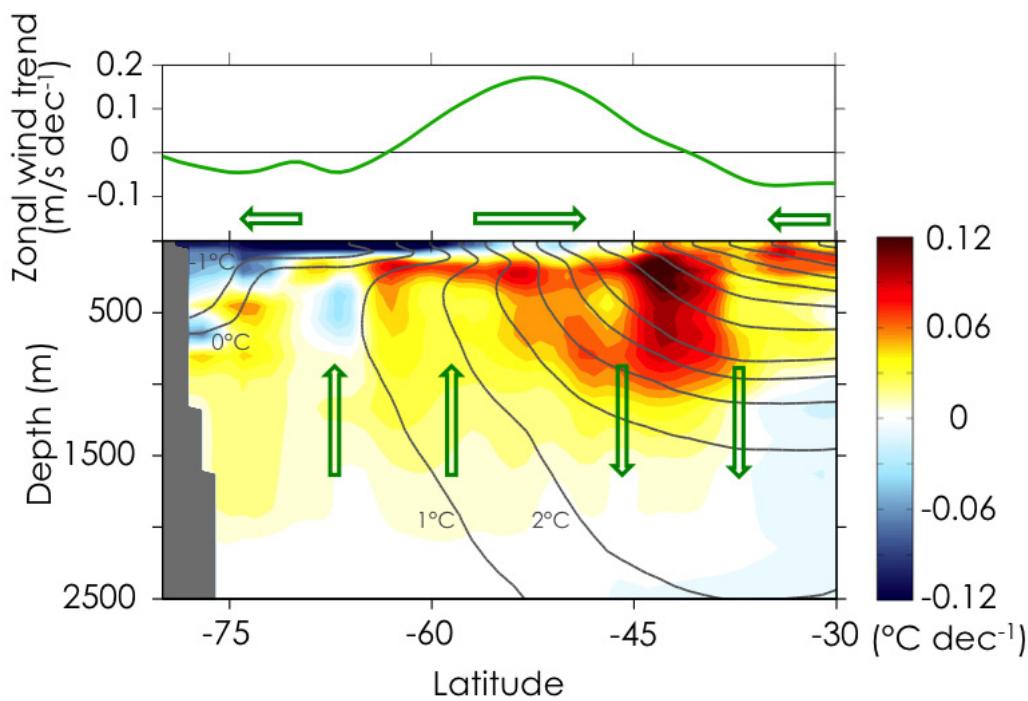


Figure 3. Trends in annual, zonal-mean ocean potential temperature and zonal-mean zonal winds over 1980-2014. Black lines are contours of the climatological zonal-mean mean ocean temperature averaged over 1980-2014. Green arrows are a schematic representation of the approximate ocean circulation that has been induced by the westerly wind trends. Generally the ocean temperature trends can be linked to anomalous advection of the ocean mean state temperature by these anomalous currents. The wind trends have driven anomalous northward surface currents that transport relatively cold waters to the north, driving surface cooling south of $\sim 45^{\circ}\text{S}$. The wind trends have further driven anomalous divergence at the ocean surface, and hence anomalous upwelling, south of $\sim 55^{\circ}\text{S}$; over much of this region, ocean temperature increases with depth, so this amounts to enhanced upwelling of relatively warm waters. North of about $\sim 55^{\circ}\text{S}$, the winds have driven anomalous convergence, and the subsurface flow appears to be that of enhanced subduction. The annual and zonal-mean winds trends are from ERA-Interim (Dee et al. 2011).

The timescale at which the upper ocean transitions from the fast surface cooling to the eventual warming in response to westerly wind forcing is of critical importance to sea ice trends (Marshall et al. 2014b). Yet, it differed markedly between the two models analyzed in Ferreira et al. (2015), with the comprehensive climate model in their study transitioning over just a few years, and the more idealized model transitioning over decades. The timescale appears to be largely set by the climatological meridional temperature gradient at the ocean surface, which governs the magnitude of the initial cooling, and by

the temperature gradient between the sea surface and deep ocean, which governs the rate of slow warming (Ferreira et al. 2015).

It is not known what the Southern Ocean response to westerly wind trends should be, but following Fan et al. (2014) we can look to the observations since 1950 as a guide (Figure 2). As noted above, Southern Ocean SSTs have decreased concurrently with an increase in zonal-mean westerly winds since ~ 1980 . While the wind data are sparse (see Fan et al. 2014), the time-series of zonal-mean wind shows an intriguingly strong *decrease* in strength from about 1950 to 1980, concurrent with a significant increase in SSTs and decrease in sea ice extent from 1964 to the beginning of the satellite era. We view

these observations as strong evidence that the observed trends in Southern Ocean sea ice and SSTs since 1950 have been primarily driven by changes in atmospheric circulation.

These results further lead us to speculate that it may be biases in the ocean components of comprehensive climate models that are the main reason they exhibit Southern Ocean warming and sea ice loss in response to ozone depletion, which is at odds with the observed trends over recent decades. We suggest that a strong

test of this mechanism would thus be the simulation of stratospheric ozone depletion within those climate models that accurately simulate the observed Southern Ocean mean state (i.e., the climatological temperature gradients in Figure 3).

Another suggestion is that the recent sea ice expansion can be explained by natural variability alone, based on GCM simulations (Polvani and Smith 2013; Zunz et al. 2013; Mahlstein et al. 2013). Yet, much of the natural variability of Southern Ocean sea ice extent in models is driven by changes in the strength of deep ocean convection (e.g., Latif et al. 2013). While variability in deep ocean convection is an intriguing mechanism for sea ice expansion, it seems inconsistent with the observations, which do not appear to reflect such changes over the satellite era. However, the possibility remains that natural variability has contributed substantial westerly wind trends over recent decades (Deser et al. 2012; Thomas et al. 2015) and, in turn, to sea ice expansion.

