Report from the ACE Workshop on Ocean Productivity and Carbon Cycle (OPCC)

Summary:
A workshop in support of the NASA Aerosol-Cloud-Ecosystems (ACE) mission was held at the Earth Research Institute (ERI) at UC Santa Barbara June 6-8, 2011. The goals of the workshop were to discuss ocean productivity and carbon cycle processes and parameters and how ACE satellite observations along with model assimilation and in situ data will be used to constrain their retrieval. The participants decided on a list of essential ocean productivity and carbon cycle parameters (OPCC) and discussed the next steps in developing satellite algorithms for their determination from satellite observations.

Background:
The Aerosol-Cloud-Ecosystem (ACE) mission is one of the future NASA Earth science missions recommended in the National Research Council’s (NRC) 2007 Decadal Survey. ACE obviously has many objectives including cloud-aerosol indirect radiative forcing of atmospheric heating and ocean ecosystems. This means that ACE will include many sampling tools including cloud radars, aerosol lidars, an imaging polarimeter and an advanced ocean color sensor. Originally ACE was designated as a Tier 2 mission in the Decadal Survey but the advanced ocean color imager was accelerated in the NASA’s Climate Architecture Plan (2010). This mission known as Pre-ACE (or PACE). PACE has a nominal launch date of 2019 and the time for mission planning is now.

Science planning for the ocean ecosystems portion of the ACE mission has been started by the ACE Ocean Ecology Science Working Group. Presumably these plans will be valid for PACE. The ACE Ocean Ecology Science Working Group developed the following science questions (ACE Ocean Ecosystems White Paper, 2010).

• SQ-1: What are the standing stocks, composition, & productivity of ocean ecosystems? How and why are they changing?
• SQ-2: How and why are ocean biogeochemical cycles changing? How do they influence the Earth system?
• SQ-3: What are the material exchanges between land & ocean? How do they influence coastal ecosystems, biogeochemistry & habitats? How are they changing?
• SQ-4: How do aerosols & clouds influence ocean ecosystems & biogeochemical cycles? How do ocean biological & photochemical processes affect the atmosphere and Earth system? These questions link directly to Question 4 of the Ocean-Aerosol Interactions element of the ACE program.
• SQ-5: How do physical ocean processes affect ocean ecosystems & biogeochemistry? How do ocean biological processes influence ocean physics?
• SQ-6: What is the distribution of algal blooms and their relation to harmful algal and eutrophication events? How are these events changing?

The ACE Ocean Ecology Science Working Group has expertise to develop plans for ACE that will answer many of these questions. However, the working group is lacking some of the expertise required to address SQ-2 (ocean biogeochemical cycles) fully as well as aspects of some of the other ACE science questions.
To address these shortcomings a workshop focused on Ocean Productivity and Carbon Cycle (OPCC) parameters was proposed. The OPCC parameters include net primary production, net community production, export, new production, air-sea CO2 exchanges, nitrogen fixation, etc. One of the purposes of the workshop was to prioritize the OPCC parameters that are necessary for constraining the ACE science questions. Obviously, the assessment of the ACE science questions will require a synthesis of satellite observations, field measurements (including process studies), algorithm development and model assimilation (assimilation here in the loosest sense).

Pre-Workshop Objectives:

There were several deliverables proposed for the ACE OPCC workshop in the statement of work before it occurred. These include...

- Assessment of essential OPCC parameters to achieve ACE goals,
- Create product assessment sheets for these essential OPCC parameters,
- Develop a framework for a plan for collecting data needed for algorithm/validation of the essential OPCC parameters for ACE/PACE, and
- Write a high-level vision document describing our approach for assessing essential OPCC parameters from satellite observables.

Workshop at UC Santa Barbara:

The ACE OPCC workshop brought together a broad range of scientists and engineers with interests spanning satellite ocean color remote sensing, ocean biogeochemistry, air-sea gas exchange, ocean optics and ocean modeling. Because of this wide diversity of participants, the first part of the workshop had "cross-training" tutorials aimed at getting people on one side of the problem up to speed with the other. Following an introduction to ACE/PACE (by Chuck McClain), tutorials were presented on ocean productivity measures (by John Marra) and satellite ocean color remote sensing (by Dave Siegel). Jeremy Werdell presented an overview of the NASA/GSFC in situ science work in support of satellite ocean color missions which was followed by a suite of presentations were made to bring us all up to date about what can be done in each participants’ areas of expertise (see presentation list in the appendix below). All presentations are available at [http://people.eri.ucsb.edu/~davey/OPCC](http://people.eri.ucsb.edu/~davey/OPCC).

