

Ocean Ecosystem Measurement Requirements: ACE Ocean Team Perspective

GeoCAPE Science Team Meeting
Sept. 22, 2009

Chuck McClain
NASA/GSFC

Ocean Ecology Working Group

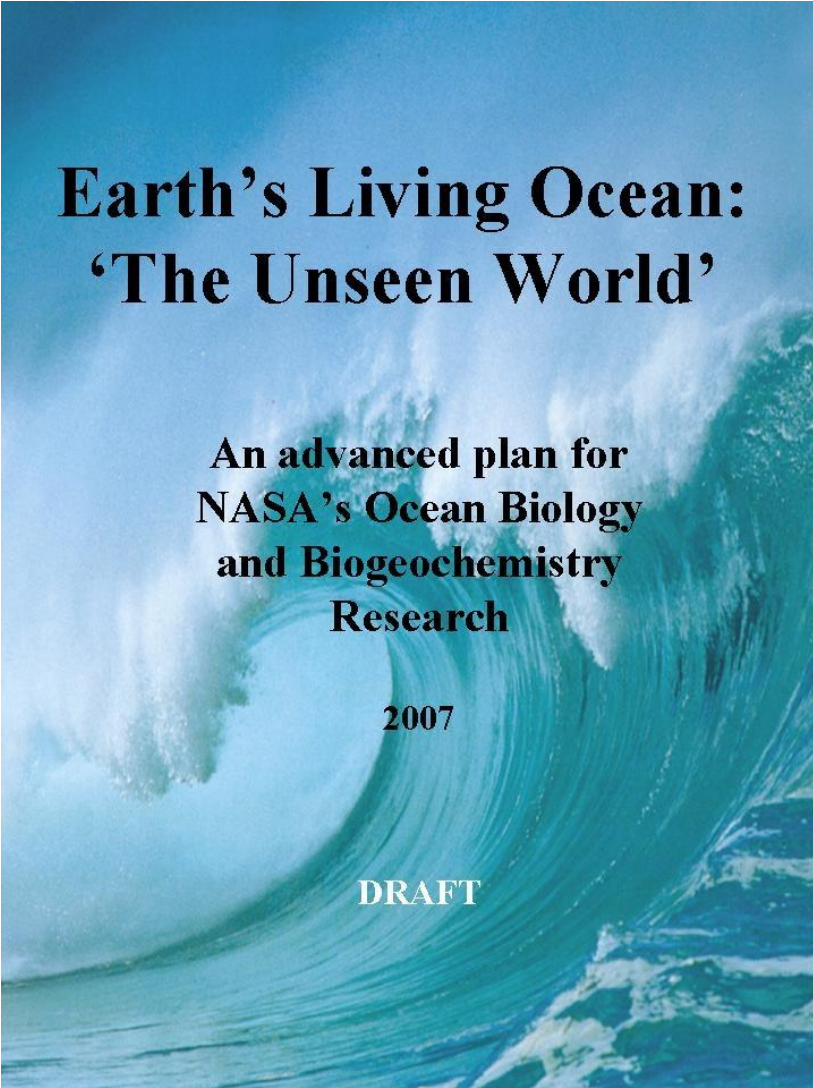
Chuck McClain: Chair

Paula Bontempi: Co-chair

- Zia Ahmad (NASA/GSFC*; **OBPG**)
- Bob Barnes (NASA/GSFC*; **OBPG**)
- Mike Behrenfeld (Oregon State U.)
- Emmanuel Boss (U. of Maine)
- Steve Brown (NIST)
- Jacek Chowdhary (NASA/GISS)
- Robert Frouin (U. California/San Diego)
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- Stan Hooker (NASA/GSFC; **field campaign WG**)
- Yong Hu (NASA LaRC)
- Stephane Maritorena (UC/Santa Barbara)
- Gerhard Meister (NASA/GSFC*; **OBPG**)
- Norm Nelson (UC/Santa Barbara; **field campaign WG**)
- Dave Siegel (UC/Santa Barbara)
- Rick Stumpf (NOAA/NOS)
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*contract staff

Community Plan for NASA Ocean Biology & Biogeochemistry Program



Earth's Living Ocean: 'The Unseen World'

An advanced plan for
NASA's Ocean Biology
and Biogeochemistry
Research

2007

DRAFT

- A plan for the NASA OBB program
- Science to Requirements to Strategies to Missions
- Community plan
- Intended as a “living document”
- Under NRC review
 - Draft statement of task completed
 - NASA, NOAA, NSF, ONR

The 4 NASA OBB Questions

- (1) How are ocean **ecosystems** and the biodiversity they support influenced by climate and environmental variability and change, and how will these changes occur over time?
- (2) How do carbon and other elements transition between ocean pools and pass through the Earth System, and how do **biogeochemical fluxes** impact the ocean and Earth's climate over time?
- (3) How (and why) is the diversity and geographical distribution of coastal marine **habitats** changing, and what are the implications for the well-being of human society?
- (4) How do **hazards** and pollutants impact the hydrography and biology of the coastal zone? How do they affect us, and can we mitigate their effects?