Mechanisms driving the observed local-scale patterns of sea ice change

What has driven the local-scale patterns of sea ice and SST trends over the satellite era? Holland and Kwok (2012) argue that winds, especially the meridional component, are the principle cause of regional sea ice trends, and that changes in sea ice advection have been a dominant factor in driving the apparent sea ice loss around West Antarctica. Trends in surface winds over the Southern Ocean also impact ocean waves, and an overall decrease in wave heights has been related to a reduction in the breakup of sea ice (Kohout et al. 2014). While local-scale wind and wave forcings appear to be factors in driving the observed pattern of sea ice trends, it is less clear how changes in sea ice motion and breakup can cause concurrent trends in SSTs. One possibility is that sea ice trends are able to modify SSTs through sea ice-ocean feedbacks (Goosse and Zunz 2014). However, such mechanisms do not account for the concurrent trends in Southern Ocean SSTs that extend far beyond the sea ice edge (Figure 1). We thus view these wind and wave height changes as the proximate causes of local-scale patterns

of sea ice change, as opposed to fundamental drivers of sea ice and SST trends over the whole of the Southern Ocean.

Recent changes in atmospheric circulation patterns, and hence winds, over the Southern Ocean have been linked to teleconnections via atmospheric Rossby waves emanating from the tropical Pacific and/or Atlantic (e.g., Ding et al. 2011; Li et al. 2014; Simpkins et al. 2014; Schneider et al. 2015). Many have attributed patterns of warming and cooling in the tropics to natural variability, so perhaps we should not expect GCMs to reproduce the observed patterns of local-scale wind changes over the last few decades. Moreover, even if a simulation should randomly exhibit reasonable tropical variability, the teleconnections to the Antarctic may be poor if the location or strength of the atmospheric subtropical and mid-latitude jets is biased. Indeed, several recent studies have found fault with the ability of CMIP5 models to simulate recent decadal-scale trends in Antarctic circulation features such as the Amundsen-Bellingshausen Seas Low (Hosking et al. 2013). Given these findings, it is perhaps no great surprise that GCMs are unable to capture the local-scale patterns of Antarctic sea ice trends.

What is the future of Antarctic sea ice?

Given the inconsistencies between observed and simulated trends over recent decades, it is natural to ask, should we trust model projections of Antarctic sea ice over the 21st century? Our answer is: both yes and no. While stratospheric ozone is expected to recover, the westerly winds are likely to continue to increase in strength and shift poleward due to rising greenhouse gases alone (e.g., Kushner et al. 2001; Arblaster et al. 2011), though perhaps at a slower rate than has been observed (Polvani et al. 2011b; Bracegirdle et al. 2013; Barnes et al. 2014). We anticipate that, in time, the dominant effect of westerly wind enhancement will almost certainly be the slow, surface warming response described by Ferreira et al. (2015), which climate models seem able to simulate. Thus, although there is a wide spread in their projections, we believe that climate models are at least simulating the correct sign of the 21st century changes: a decline in the

total Antarctic sea ice cover. However, natural variability in large-scale Southern Ocean winds may prove to be an important driver of sea ice trends on timescales of years to decades. Moreover, model deficiencies in simulating the spatial pattern of local wind changes, in combination with substantial variability associated with teleconnections from the tropics, may continue to preclude accurate projections of the regional patterns of sea ice trends for the foreseeable future.

Acknowledgments

The authors thank David Schneider for providing the zonal wind data in Figure 2 and Yavor Kostov, Lorenzo Polvani, Claire Parkinson, Judy Twedt, and Clara Deser for helpful comments on this article. Armour and Bitz are grateful to the National Science Foundation for support through grant PLR-1341497 (Bitz) and OCE-1523641 (Armour).

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State estimation for determining the properties and sensitivities of the Southern Ocean carbon cycle

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Regardless of complexity, the goal of data assimilation techniques is to maximize the utility of observations. The methods involve using correlation scales to project observation information in time and space. Methods using empirical or statistical models are computationally efficient and desirable for many applications. These have shortcomings, however, in that they often don't obey physical constraints and may also misrepresent correlations between forcing mechanisms. More complex mapping methods use the governing physics, represented in discrete form by a numerical model, to determine spatiotemporal correlation and cross-correlation. The complex methods also have shortcomings in that model errors still exist, and these methods are computationally expensive.

The ideal mapping method complexity will depend on the application. Determining a best estimate of the current biogeochemical–ice–ocean state incorporates all knowledge of the system, including knowledge of the physics governing the system, and thus requires a complex method. The method of choice for many science applications has become known as “state estimation”. The primary difference between state estimation and “reanalysis” as performed by numerical weather prediction centers is the length of the assimilation window. Reanalyses assimilate data over a window that is less than one month and then patch the solutions together, whereas in state estimation the entire estimation period (e.g., years to decades) is assimilated in one calculation. In practice, reanalyses usually fit individual observations

more closely than state estimates, but physical budgets are not closed between the sequential assimilations.

The governing physics obeyed by state estimates offers a powerful constraint allowing one to infer air-sea fluxes. Variations in ocean properties, for example inventories of heat and carbon, imply changes in fluxes. Thus by measuring ocean carbon content we are informing air-sea carbon flux, and state estimates allow one to infer this flux.

Measurements of the Southern Ocean carbon system have been greatly augmented by the deployment of biogeochemical sensors on autonomous profiling floats. Furthermore, the software to produce state estimates of the carbon budget via the adjoint method is now mature. State estimates of biogeochemical and physical ocean properties will be available in the near future. Here, we review the development of a coupled physical–biogeochemical Southern Ocean State Estimate. We then showcase the adjoint tool used to produce this state estimate by determining the sensitivity of air-sea carbon flux to ocean properties.

A biogeochemical Southern Ocean state estimate Configuration

A Southern Ocean state estimate (SOSE; sose.ucsd.edu) is being produced at Scripps Institution of Oceanography using the machinery developed by the consortium for Estimating the Circulation and Climate of the Ocean (ECCO; <http://www.ecco-group.org>). For more information on

SOSE and ECCO, see Mazloff et al. (2010) and Wunsch and Heimbach (2013). Here, we describe the biogeochemical SOSE configuration being used to hindcast the period 2005 to 2014.

To maximize efficiency, we utilize multi-scale optimization, in which one uses model setups of varying resolution to first optimize the large scales and then progressively smaller scales. We are currently optimizing a setup with $1/3^\circ$ horizontal resolution and 52 vertical levels. The coarse state estimate will inform our first-guess solution of a $1/6^\circ$ resolution setup, which will in turn be optimized and used to drive a high-resolution $1/12^\circ$ setup. The vertical resolution will be increased to 104 levels for the $1/12^\circ$ setup.