Discussions were focused on 1) what are the essential OPCC parameters, 2) what is needed to measure them (or model them based upon satellite observations) and 3) what are the appropriate next steps, particularly for field and model experiments. For each essential OPCC parameter a subset of the participants list was identified who will assist with the OPCC product assessment sheets.

The group also discussed what appropriate cal/val plans would be for the OPCC parameters that are a focus of the ACE/PACE mission. Conclusions were tabled for a future ACE workshop on the topic. It is also planned that this document be used as a starting point for an EOS workshop report article on the ACE/PACE OPCC workshop.
Essential OPCC Parameters:

The workshop participants focused on the following OPCC parameter suite with the goal of constraining the ACE/PACE ocean productivity and carbon cycle questions. One advantage of the nominal ACE/PACE sensor is its hyperspectral (5 nm) sampling that should enable advanced ocean color algorithms for phytoplankton functional types (PFT) and the particle size distribution (PSD). These retrievals would be critical for helping validate and provide data to assimilate into advanced couple ocean ecosystem and biogeochemical models as well as be useful for biomass partitioning estimates of NPP, export production (EP) and net community production (NCP), which will be essential for parameterizing other biogeochemical fluxes such as export.

The eight essential OPCC parameters are…

- Phytoplankton Functional Type / Particle Size Distribution (PFT/PSD)
- Net Primary Production (NPP)
- Net Community Production (NCP)
- Export Production (EP) & Export Flux Attenuation
- Surface pCO$_2$ and pH
- Air-Sea CO$_2$ and O$_2$ Fluxes
- Calcification Rate
- Nitrogen Fixation

These eight OPCC parameters enable the ACE mission to make many contributions towards the description of the structure and functioning of pelagic ecosystems, the structure and functioning of pelagic ecosystems, the dynamics of the carbon cycle and of the biological pump, ocean acidification, air-sea biogenic gas fluxes and the nitrogen cycle. In the following, we briefly address each and present the methods available to measure them in the field.

*Phytoplankton Functional Type / Particle Size Distribution (PFT/PSD):*

Phytoplankton functional types (PFT) provide information of the composition and potential functioning of the phytoplankton community. Examples include nitrogen fixers (e.g. *Trichodesmium*), calcifiers (coccolithophores), dimethyl sulfide (DMS) producers (e.g., *Phaeocystis*) and silicifiers (e.g., diatoms). The groupings are not necessarily related to physiological characteristics, but are often based on functionality (export of organic carbon to the deep ocean vs. local recycling) or other characteristics, such as cell size (pico, nano and microphytoplankton), which can also be assessed through determinations of the the particle size distribution (PSD). Further determination of the pigment- and carbon-content of PFT’s is essential for understanding the carbon cycle dynamics of ACE/PACE driven by phytoplankton processes.

PFTs and the PSD are of interest to ACE/PACE because they enable relevant ecosystem and biogeochemical rate estimates to be partitioned by size and function. Incorporation of PFTs into biogeochemical models may improve the predictive capabilities of such models.

In situ methods for determining PFT’s and the PSD include chemotaxonomic analyses from HPLC phytoplankton pigment analyses, microscopic imagery or flow cyrometer cell counts and characterization, optical and electrostatic determinations of the PSD and measurements of particulate inorganic carbon (PIC) concentrations.
Net Primary Production (NPP):

Net primary production (NPP) by ocean phytoplankton represents roughly half of the net plant production of the Earth and is the major conduit for biologically sequestering atmospheric carbon dioxide into moderate- and long-lifetime organic ocean carbon pools. In addition to being a key climate-controlling process, its quantification allows investigations into energy transfer throughout marine foodwebs and is a critical attribute in near-shore waters with respect to the potential for harmful algal blooms and changes in water quality. Understanding the magnitude, change and its partitioning by size and phytoplankton function is central answering the questions posed by the ACE Ocean working group.