NASA Ocean Biogeochemistry Climate Data Records

- CDRs drive sensor stability and derived product accuracy requirements
- Ocean Products
 - **Normalized water-leaving radiances**
 - **Chlorophyll-a & other plant pigment concentrations**
 - **Primary production**
 - **Inherent optical properties (IOPs; spectral absorption & scattering coefficients)**
 - **Particulate organic carbon concentration**
 - **Calcite concentration**
 - **Colored dissolved organic matter (CDOM)**
 - **Photosynthetically available radiation (PAR)**
 - Particle size distributions & composition (biogenic, mineral, etc.)
 - Functional/taxonomic group distributions
 - Phytoplankton carbon
 - Physiological properties (e.g., C:Chl, fluorescence quantum yields)
- Ocean-Aerosol Products TBD
- Requirements for in situ observations
 - On-orbit “vicarious” calibration with an expanded measurement network)
 - Improved in situ instrumentation & measurement protocols
 - Coordinated process study-cal/val field experiments

Current OBB CDRs

Candidate OBB CDRs

Research products



ACE Ocean Ecosystems STM

Goddard
Space
Flight Center

Category	Focused Questions*	Approach	Maps to Science Question	Measurement Requirements	Instrument Requirements	Platform Requirements	Other Needs
Ocean Biology	1 What are the standing stocks, composition, & productivity of ocean ecosystems? How and why are they changing? [OBB1]	Quantify phytoplankton biomass, pigments, optical properties, key groups (functional/HABS), and productivity using bio-optical models & chlorophyll fluorescence	1 2 6	Water-leaving radiances in near-ultraviolet, visible, & near-infrared for separation of absorbing & scattering constituents and calculation of chlorophyll fluorescence	Ocean Radiometer <ul style="list-style-type: none"> • 5 nm resolution 350 to 755 nm <ul style="list-style-type: none"> ▷ 1000 – 1500 SNR for 15 nm aggregate bands UV & visible and 10 nm fluorescence bands (665, 678, 710, 748 nm centers) ▷ 10 to 40 nm width atmospheric correction bands at 748, 765, 820, 865, 1245, 1640, 2135 nm • 0.1% radiometric temporal stability (1 month demonstrated prelaunch) • 58.3° cross track scanning • Sensor tilt ($\geq 20^\circ$) for glint avoidance • Polarization insensitive ($< 0.5\%$) • 1 km spatial resolution @ nadir • No saturation in UV to NIR bands • 5 year minimum design lifetime 	Orbit permitting 2-day global coverage of ocean radiometer measurements	Global data sets from missions, models, or field observations: <i>Measurement Requirements</i> (1) Ozone (2) Total water vapor (3) Surface wind velocity (4) Surface barometric pressure (5) NO ₂ concentration (6) Vicarious calibration & validation** (7) Full prelaunch characterization (2% accuracy radiometric)
		Measure particulate and dissolved carbon pools, their characteristics and optical properties	2 3	Total radiances in UV, NIR, and SWIR for atmospheric corrections			
	Quantify ocean photobiochemical & photobiological processes	2 4	Cloud radiances for assessing instrument stray light				
	Estimate particle abundance, size distribution (PSD), & characteristics	1 3 2	High vertical resolution aerosol heights, optical thickness, & composition for atmospheric corrections				
	2 How and why are ocean biogeochemical cycles changing? How do they influence the Earth system? [OBB2]	Assimilate ACE observations in ocean biogeochemical model fields of key properties (cf., air-sea CO ₂ fluxes, export, pH, etc.)	2	Subsurface particle scattering & depth profile	Lidar <ul style="list-style-type: none"> • 0.5 km aerosol vertical resolution • 2 m sub-surface resolution • $< 0.3\%$ polarization misalignment • 0.0001 km⁻¹sr⁻¹ aerosol backscatter sensitivity at 532 nm after averaging • < 4 ns e-folding transient response • Brillouin scattering capability; Receiver FOVs: 0-60 m; 0-120 m. 	Storage and download of full spectral and spatial data	(7) Full prelaunch characterization (2% accuracy radiometric)
		Compare ACE observations with ground-based and model data of biological properties, land-ocean exchange in the coastal zone, physical properties (e.g., winds, SST, SSH, etc), and circulation (ML dynamics, horizontal divergence, etc)	3 4 5 6	Broad spatial coverage aerosol heights and single scatter albedo for atmospheric correction. Subsurface polarized return for typing oceanic particles			
	3 What are the material exchanges between land & ocean? How do they influence coastal ecosystems, biogeochemistry & habitats? How are they changing? [OBB1,2,3]	Combine ACE ocean & atmosphere observations with models to evaluate (1) air-sea exchange of particulates, dissolved materials, and gases and (2) impacts on aerosol & cloud properties	4	Supporting Field & Laboratory Measurements <ul style="list-style-type: none"> • Primary production (NPP) measurement & round-robin algorithm testing • Inherent optical properties (IOPs) instrument & protocols development, field measurement comparisons (coastal and open ocean) • Measure key phytoplankton groups across ocean biomes (coast/open ocean) • Expanded global data sets of NPP, CDOM, DOM, pCO₂, PSDs, IOPs, fluorescence, vertical organic particle fluxes, bio-available Fe concentrations 			
		Assess ocean radiant heating and feedbacks	5				
	4 How do aerosols & clouds influence ocean ecosystems & biogeochemical cycles? How do ocean biological & photochemical processes affect the atmosphere and Earth system? [OBB2]	Conduct field sea-truth measurements and modeling to validate retrievals from the pelagic to near-shore environments	1 4 2 5 3 6	Modeling <ul style="list-style-type: none"> • Expand model capabilities to assimilate variables such as NPP, IOPs, and phytoplankton species/functional group concentrations. • Others (model processes, etc.)? 			
		What is the distribution of algal blooms and their relation to harmful algal and eutrophication events? How are these events changing? [OBB1,4]					

* ACE focused questions are traceable to the four overarching science questions of NASA's Ocean Biology and Biogeochemistry Program [OBB1 to OBB4] as defined in the document: *Earth's Living Ocean: A Strategic Vision for the NASA Ocean Biological and Biogeochemistry Program* (under NRC review)