The domain is from 78°S to the equator. Isotropy in discretization (Mercator projection) is achieved to 30°S , and then the meridional grid size increases gradually toward the equator. Topography is prescribed usingETOPO1 (Amante and Eakins 2009), with partial bottom cells to better resolve variations in ocean depth. An atmospheric boundary layer scheme is employed where fluxes of heat, freshwater (salt), and momentum are determined by bulk formulae (Large and Yeager 2009). The atmospheric state is optimized using the adjoint method, but constrained to be consistent with the ERA-Interim reanalysis (provided by the European Centre for Medium-Range Weather Forecasts, ECMWF). Similarly, the initial conditions are optimized and constrained to be consistent with a coarse global state estimate (Forget 2010). Runoff is prescribed at the continental boundary.

The biogeochemistry component of the model is adapted from the Biogeochemistry with Light, Iron, Nutrients, and Gases model (BLING; Galbraith et al. 2010). This intermediate complexity model includes a full description of the carbon system and a simple representation of phytoplankton community production, parameterized as a function of temperature with limitation terms from deficiencies of light, iron, and phosphate. With only six prognostic variables, it is relatively computationally inexpensive to run and thus well suited for data

assimilation. First-guess initial and open boundary conditions for the biogeochemical fields are derived from global climatologies (GLObal Ocean Data Analysis Project version 2 (GLODAPv2), World Ocean Atlas) and optimized using the adjoint method.

Model-observation synthesis: Determining the state estimate

Physical observations constraining the state estimate include Argo float profiles, conductivity-temperature-depth (CTD) synoptic sections, instrument-mounted seal profiles, expendable bathythermographs (XBTs), altimetric observations, microwave radiometer-observed sea surface temperature, inverted echo sounders, and bottom pressure gauges. Observations of sea ice concentration from the National Snow and Ice Data Center (NSIDC; Cavalieri et al. 1996, updated yearly) are assimilated. Biogeochemical observations come mainly from Argo floats, underway $p\text{CO}_2$ measurements, and the GLODAPv2 calibrated data product. A collection of iron measurements for the Southern Ocean is also available (Tagliabue et al. 2012).

The adjoint method optimization, also known as 4-dimensional variational assimilation (4D-Var), is used to bring the model into agreement with the observations. Model ability to reproduce the observations is measured with a cost function, J , which is the sum over time and space of squared model-data differences weighted by a prescribed uncertainty. The weight assigned to each data point is determined by combining the measurement error with the model representation error. Optimization is sought by iteratively reducing J by adjusting the control vector, u , which consists of the initial conditions and the surface boundary (atmospheric state) conditions. The adjoint model calculates the cost function gradients with respect to the controls, $\nabla_u J$, thereby increasing the efficiency of the optimization algorithm.

Examples of other biogeochemical and ecological data assimilation efforts in ocean models of varying complexity are described in Gregg (2008) and Gregg et al. (2009). It is noteworthy that coupled physical-biological models

often assimilate either physical data or biogeochemical data, but rarely both (a notable exception is the study of Schlitzer (2002)). In several studies, the assimilation of chlorophyll data was shown to significantly improve the simulation (Nerger and Gregg 2007; Ford et al. 2012; Tjiputra et al. 2007). These recent studies employ Kalman filter methods for data assimilation and produce sequential reanalyses. In contrast, the state estimate we are producing is determined by running the *free* model forward in time using the adjusted control vector. In that important sense, the state estimate is dynamically self-consistent (i.e., there are no non-physical jumps in properties), and this is the primary reason the adjoint method of optimization is chosen for this work.

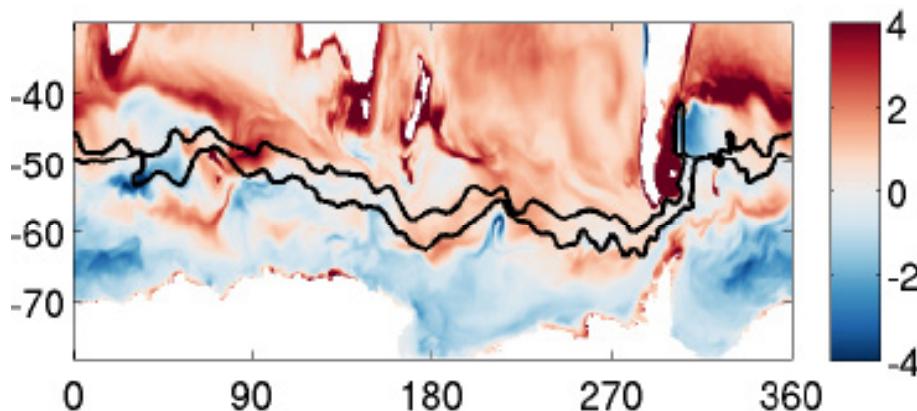


Figure 1. October mean air-sea CO_2 flux [$\text{mol m}^{-2} \text{yr}^{-1}$] in the model run. Positive fluxes are defined as ocean uptake (i.e., red implies an increase in oceanic carbon inventory). Black contours denote the approximate Subantarctic Front and Polar Front locations as determined in Orsi et al. (1995).

Assimilation of observations in SOSE will be performed with the adjoint of the coupled model, meaning that both biogeochemical and physical constraints will contribute to determining the state. Dutkiewicz et al. (2006) have shown that the adjoint methodology can be applied to a physical-biogeochemical model. Our model, though slightly more sophisticated than the one used by Dutkiewicz et al. (2006), has been made compatible with

the adjoint method. As an example of what the adjoint offers, we present the results of a carbon flux sensitivity experiment in the next section.

The utility of the adjoint model: An example sensitivity experiment

The adjoint model yields the partial derivatives of a cost function with respect to model state and model inputs. In state estimation, the cost function is the weighted model-data misfit. One can, however, design a different cost function. Dutkiewicz et al. (2006) evaluate two cost functions; one being global biological productivity and the other being global air-sea carbon fluxes. They find the Pacific and Southern Oceans to be most sensitive to sustained atmospheric iron source inputs.

Following that work, we use our $1/3^\circ$ setup to determine the sensitivity of October air-sea carbon exchange poleward of 40°S . The purpose is two-fold. First, we wish to demonstrate the power of the adjoint model in revealing the sensitivities of the system. Second, we wish to understand the controls on carbon flux. Fluxes themselves are challenging to observe, but knowing their sensitivities can guide how to infer them from properties that are more readily observed.