Classical in situ methods for determining NPP are based upon incubation methods where the rate of $^{14}$C or $^{13}$C labeled bicarbonate incorporation is measured. Other incubation methods are possible using other tracers (dissolved oxygen, $^{15}$N, etc.). For all of these methods, several assumptions need to be made. Values of NPP are equal to the gross rate of phytoplankton production (GPP) minus the autotrophic respiration ($R_A$; or NPP = GPP - $R_A$). New methods such as triple oxygen isotopes enable some of these assumptions to be tested (see below). Further, NPP can also be expressed as the product of phytoplankton biomass and the phytoplankton growth rate (NPP = $B_{ph}$ * $\mu_{ph}$) and in situ methods for constraining NPP following this approach are under development.

Net Community Production (NCP):

The net balance between phytoplankton production and the food web respiration of organic carbon defines the net community production rate (NCP). Determinations of NCP quantify the net conversion of DIC to POC and put important constraints on the air-sea exchanges of CO$_2$. Values of NPP, the difference between phytoplankton production and phytoplankton respiration, do not account for respiration by the heterotrophic community and hence estimates of NPP are not useful for addressing upper ocean Carbon cycle dynamics by themselves.

Values of NCP can be assessed by evaluating the time rate of change of upper ocean inorganic or organic carbon stocks or through the measurement of changes of stocks of other constituents that are in approximate stoichiometric relationship with changes in carbon (such as dissolved oxygen, organic nitrogen, inorganic nutrients, etc.). Especially useful are powerful geochemical methods that determined NCP from the difference of simultaneous measurements of dissolved oxygen and argon concentrations. Both oxygen and argon have similar gas transfer characteristics but oxygen will respond to biological processes and argon will not. This method can be made on instantaneous samples which is attractive in developing an in situ data base of NCP observations.

Export Production (EP) & Export Flux Attenuation:

The bulk of the organic material and biominerals produced in sunlit surface waters decomposes or is remineralized in the upper ocean via zooplankton grazing, microbial hydrolysis or dissolution. However, a fraction of this fixed carbon is transported, by sinking and other processes, into the deep sea, and is exported from the surface ocean. This flux of sinking matter from the euphotic zone defines export production (EP). During transit to depth much of this exported material is respired or dissolved, whereas another fraction survives to reach the deep sea and eventually the sediments. The Martin curve has historically been used to describe the decrease of sinking material ($C_{flux}$) with depth or $C_{flux}(z) = EP (z/z_0)^b$, where the parameter b describes the rate of loss of material or flux attenuation during transit and EP the flux of material.
leaving the euphotic zone. The characteristics of the flux attenuation rate, b, are related to the rates of NPP and NCP of the euphotic zone (and their changes in time) and the composition of the particulate materials comprising the sinking flux (contributing to the “ballast” flux).

Particle interceptor traps (frequently termed sediment traps) have been used historically to collect and quantify sinking particles. Time series traps allow the continuous collection of sinking material over time scales of days to years and rates of export flux attenuation may be estimated from deployments of a series of traps at different depths. Marine aggregate camera systems and pumps yield data on standing stocks of large particles at different depths, which under the assumption of steady state and knowledge of the sinking velocities of the respective particles may be used to calculate sedimentation rates with depths. Geochemical approaches are also useful. The ratio of the particle reactive radionuclide $^{234}$Th to its soluble and long lived parent $^{238}$U in the surface ocean can be used to estimate the uptake of $^{234}$Th onto marine particles, and their export out of the surface ocean, reflecting average export from the upper layer in the 2-3 weeks preceding measurements. Similar to O$_2$/Ar approaches for estimating NCP, measurements of $^{234}$Th can be made on single samples greatly simplifying the logistics for constraining EP.