** See ACE Ocean Ecosystem white paper for specific vicarious calibration & validation requirements

Measurement Requirements

Ocean Radiometer

- Water-leaving radiances in near-ultraviolet, visible, & near-infrared for separation of absorbing & scattering constituents and calculation of chlorophyll fluorescence
- Subsurface particle scattering & depth profile
- Total radiances in UV, NIR, and SWIR for atmospheric corrections
- Cloud radiances for assessing instrument stray light

Lidar

- High vertical resolution aerosol heights, optical thickness, & composition for atmospheric corrections
- Subsurface particle scattering & depth profile

Polarimeter

- Broad spatial coverage aerosol heights and single scatter albedo for atmospheric correction.
- Subsurface polarized return for typing oceanic particles

Pigment separation & phytoplankton functional group identification

Marine particulates

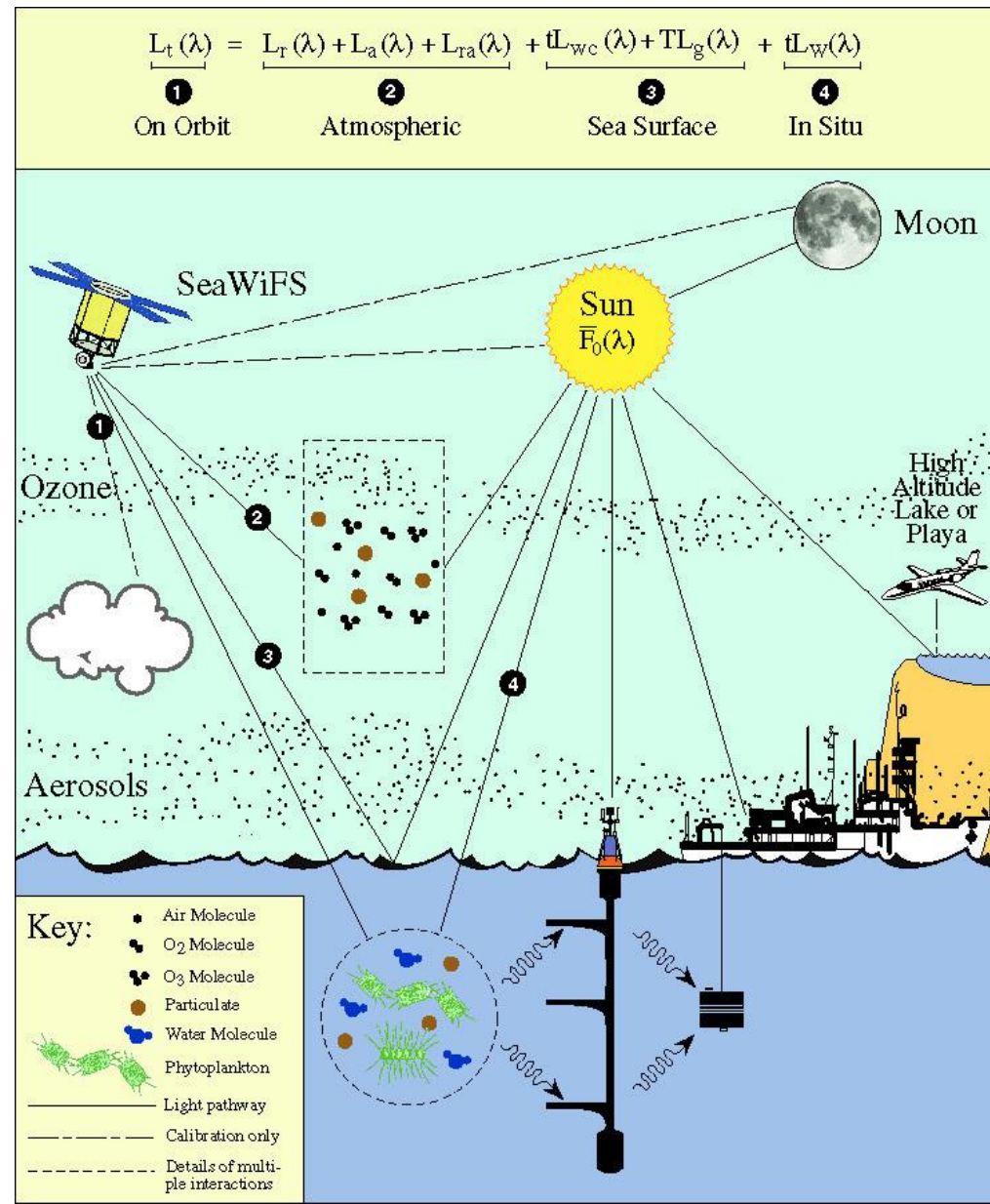
Atmospheric correction

Instrument artifact correction

Calibration/Validation Paradigm

Program Elements:

- **Laboratory** - prelaunch sensor calibration & characterization
- **On-orbit** - solar and lunar observations are used to track changes in sensor response
- **Field** - comparison of satellite data retrievals to in-water, above-water and atmospheric observations
 - Vicarious calibration - adjust instrument gains to match water-leaving radiances
 - Product validation (water-leaving radiances, chl-a, etc.)