Over 50% of the variance in the air-sea carbon exchange time series in our model can be explained by the seasonal cycle (not shown). October is a time when the ocean is generally outgassing carbon to the atmosphere poleward of the Antarctic Circumpolar Current (ACC) and taking up carbon from the atmosphere equatorward of the ACC (Figure 1). This pattern is typical of the Austral spring months from September to December. The uptake is

greatest in the confluence regions and downstream of land. Some uptake occurs along Antarctica.

The overall sensitivity of this October air-sea exchange to other model properties can be quantified and compared by weighting with a typical perturbation size of that property. We take the sensitivity maps (i.e., partial derivatives) of carbon flux to a property and multiply by the temporal standard deviation of that property to find how carbon is sensitive to a typical anomaly in units of carbon flux. Doing this to all prognostic variables, and then calculating the spatial root-mean-square of these normalized sensitivities, reveals that carbon flux is most sensitive to anomalies of dissolved inorganic carbon (DIC), alkalinity, temperature, and iron (Figure 2). The sensitivity maximum is on October 1, as perturbations at this time will have the greatest influence on October mean carbon flux. The decay shows how long sensitivity persists. This decay rate is similar for anomalies of alkalinity and DIC perturbations, slowest for nutrients and iron, and fastest for temperature.

The air-sea carbon flux poleward of 40°S is sensitive to September upper ocean DIC concentration almost everywhere (Figure 3a). The sign is always negative, implying adding DIC will decrease the carbon flux into the ocean, and thus increase ocean outgassing of CO₂. The greatest sensitivity is found along the ACC, and particularly around the Kerguelen Plateau and in the Southeast Pacific sector. In the depth range of 300-600 m, the carbon flux is sensitive to September DIC concentration only in a few regions where there is a transport pathway to the surface (Figure 3b). These locations are primarily associated with mode water formation in the Southeast Indian and Pacific sectors. A few regions around Antarctica can also

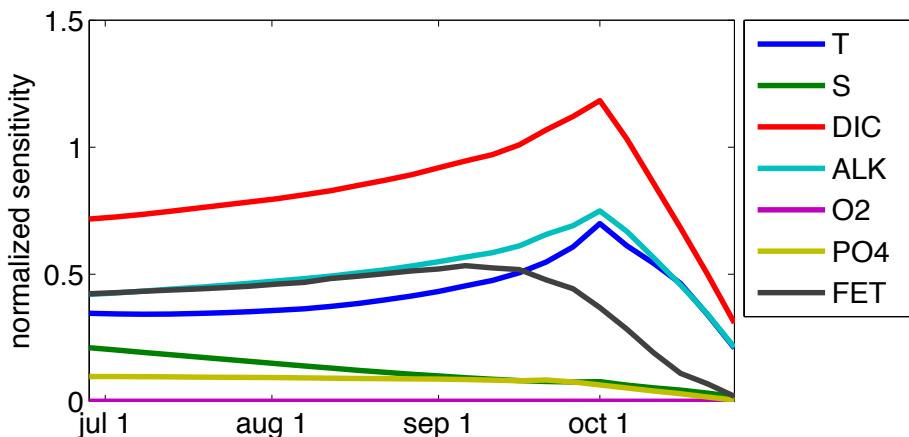


Figure 2. Temporal evolution from July 1 to October 30 of the sensitivity of October air-sea CO₂ flux poleward of 40°S to various physical and biogeochemical properties (colored lines). Sensitivity is calculated as the root-mean-square of adjoint gradients normalized by the spatially varying temporal standard deviation of the respective property.

influence carbon flux. The sensitivity to alkalinity (not shown) looks qualitatively very similar to DIC, though with the opposite sign.

The sensitivity of air-sea carbon flux poleward of 40°S to September iron concentration is always positive, implying that adding iron will always increase the flux into the ocean (Figure 3c). As with DIC a sensitivity is found everywhere in the upper ocean, but the patterns are quite different. The sensitivity is strongest in the regions where the ocean is most iron-limited. Many of these locations coincide with regions of ocean outgassing in the October mean (Figure 1). An exception is a lack of sensitivity at the highest latitudes, as these are likely ice-covered and light-limited. The sensitivity at depths 300-600 m mirrors the sensitivity to DIC, as both of these are governed by the ability to be transported into the euphotic zone.

The sensitivity of air-sea carbon flux to September temperature reflects two phenomena. The first is the temperature effect on solubility, and thus the sensitivity is negative almost everywhere, implying that decreasing