*Surface pCO$_2$ and pH:*

One of the major goals of the ACE/PACE missions is to improve our understanding of the ocean’s carbon cycle, which requires the assessment of state of the surface inorganic carbon system. As CO$_2$ dissolves in seawater, it disassociates into dissolved CO$_2$, bicarbonate and carbonate ions. This disassociation means that the oceans can hold a lot of dissolved inorganic carbon and the oceans contain about 85% of the active carbon reservoir on Earth. Cold seawater can hold more CO$_2$ than warm water, so waters that are cooling (i.e. poleward-moving western boundary currents) tend to take up carbon, and waters that are upwelling and warming (i.e. coastal zones and the tropics) tend to emit carbon. This is the basic reason for the pattern of upper layer pCO$_2$ values and the global sea-to-air CO$_2$ flux. The state of the bicarbonate system also controls acidity of the oceans (pH), which has important ramifications for many calcifying marine organisms. Clearly ACE/PACE needs to develop techniques to constrain surface pCO$_2$ and pH distributions model synthesized from satellite and in situ observations.

Direct measurements of the inorganic carbon system (pH, pCO$_2$, Talk & DIC) have been in place for many years as well as algorithms that allow the entire system to be constrained with only two of the components measured.

*Air-Sea CO$_2$ and O$_2$ Fluxes:*

One of the challenges facing the ACE/PACE missions is the remote estimation of the air-sea carbon dioxide fluxes. The simultaneous determination of air-sea oxygen fluxes puts important constraints on the ocean carbon cycle as well. Once assessments of the surface pCO$_2$ and dissolved oxygen distribution are available (with corresponding determinations of atmospheric CO$_2$ and O$_2$ levels to quantify air-sea differences) then estimates of the air-sea fluxes of CO$_2$ and O$_2$ can be easily determined knowing the exchange coefficient (which is a function of the wind speed) and the gas solubility (a function of temperature and often salinity).

In situ methods for determining air-sea CO$_2$ and O$_2$ fluxes require measurements of the air-sea differences in pCO$_2$ and O$_2$ concentrations, the exchange coefficient and a solubility model for the dissolved gas in question. Coupled atmosphere/ocean model inversions provide another path towards constraining air-sea fluxes of CO$_2$ and O$_2$. 
**Calcification:**

One of the most important repercussions of changes in ocean acidity is the potential effects that increasing acidity may have on the calcification rate of many organisms. Calcification involves the formation of solid CaCO$_3$ structures from seawater, such as the CaCO$_3$ laths found in coccolithophores as well as physical structures for many invertebrates (cf., corals, shellfish, etc.). Understanding the calcification rate is therefore useful for monitoring the effects of changes of ocean pH on ecosystem function as well as the formation of ballast materials which can affect the transmission of export production to depth. This area of research couples with the determination essential OPCC parameters for PFTs above (coccolithophores, etc.) and the monitoring of pH from satellite/model synthesis.

In situ methods for determining calcification rates via include the $^{14}$C bicarbonate microdiffusion PIC incorporation method and by the mass balance assessment of changes in PIC stocks.

**Nitrogen Fixation:**

Ultimately all new production in the ocean comes from nitrogen fixation. Hence, the prevalence of N limitation of net primary productivity in the bulk of the ocean is in turn driven by limits on the fixation of new nitrogen from N$_2$ in these systems. Changes in oceanic N inventory over time is driven by a balance between nitrogen fixation and denitrification and the state of the system has important ramifications for the efficiency of biological pump and the nature of the pelagic ecosystems, particularly in tropical and subtropical biomes. Trichodesmium is an important, although not the only, diazotroph in the sea and much previous work has been focused on the dynamics of Trichodesmium populations. This area of research again couples to the determination of PFTs above (Trichodesmium, etc.).

In situ methods for determining include $^{15}$N$_2$ incorporation and acetylene reduction incubations, geochemical mass balances, characterization of nifH genes.

**Constraining Essential OPCC Parameters from ACE/PACE:**

The determination of the essential OPCC parameters will require a synthesis of ACE/PACE satellite observations, field measurements (including process studies), algorithm development exercises and numerical modeling including data assimilation. Clearly, advanced coupled ocean-ecosystem-biogeochemical data assimilative capabilities are going to be needed to derive the OPCC essential variables from ACE/PACE observations. Further, data sets for developing and validating advanced satellite ocean color algorithms for the OPCC parameters. This discussion of what this integrated ACE/PACE algorithm/validation plan will be was left for future meeting. However, suggestions of field/modeling process experiments in support of these goals were discussed and presented below.