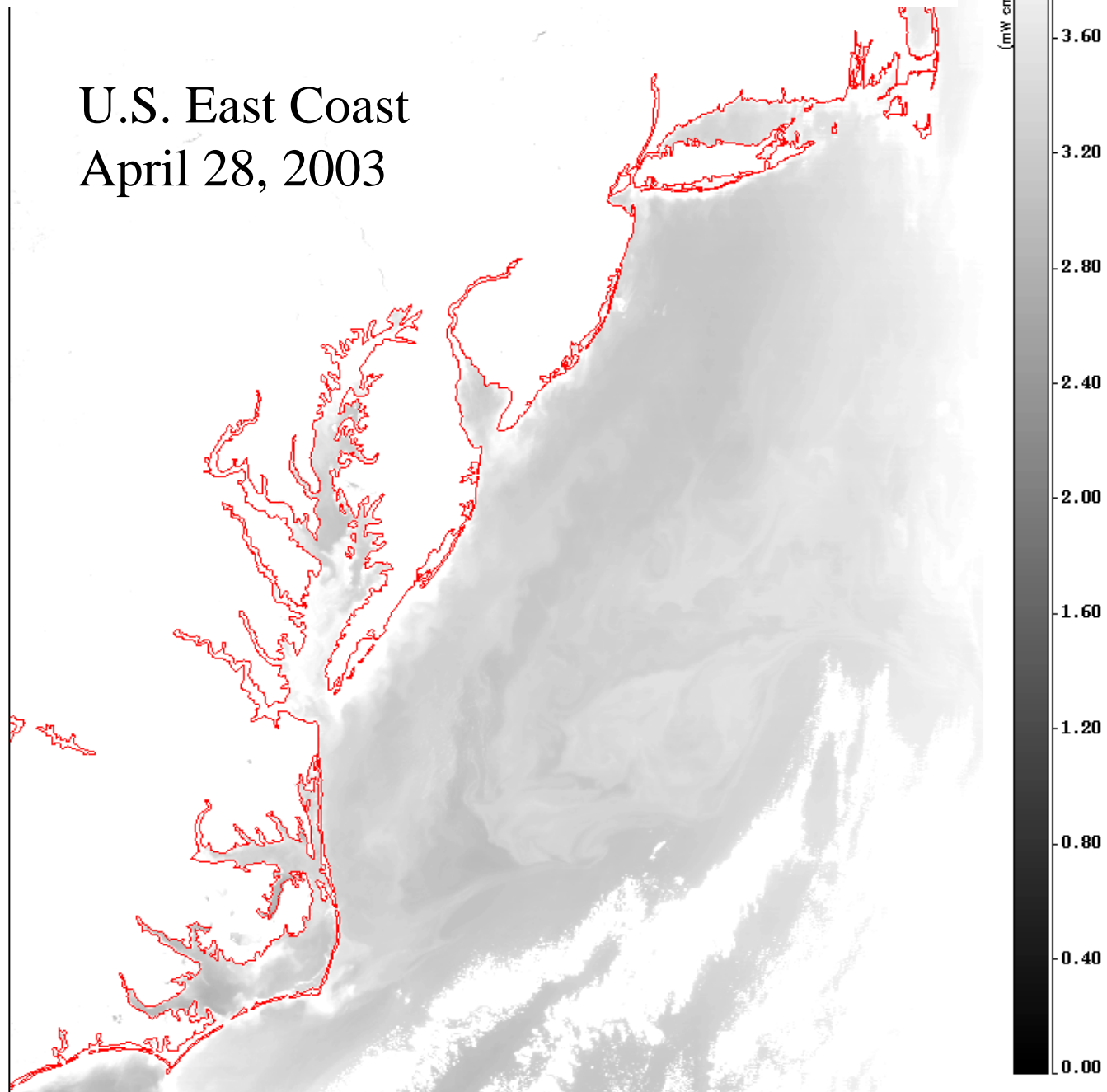
Atmospheric Correction: An Example

U.S. East Coast
April 28, 2003

Green wavelength
551 nm

Total top-of-the-
atmosphere radiance

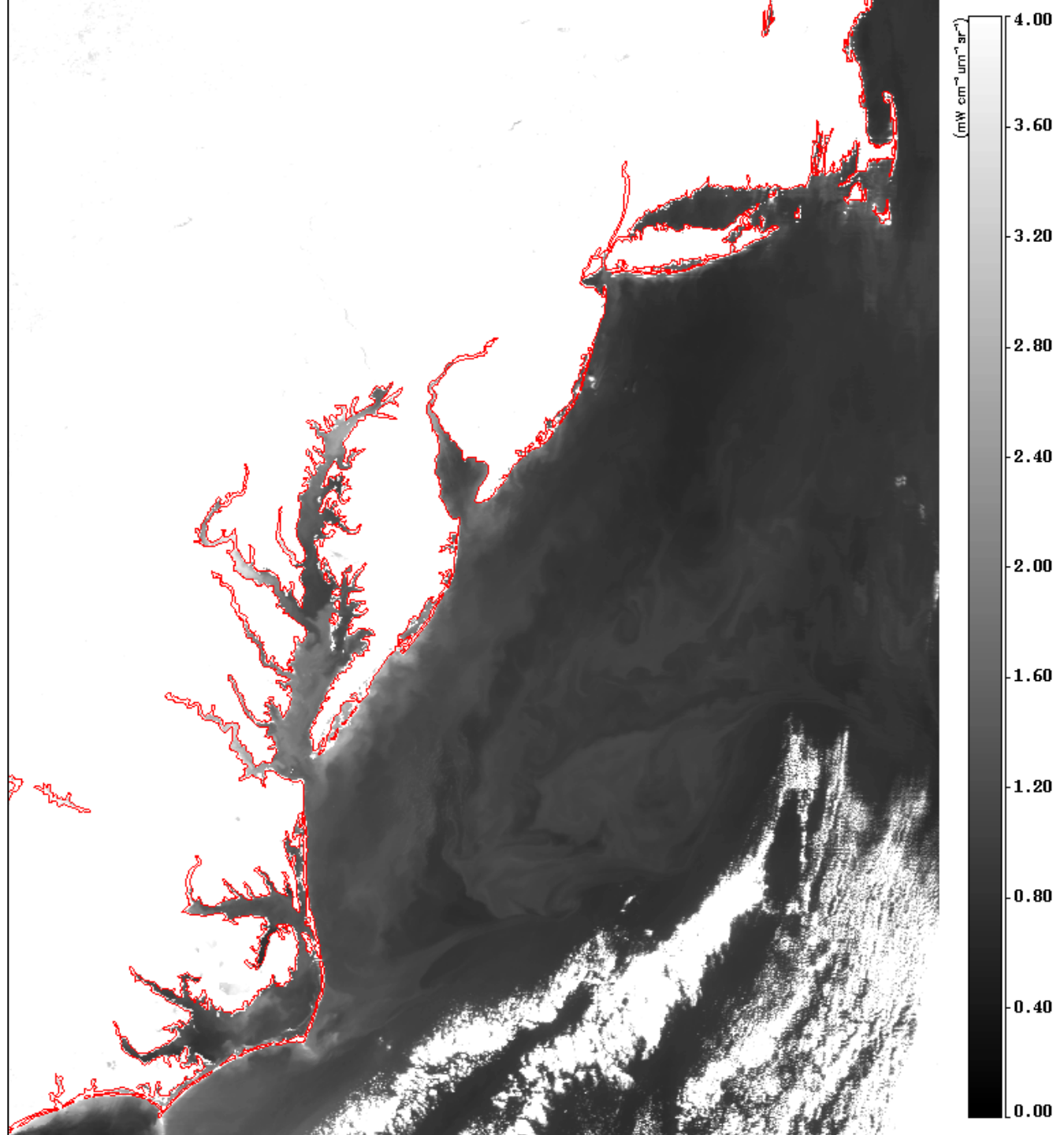
$0 - 4 \text{ mW/cm}^2 \text{ sr } \mu\text{m}$