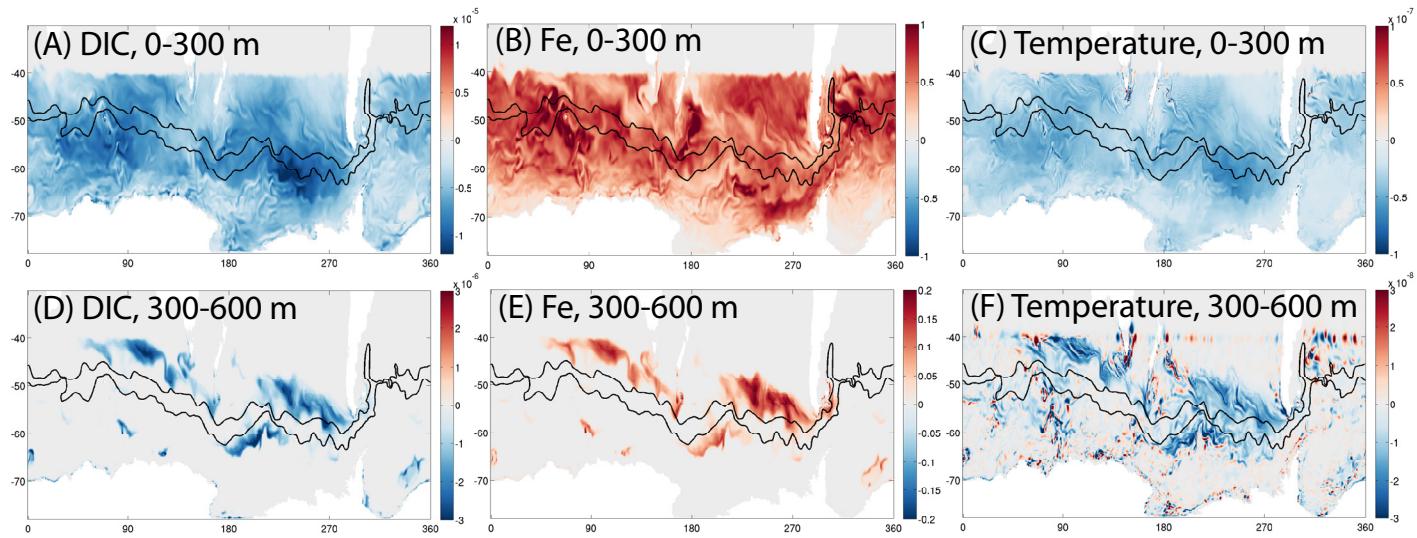


Figure 3. Spatial patterns of the sensitivity of the October air-sea CO_2 flux poleward of 40°S to DIC concentration in September (a) in the upper 300 m and (b) at depths 300 m to 600 m. The sensitivity to September iron concentration (c) in the upper 300 m and (d) at depths 300 m to 600 m. The sensitivity to September temperature (e) in the upper 300 m and (f) at depths 300 m to 600 m.

temperature increases carbon flux into the ocean (Figure 3e). The other is the effect of temperature perturbations on the circulation. This effect is more noticeable below the mixed layer where temperature has less impact on solubility (Figure 3f). The influence of the circulation on carbon flux poleward of 40°S is noticeable at 40°S where properties can be exchanged across the arbitrary cost function integration domain. It is also noticeable in regions where temperature anomalies can induce or enhance shelf exchanges (e.g., downstream of New Zealand) or cross-front transport (e.g., into the Argentine Basin or across the Polar Front).

The sensitivity to salinity (not shown) looks much like the sensitivity to temperature, but without the large-scale solubility component (i.e., without the relatively smooth domain-scale negative sensitivity pattern). While the sensitivity to the solubility component in temperature tends to decay rapidly, the sensitivity to circulation changes tends to grow slowly in numerous locations,

as can be seen by the growing influence of salinity perturbations back in time (Figure 2).

Conclusions

Constraining biogeochemical observations to models via the adjoint method is feasible, and given the growing biogeochemical observational capabilities efforts have begun to produce state estimates of the carbon cycle. In this paper we introduced one underway state estimation effort. We demonstrate the utility of the adjoint model used in this effort by using it to map the sensitivities of the October air-sea carbon exchanges to anomalies in model state. We find this air-sea exchange is most sensitive to September anomalies of DIC, iron, alkalinity, and heat. Moderate sensitivities are also found to anomalies of macronutrients and salinity.

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Biogeochemical metrics for the evaluation of the Southern Ocean in Earth system models

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Observationally-based metrics are an important step in reducing the uncertainty in model simulations of the future climate. Especially as the community is shifting toward Earth system models with explicit carbon simulations, the need for more direct observations of biogeochemically (BGC) important parameters is essential. We present three biogeochemical metrics and discuss why they are important, the observations on which the metrics are based, and the quality and biases seen in the Earth system models' simulations. This analysis emphasizes the importance of the advent of a BGC Argo array as a critical tool for climate model assessment and refinement.

Introduction

The exchange of heat and carbon dioxide between the atmosphere and ocean are major controls on Earth's climate under conditions of anthropogenic forcing. The Southern Ocean south of 30°S, occupying just over a quarter of the surface ocean area, accounts for a disproportionate share of the vertical exchange of properties between the ocean's deep and surface waters and between the surface ocean and the atmosphere. Model simulations and observational analyses of the Southern Ocean have indicated that: 1) it may account for up to half of the annual oceanic uptake of anthropogenic carbon dioxide from the atmosphere (cf., Gruber et al. 2009, Frölicher et al. 2015); 2) vertical exchange there is responsible for supplying nutrients that fertilize three-quarters of the biological production in the global ocean

north of 30°S (Sarmiento et al. 2004, Marinov et al. 2006); and 3) it may account for up to $75 \pm 22\%$ of the excess heat that is transferred from the atmosphere into the ocean each year (Frölicher et al. 2015). Unfortunately, uncertainty in these estimates and future climate projections remains high, and the carbon cycle represents one of the biggest challenges in this regard. There is an obvious need for improved observational data and model fidelity, especially as the scientific community is working toward more accurate estimates of the present and future carbon budgets.

Despite the crucial role of the Southern Ocean in the Earth system, our understanding of key underlying mechanisms remains inadequate, and the model studies that have focused on mechanisms of heat and carbon uptake to date remain highly controversial. Model uncertainty comes from incomplete physics and biogeochemistry, and from the use of parameterizations required in place of unresolved processes, such as cloud physics and stirring by mesoscale eddies. Equally important is the deficit of observational data to test the models due to the great difficulty of obtaining observations in this region. Quantifying the actual air-sea exchanges of carbon through direct observations remains beyond our capability, so we are dependent on the observations in the ocean from ships, buoys, and, most recently, the [Southern Ocean Carbon and Climate Observations and Modeling \(SOCCOM\)](#) BGC-Argo float

array. We do not have anything approaching an adequate spatial or temporal set of observations with which to definitively evaluate the biogeochemistry in Earth system model simulations. Despite significant recent advances in model development and observational coverage, it seems unlikely that modeling biases and observational gaps will be eliminated in the near future. There is an obvious need for quantitative information that would assist model validation and development and inform observational efforts on what information is most critical in this regard.

Here we describe several observationally-based data/model metrics that, with the advent of new biogeochemically-equipped floats, will be able to quantify the success of simulations and will allow for demonstrable progress and the reduction of model uncertainty in the projections of future climate. These metrics will become more robust as the coverage of the BGC-Argo array expands its scope in both space and time. Standardized metrics are especially critical for processes with large biases and inter-model differences like those that typify simulations of the Southern Ocean. We cannot expect all models to simulate all aspects of the ocean physics and biogeochemistry perfectly, so metrics should focus on processes that are most critical for the ocean's role in climate, such as heat and carbon uptake. The metrics presented here are an outgrowth of the US CLIVAR Working Group on the Southern Ocean Heat and Carbon Uptake, and a more complete discussion can be found in the full manuscript (to be submitted to the *Journal of Climate*).