It was also noted that there are many supporting measurements that we assume will be available (from other sources) for use by the ACE/PACE mission. These parameters include mixed layer depth (MLD), sea surface temperature (SST), vector winds, sea surface height (SSH), sea surface salinity, daily integrated incident spectral solar irradiance, horizontal currents and model assessment of vertical water mass exchanges in the upper 500 m. In particular, there was concern that help was needed from the physical oceanography community to improve upper ocean vertical water mass exchanges.
Required Field / Modeling Studies to Accelerate the PACE of ACE:

The group spent a good deal of time detailing what field and modeling studies would be useful for accelerating the technologies required to retrieve OPCC parameters from the ACE mission. The five following suggestions grew organically out of discussions.

Characterization of OPCC Dynamics Across a Range of Ocean Biomes:

There are a variety of approaches that are used to derive the essential OPCC parameters as addressed above. Some are isotope incorporation methods while others measure relative concentrations of biogenic and inert gases and still others use mass balance approaches. Each has their advantages and disadvantages and inherent time scales, which are likely to be both context and/or location sensitive. The goal here is to understand the interrelationships among measurements of GPP, NPP, NCP and EP across a range of time evolving pelagic ecosystems.

The workshop participants concluded that a series of process studies across important pelagic ecosystems ranging from subtropical gyres to subpolar blooms to productive coastal waters under different time-evolving states are critical here. Besides OPCC parameters supporting measurements of phytoplankton pigment / biomass, PFT/PSD, inherent optical property characteristics and water-leaving radiance spectra must be measured. Further, mass balance approaches require determinations of stock concentrations to be followed over time. Thus, these OPCC intercomparison experiments need to be conducted in a Lagrangian frame following the water parcel as it evolves. These coupled experiments will enable a wide variety of approaches to be compared and will provide first order progress towards constraining OPCC parameters from satellite observations.

PFT/PSD Intercomparison:

The robust determination of PFT and PSD characteristics from satellite ocean color observations is a central goal of the ACE/PACE mission. It is planned that the hyperspectral observations planned for ACE/PCE will enable phytoplankton spectral properties to be deconvolved at least to a functional level. As described above, a variety of in situ methods have been developed and PFT and size are obvious entrees into coupled ecosystem/carbon cycle data assimilation models.

There have been several intercomparison activities aimed at evaluating methods for assessing PFTs and an IOCCG working group has been convened on the remote characterization of PFT’s using ocean color imagery (http://www.ioccg.org/groups/PFT.html). However, we envision that more detailed work is required where appropriate field and imagery data sets are collected across a range of conditions. Both field and laboratory studies are needed to compare various approaches for characterizing PFT and the PSD. Again a set of intercomparison cruises comparing the various direct and indirect methods of assessing PFT/PSD is needed across a range of biomes. Methods to compare include chemotaxonomic analyses from HPLC phytoplankton pigment analyses, microscopic imagery or flow cytometer cell counts and characterization, optical and electrostatic determinations of the PSD. These must be supported by optical measurements of hyperspectral reflectance spectra, phytoplankton absorption and related inherent optical properties. Simultaneous measurements of the particulate organic and inorganic carbon (POC and PIC) concentrations of bulk seawater and of the different PFT/PSD components are also needed.

Expanding Existing Observational Programs to Include OPCC Parameters:
The time to collect the data required to build OPCC algorithms is now, not after the ACE/PACE missions are launched. Long line observations of appropriate variables seem like a good way of expanding our global data set cheaply and easily. Opportunities exist from CLIVAR / Repeat Hydrography, Atlantic Meridional Transect (AMT), TOGA/TAO refurbishment and similar cruises. The goal here is to expand these measurements suites made from these to include the eight essential OPCC parameters along with standard ocean color observations. This requires support from NASA to enable these “cruise of opportunity” to expand the available data set of OPCC parameters.