Green wavelength
551 nm

Total top-of-the-
atmosphere radiance
corrected for ozone
absorption and
Rayleigh (gas
molecule) scattering

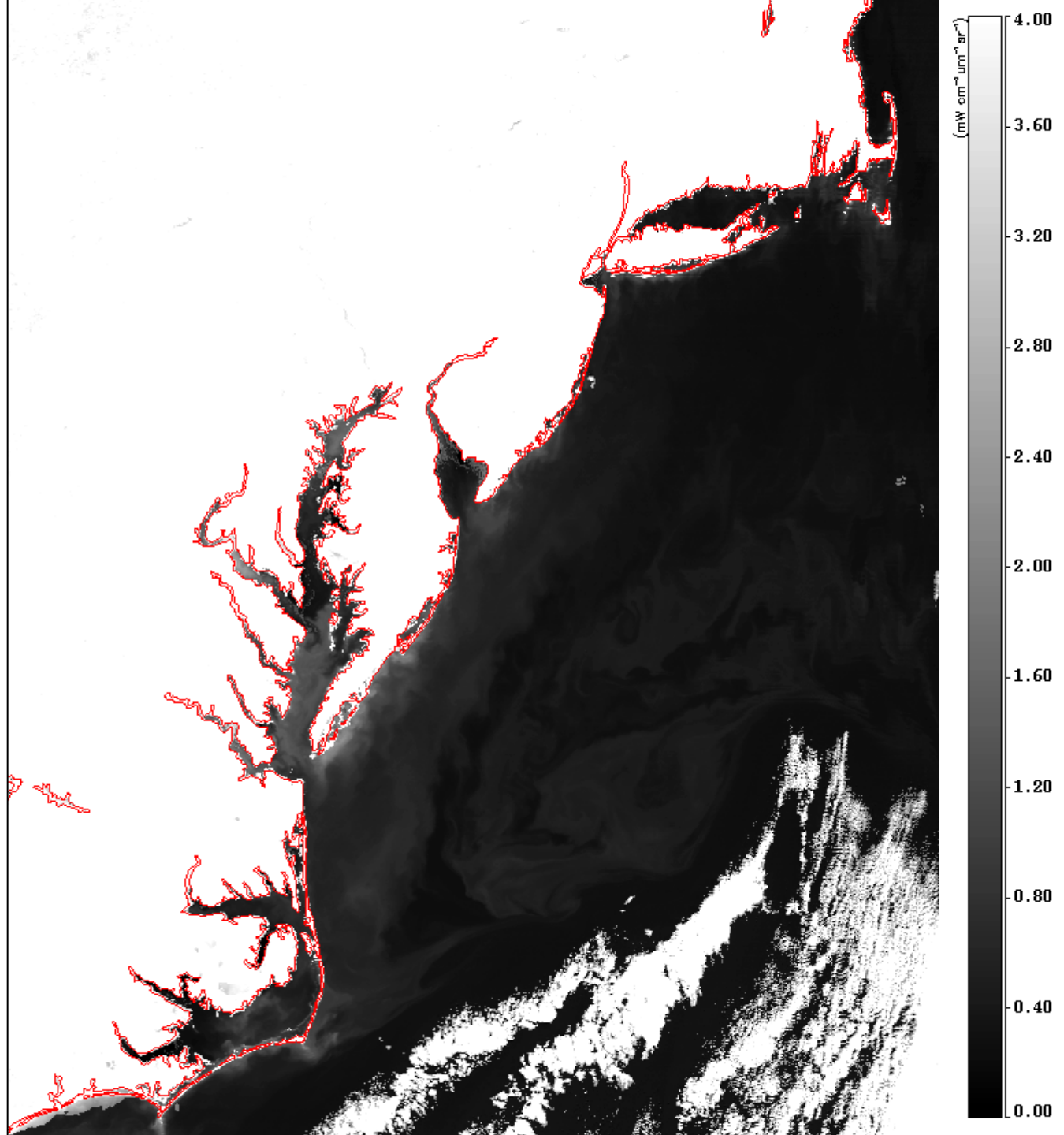
$0 - 4 \text{ mW/cm}^2 \text{ sr } \mu\text{m}$