Metrics

For this analysis, we compare a small subset of the historical simulations from the CMIP5/IPCC-AR5 archive at the Department of Energy's Program for Climate Model Diagnosis and Intercomparison (PCMDI) to the observations of surface dissolved inorganic carbon (DIC), air-sea CO₂ flux and surface pH. For each of these metrics, we discuss why the metric is important, the observations on which the metric is based, and the quality and biases seen in the Earth system models' simulations. The Earth-

system models chosen for this analysis are: 1) CanESM2 (Canadian Centre for Climate Modeling and Analysis, Canada); 2) ESM2M (Geophysical Fluid Dynamics Laboratory, USA); 3) HadGEM2 (Met Office Hadley Centre, UK); 4) MIROC-ESM (Model for Interdisciplinary Research on Climate, Japan); and 5) MRI-ESM2 (Meteorological Research Institute, Japan).

Wherever possible, model simulations should be compared to actual observations. Unfortunately, ocean data and atmospheric data over the ocean rarely provide enough coverage in space or time to form a complete picture of the biogeochemistry. As a result, we will rely on atlases and reanalyses to fill in the gaps. The advent of profiling Argo-like floats equipped with BGC sensors are expected to bring a wealth of new data that can potentially revolutionize our understanding of the carbon cycle in the real ocean and dramatically improve the accuracy of the metrics discussed here.

Dissolved Inorganic Carbon

The total amount of carbon in the surface ocean, along with the pH, determines the surface pCO₂ and therefore greatly affects the air-sea exchange of carbon. Significant biases in simulated DIC will almost certainly lead to large biases in simulated uptake of CO₂ in transient forcing scenarios, and therefore the global atmospheric temperature response to these scenarios.

The gold standard of carbon data in the ocean continues to be the GLODAP dataset (Figure 1a; Key et al. 2004), although this is soon to be replaced by GLODAP v2, which is slated to become available in 2016. GLODAP data will serve as our observational benchmark for DIC and are available from CDIAC (http://cdiac.ornl.gov/ftp/oceans/GLODAP_Gridded_Data/). The other significant (and global) resource is the Takahashi surface ocean pCO₂ dataset, which is not used here for DIC. In the near future, we expect BGC-sensored floats to provide a much better resolved dataset in both space and time (seasonally) that will eventually give us an observational basis for the estimation of trends.

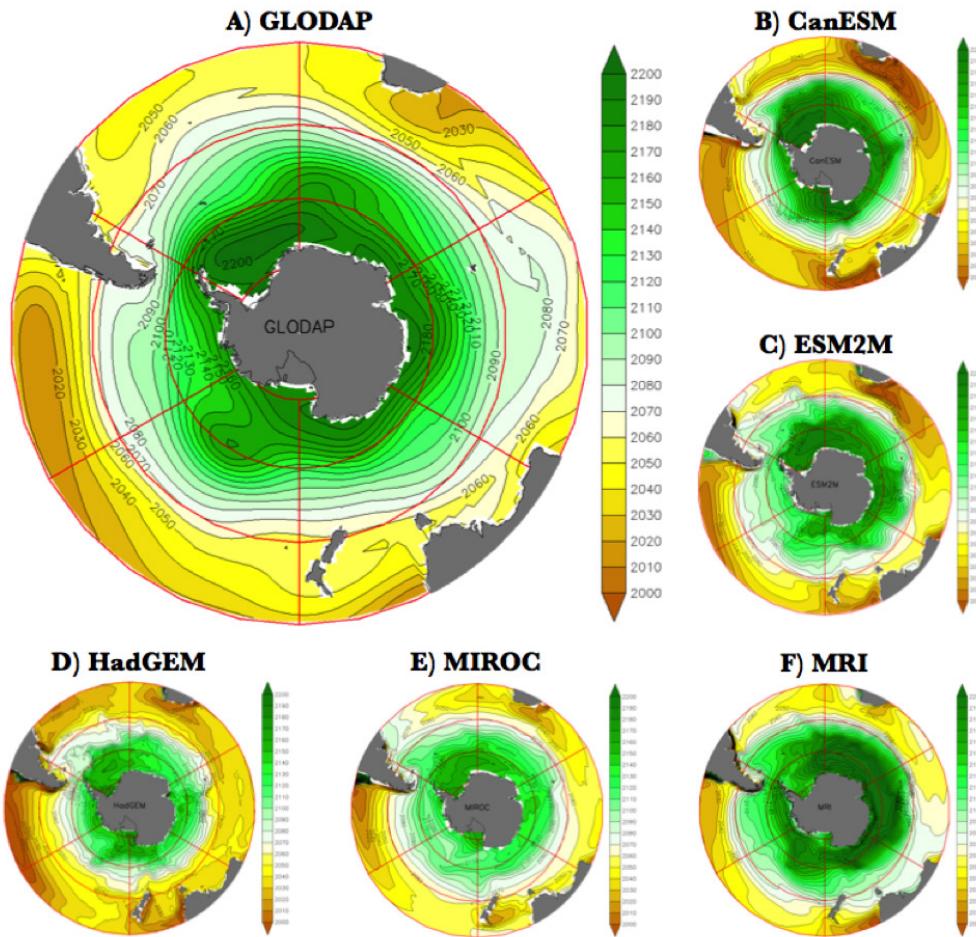


Figure 1. Surface (0-100 m) concentrations of dissolved inorganic carbon (DIC; $\mu\text{mol}/\text{kg}$) from observations (a) and model simulations (b-f). The observations are from the GLODAP dataset (Key et al. 2004), available through CDIAC. All model simulations cover years 1986-2005 from the HISTORICAL forcing scenario. Panel a) GLODAP; b) CanESM2; c) GFDL-ESM2M; d) HadGEM2-ES; e) MIROC-ESM; and f) MRI-ESM1.

Earth system models simulate significantly different amounts of total carbon, globally and in each of the different reservoirs (atmosphere, ocean, vegetation, and soil). The amount of carbon in each reservoir can potentially affect the modeled transient response (uptake or degassing) based on potentially unrealistic initial conditions. Focusing on the Southern Ocean (Figure 1), most models can simulate a general pattern of the observed surface DIC distribution, with the local maxima

in the Weddell Sea and near the Ross Sea, but they also exhibit biases in simulated magnitudes of the DIC concentrations.

Surface pH

Ocean acidification, the decrease in oceanic pH due to the absorption of carbon dioxide, is an acknowledged and growing concern. Southern Ocean acidification is projected to lead to aragonite undersaturation in as little as 15 years (McNeil and Matear 2008). Monitoring and accurately simulating the Southern Ocean surface pH and its trend is critical. Small differences can potentially have large effects on simulated acidification trends as calcification rates are especially sensitive to small changes in pH. As noted above, pH influences the surface pCO_2 and carbon uptake.