Observing System Simulation Experiments:

Data assimilation techniques provide a powerful mechanism to examine how new observational systems such as ACE will advance the representation of key processes in the ocean. A class of experiments called "Observing System Simulation Experiments" (OSSE) involve twin simulation experiments: A model is sampled in a way that resembles real observations and those observations (with uncertainties) are then assimilated into an alternative model. This twin model provides a mechanism to determine regions of high sensitivity or influence of those "new" observations, examine how much value is added for each measurement type, and provide estimates of how much the "new" measurements will help constrain uncertainties in budgets (e.g. air-sea CO₂ flux). Such experiments have been successfully undertaken to examine how ARGO floats would benefit ocean circulation estimates and how satellite derived salinity will help constrain salinity budgets. Such experiments will be an essential part of examining how each OPCC parameters will impact the ACE/PACE key science questions, and provide framework for examining the consequence of each parameter measurement uncertainties. In particular experiments can be designed to provide quantitative limits of errors estimates for the usefulness of each measurement type.

Airborne Lidar and OPCC Parameters

The complete ACE mission includes lidar observations of aerosol loads and characteristics, along with the full suite of other proposed observational sensors. With respect to ACE Ocean Science Goals, these additional measurements of the mission have clear value for improving atmospheric corrections during retrievals of ocean water leaving radiances. In addition to atmospheric corrections, the existence of a profiling LIDAR in the ACE instrument suite provides new opportunities for actively probing ocean ecosystems to depths below those detectable with the passive ocean radiometer. Studies to date, including airborne lidar demonstrations, indicate that an eye-safe ACE lidar could provide meaningful returns from below the ocean surface to depths approaching 3 optical attenuation lengths. In the clearest oceans, this translates to many tens of meters below the surface. Based on optical modeling, these measurements would commonly reach below the active mixing layer to depths where strong vertical gradients in ecosystem properties exist. Thus, by combining LIDAR and passive ocean measurements, the ACE mission could provide the first truly 3-D view of ocean ecosystems and tremendous new insights into the link between ecosystem dynamics and ocean physics. Further, LIDAR retrievals from within the surface mixed layer will provide impendent assessments of particulate scattering coefficients for comparison to retrievals from passive ocean color data. To realize these benefits from the ACE LIDAR, additional optical modeling studies are needed for algorithm development. Field studies are also needed that combine continuous, in-line measurements of ocean optical properties with simultaneous airborne lidar measurements.
Future Planning Needed:

This workshop did not get us towards an integrated ACE/PACE algorithm/validation plan. This has to happen in the future and a meeting is planned in the near-future to address this issue.

An important step in the planning of the ACE/PACE missions will be to have an integral modeling component. Biogeochemical data assimilation frameworks will strongly benefit from these parameters, but such frameworks will also provide a mechanism to help optimize the measurement network design through OSSE type experiments.

References:

ACE Ocean Ecology White Paper Draft, 2010:

ACE Ocean Ecology White Paper Appendix Draft, 2010:

NASA Climate Architecture Plan, 2010:
http://science.nasa.gov/media/medialibrary/2010/07/01/Climate_Architecture_Final.pdf.
Appendices:

1. Agenda:

Monday June 6 (there will be breaks - do not worry)
8:30 Meet - coffee/sweets will be available
9:00 Goals objectives of the workshop – Dave Siegel
9:10 ACE/PACE - plans and white paper science questions – Chuck McClain
10:00 Biogeochemical cycle overview relevant for ACE - John Marra
11:00 Satellite ocean color paradigm tutorial – Dave Siegel
12:00 Lunch
1:00 Regroup - discuss directions
1:30 Status of in situ science in support of satellite ocean color missions - Jeremy Werdell
2:00 Presentations by participants - 15 minutes max each
5:00 Regroup discuss
6:30 Group Dinner

Tuesday
8:30 Meet up - coffee/sweets will be available
9:00 Regroup discuss working groups (approaches to answering ACE SQ's, cal/val/algo plans, standards, others??)
9:30 Complete participant presentations...
12:00 Lunch
1:00 Working groups
3:00 Decide on goals and writing responsibilities....
5:00 Regroup discuss
6:30 Group Dinner

Wednesday
8:30 Meet up
9:00 Regroup discuss working groups (approaches to answering ACE SQ's, cal/val/algo plans, standards, others??)
12:00 Breakup

WRT presentations, please remember that 1/3 of the room knows everything about what you and another 1/3 will know practically nothing. We want to get everyone up to about the same level. So, please think about your presentation along the lines of teaching rather than presenting your latest, greatest research results. OK? Let me know if you want any specific guidance about your presentation. ALSO, PLAN FOR 15 MINUTES!!
### 2. Participant and Presentation List

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