Green wavelength
551 nm

Total top-of-the-
atmosphere radiance
corrected for ozone
absorption, Rayleigh
& aerosol scattering

0 – 4
 $\frac{\text{mW}}{\text{cm}^2 \text{ sr } \mu\text{m}}$

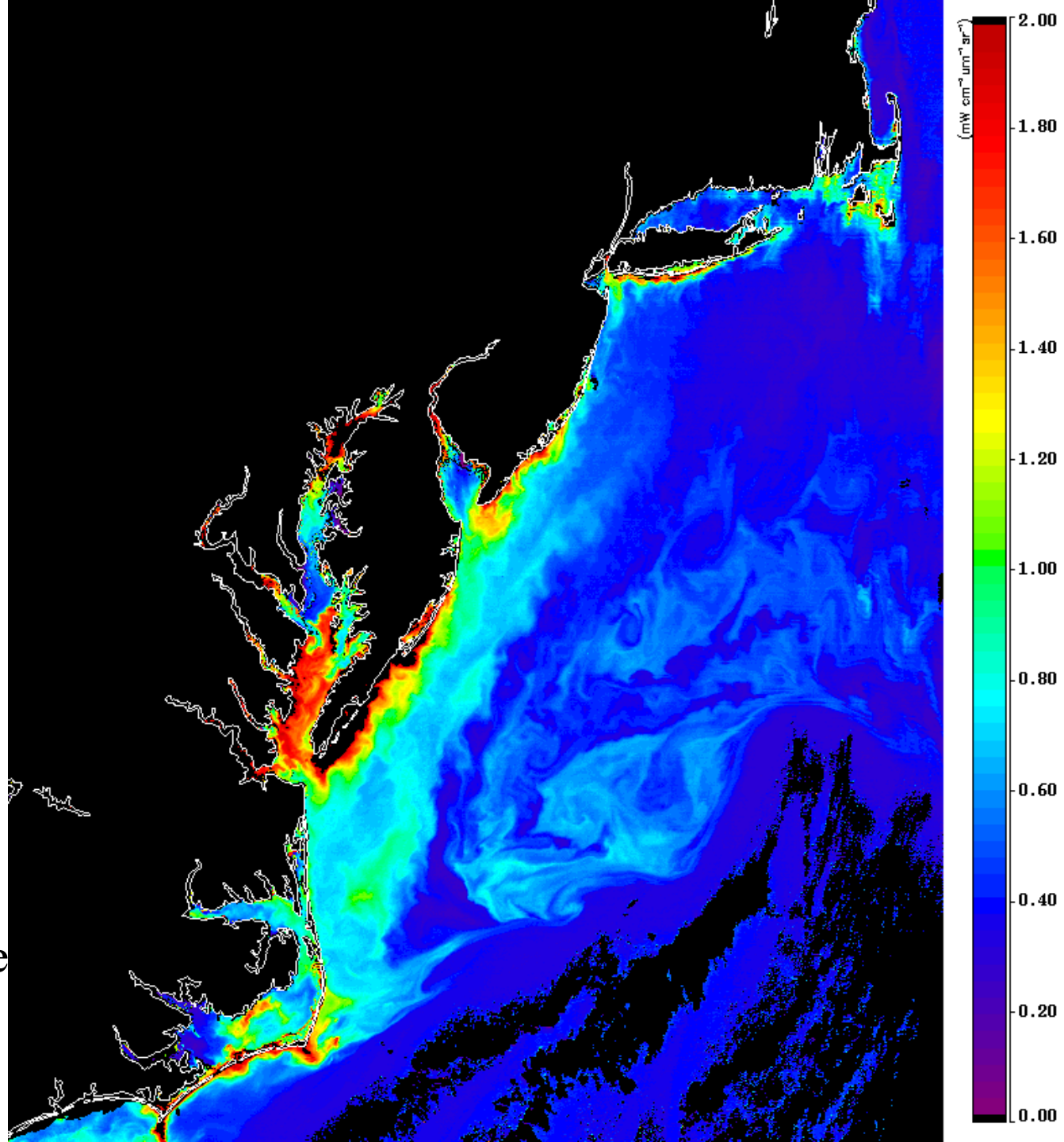


Green wavelength
551 nm

Normalized water-
leaving radiance

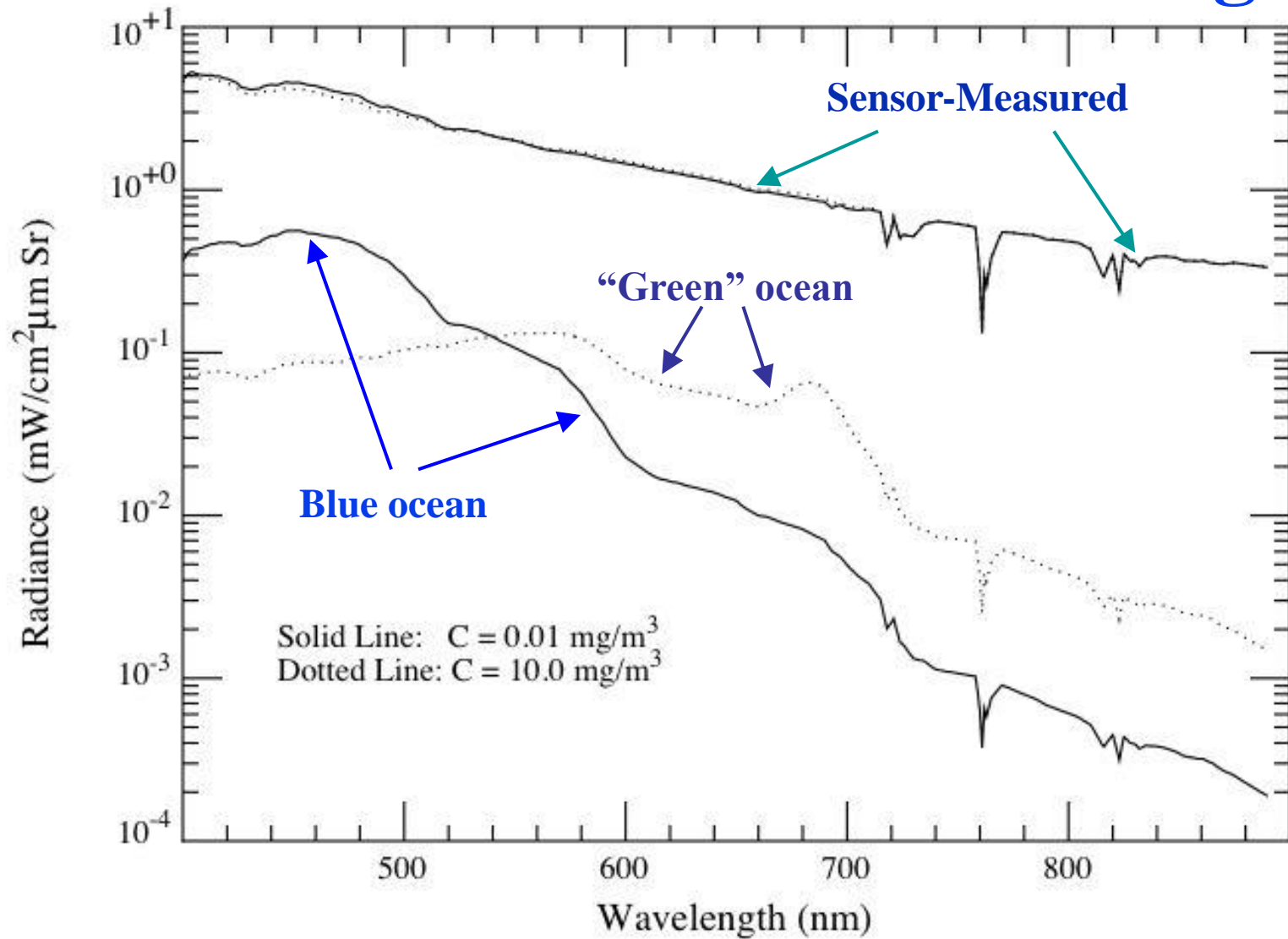
$0 - 2 \text{ mW/cm}^2 \text{ sr } \mu\text{m}$