The CDIAC dataset (NDP-094, Takahashi et al. 2014) is used here to provide

gridded monthly surface pH data in the Southern Ocean (Figure 2a), although the BGC-Argo floats should shortly surpass these limited observations and provide depth information, as well as give us the opportunity to observe trends in real time. This new source of pH data will be essential for assessing acidification issues in the Southern Ocean, where it has been projected to become critical in as little as two decades (McNeil and Matear, 2008).

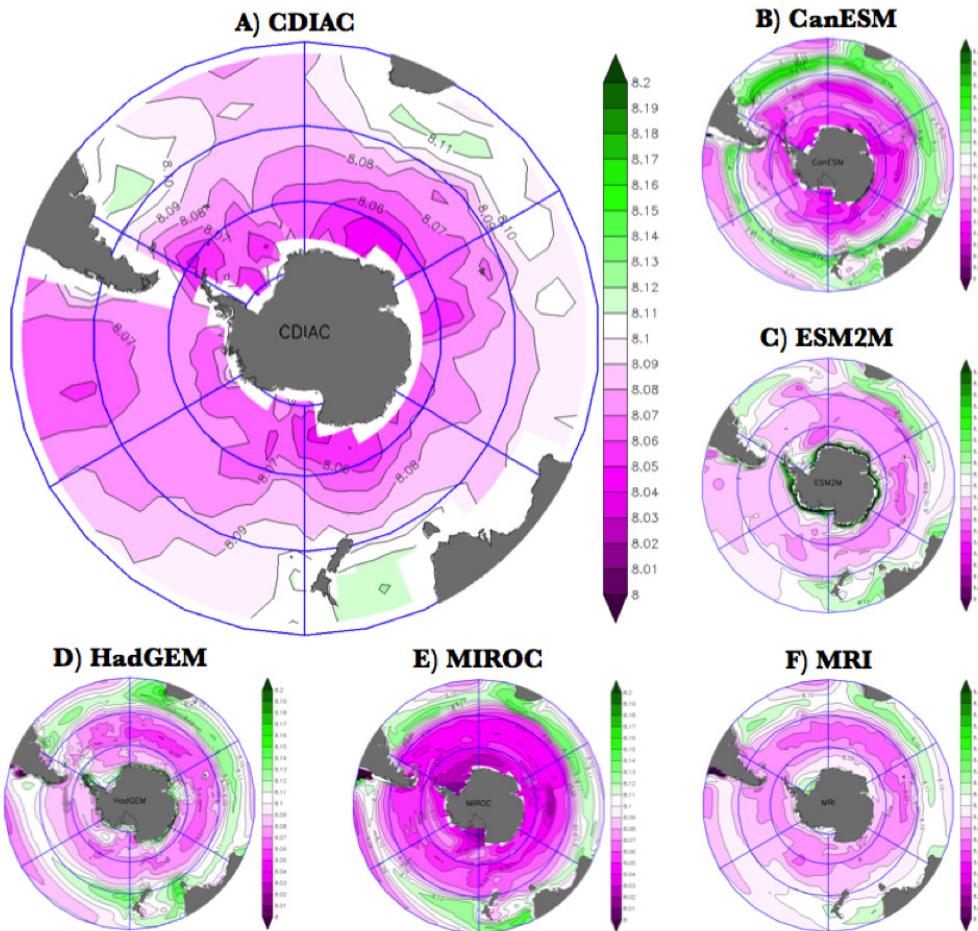


Figure 2. Annual mean surface pH from observations (a) and the model simulations (b-f). The observations are taken from the recent Takahashi et al. (2014) climatology, available through CDIAC, which has a fairly coarse $5^\circ \times 5^\circ$ resolution and should be indicative of 2005 conditions. The pH observations include data primarily from the GLODAP, CARINA, and LDEO databases taken from the top 50 m of the water column. Model simulations cover years 1986-2005 from the HISTORICAL forcing scenario. Panel a) CDIAC; b) CanESM2; c) GFDL-ESM2M; d) HadGEM2-ES; e) MIROC-ESM; and f) MRI-ESM1.

The Ekman-driven surface divergence brings old, carbon-rich, low pH water to the surface. Models generally capture this transport with some differences between the specific pH values present (Figure 2). Several of the simulations have excessively alkaline waters north of the Antarctic Circumpolar Current (ACC) and several have too acidic water in the upwelling region. Seasonal differences seen in the observations are seen in some of the simulations, but not in others (not shown), indicating

that the seasonality of the upwelling is not necessarily well simulated even if the annual mean picture is more-or-less correct.

Air-Sea CO₂ Flux

The uptake of carbon dioxide by the Southern Ocean, and its subsequent removal from contact with the atmosphere is one of the most important aspects of climate change that is needed to reduce the uncertainty in future climate projections. As noted above, this flux depends on the amount of carbon in surface water, the pH and the buffering capacity, and the wind speed that controls the speed of the air-sea exchange. All of these factors are affected by anthropogenic carbon increases. Although early studies concluded that the Southern Ocean sink of anthropogenic carbon dioxide was weakening due to atmospheric warming (Le Quéré et al. 2007), more recent studies have concluded that the slowdown in the carbon uptake seen in

the 1990s has ceased, and the uptake has been increasing steadily since the early 2000s (Landschützer et al. 2015).

The Takahashi CO₂ flux observations shown in Figure 3a are derived from measurements of the surface ocean $p\text{CO}_2$, the atmospheric $p\text{CO}_2$, and the wind speed. Although the flux is not a direct measurement, it is likely more reliable than estimates of, for example, the total heat or freshwater fluxes.