Normalized: Lw is
transformed to radiance
normal to the surface
taking into account the
ocean BRDF



**Ocean Radiometer
Measurement Requirements:
Spectral Coverage**

Ocean Color Remote Sensing

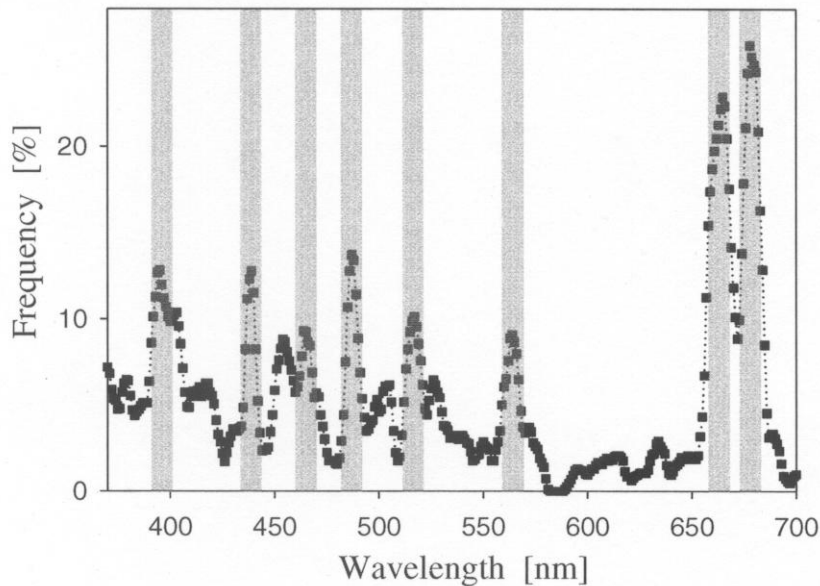


- ▶ Atmospheric Correction (removes > 85% TOA radiance)
- ▶ Calibration (0.5% error in TOA introduces ~ 5% error in Lw)