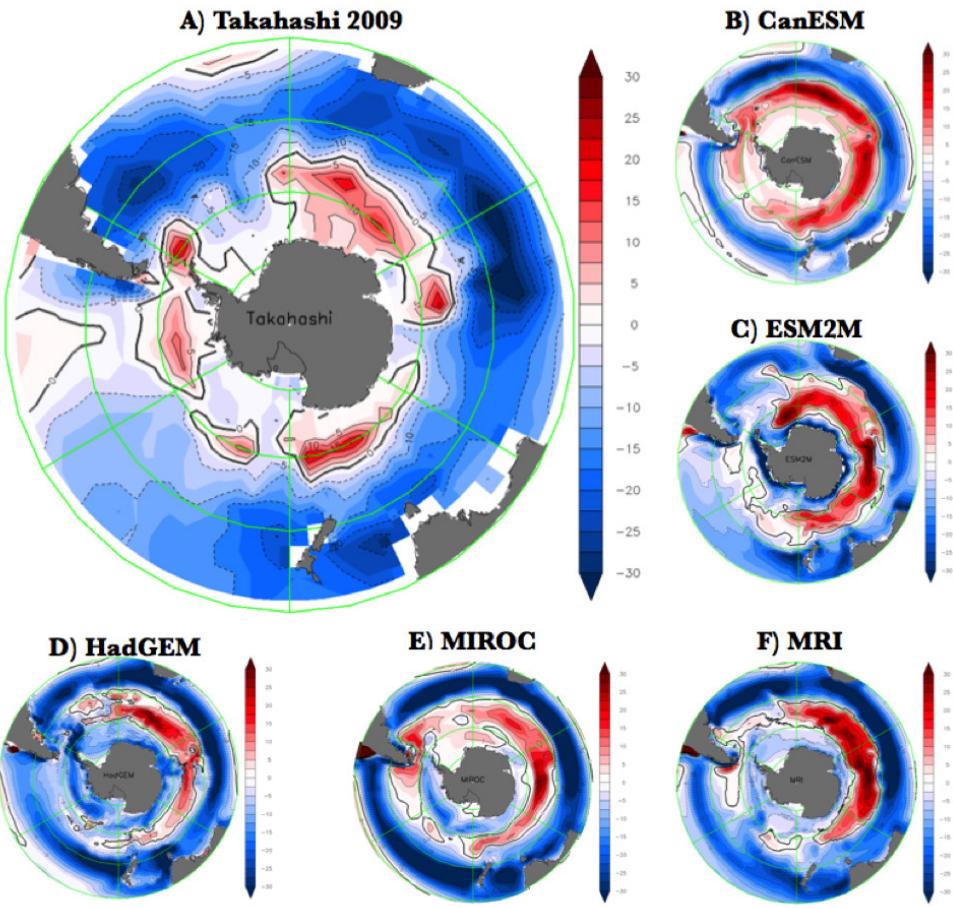


Figure 3. Annual mean surface flux of carbon ($\text{gC}/\text{m}^2/\text{yr}$) from observations (a) and model simulations (b-f). The observations are from the [2009 Takahashi dataset](#). Model simulations cover years 1986-2005 from the HISTORICAL forcing scenario. Panel a) GLODAP; b) CanESM; c) GFDL-ESM2M; d) HadGEM2-ES; e) MIROC-ESM; and f) MRI-ESM1. In these panels, red shading indicates degassing from the ocean into the atmosphere, while blue shading indicates uptake by the ocean

The models generally get the pattern of CO_2 flux correct with outgassing at approximately 60°S where the upwelling of old, carbon-rich circumpolar deep water due to Ekman divergence under the Southern Hemisphere westerlies - is most intense, and uptake at about 35°S where the Ekman convergence leads to subduction. Most of the models shown in Figure 3, however, due to their equatorward-shifted winds, overestimate both the uptake and the outgassing of carbon over the Southern Ocean.

prospect of new data generated as part of the Southern Ocean Observing System (SOOS) efforts.

While the concept of an observationally-based metric is easy to understand, generating the datasets for those comparisons requires great care. All modeling centers should be encouraged to provide data for the comparison against the most important physical and BGC metrics, and make sure that these data are provided in standard and budget-conserving grids. While metrics are essential

Discussion

Consistent, observationally-based metrics are the clearest, most objective way to make progress in reducing the uncertainty in our future climate projections. We have presented some of these metrics related to the Southern Ocean biogeochemistry here. Our way forward requires two essential tracks. First, we collectively must carry out rigorous assessments of all model simulations against these and potentially other observationally-based metrics in order to evaluate the biases in the models, reduce our inter-model differences, and reduce the uncertainty in our projections of the future. Second, we need to encourage and bring about the continued expansion of the available observational data from the nascent BGC-Argo efforts as well as the

to the overall assessment and improvement of coupled climate and Earth system models, not every metric is relevant to every study and it remains the responsibility of the individual researcher to understand and apply the specific metrics that increase confidence with respect to individual hypotheses.

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Acknowledgments

This work was funded in part by SOCCOM, the Southern Ocean Carbon and Climate Observations and Modeling Program (NSF-PLR #1425989).

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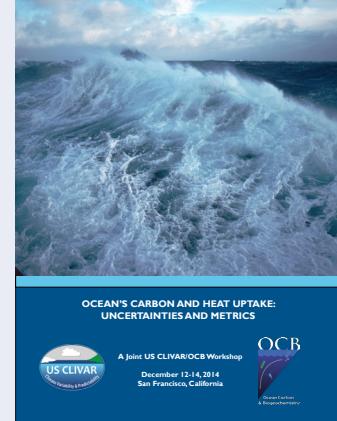
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ANNOUNCEMENTS

Workshop Report: Ocean's Carbon and Heat Uptake: Uncertainties and Metrics

A workshop jointly sponsored by the US CLIVAR and OCB Programs was convened in December 2014 on "Ocean's Carbon and Heat Uptake: Uncertainties and Metrics" and the challenges of improving observations, process understanding, and modeling. The rationale for holding this workshop, organized by the Ocean Carbon Uptake and Southern Ocean Working Groups, was that despite the fact that the ocean has absorbed over 90% of the anthropogenic heat imbalance and over 30% of the anthropogenic carbon emissions, our ability to observe and simulate the "how," the "where," and the "how fast" these uptakes occur has significant shortcomings. Due to the scope and logistical difficulties of the task, our observing network is at best incomplete, and in some cases, non-existent, and our efforts at simulating past, present, and future climate have large uncertainties due to inter-model differences and a lack of benchmarks.



Thanks to Working Group members for your contributions and efforts.

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This material was developed with federal support of NASA, NSF, and DOE (AGS-1502208), and NOAA (NA11OAR4310213). Any opinions, findings, conclusions, or recommendations expressed in this material are those of the authors and do not necessarily reflect the views of the sponsoring agencies.