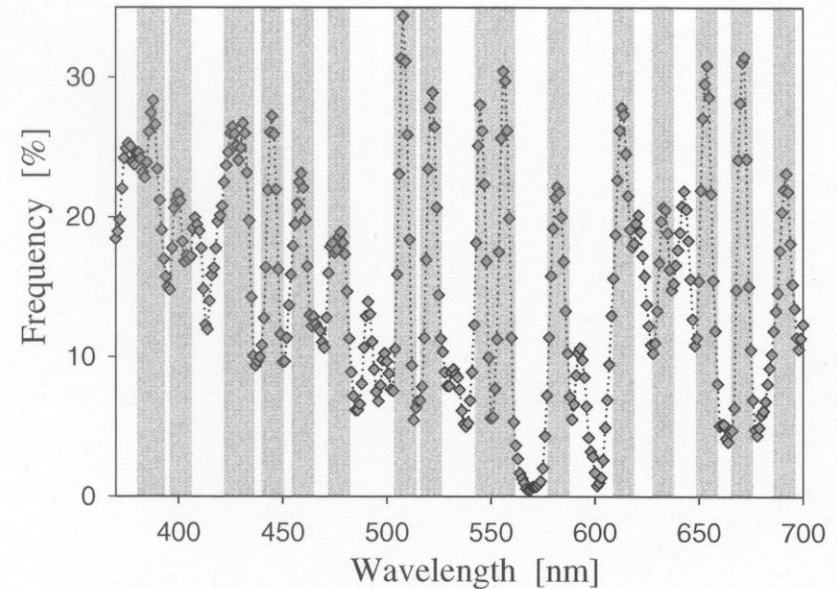
Spectral Band Considerations

- Multispectral bands
 - Particle absorption & scattering spectral features, e.g., phytoplankton pigments & suspended sediments
 - Dissolved constituent absorption spectral features, e.g., CDOM
 - Fluorescence peaks, e.g., chlorophyll
 - Atmospheric absorption bands of various gases (O_3 , O_2 , NO_2 , water vapor, etc.)
 - Atmospheric correction ancillary data availability
 - Band centers & bandwidths
 - Signal-to-Noise Ratios (SNRs)
- Hyperspectral data
 - Ocean reflectance 2nd & 3rd derivative spectral peaks
 - Bandwidths
 - SNR vs spatial variability scales

Phytoplankton Functional Groups: Spectral Derivative Analyses



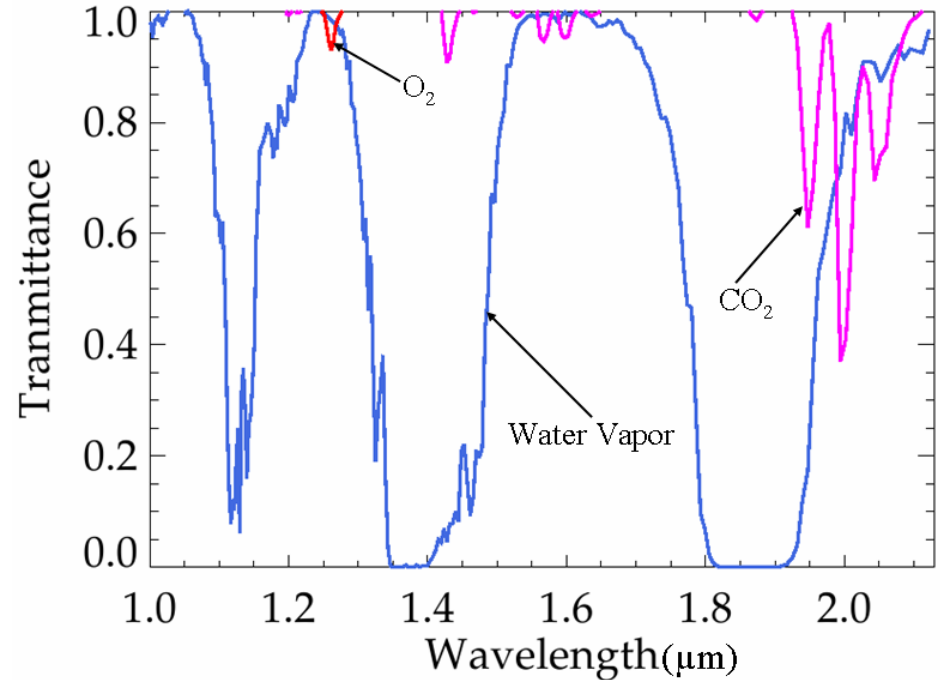
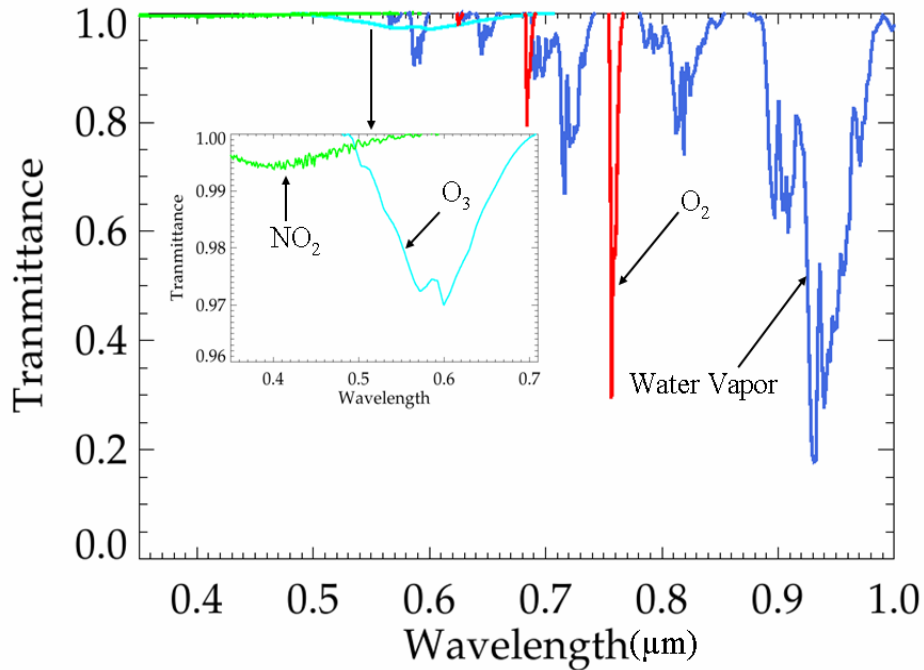
Spectral distribution of the frequency where the 1st-order derivative of ocean reflectance = 0.



Spectral distribution of the frequency where the 2nd-order derivative of ocean reflectance = 0.

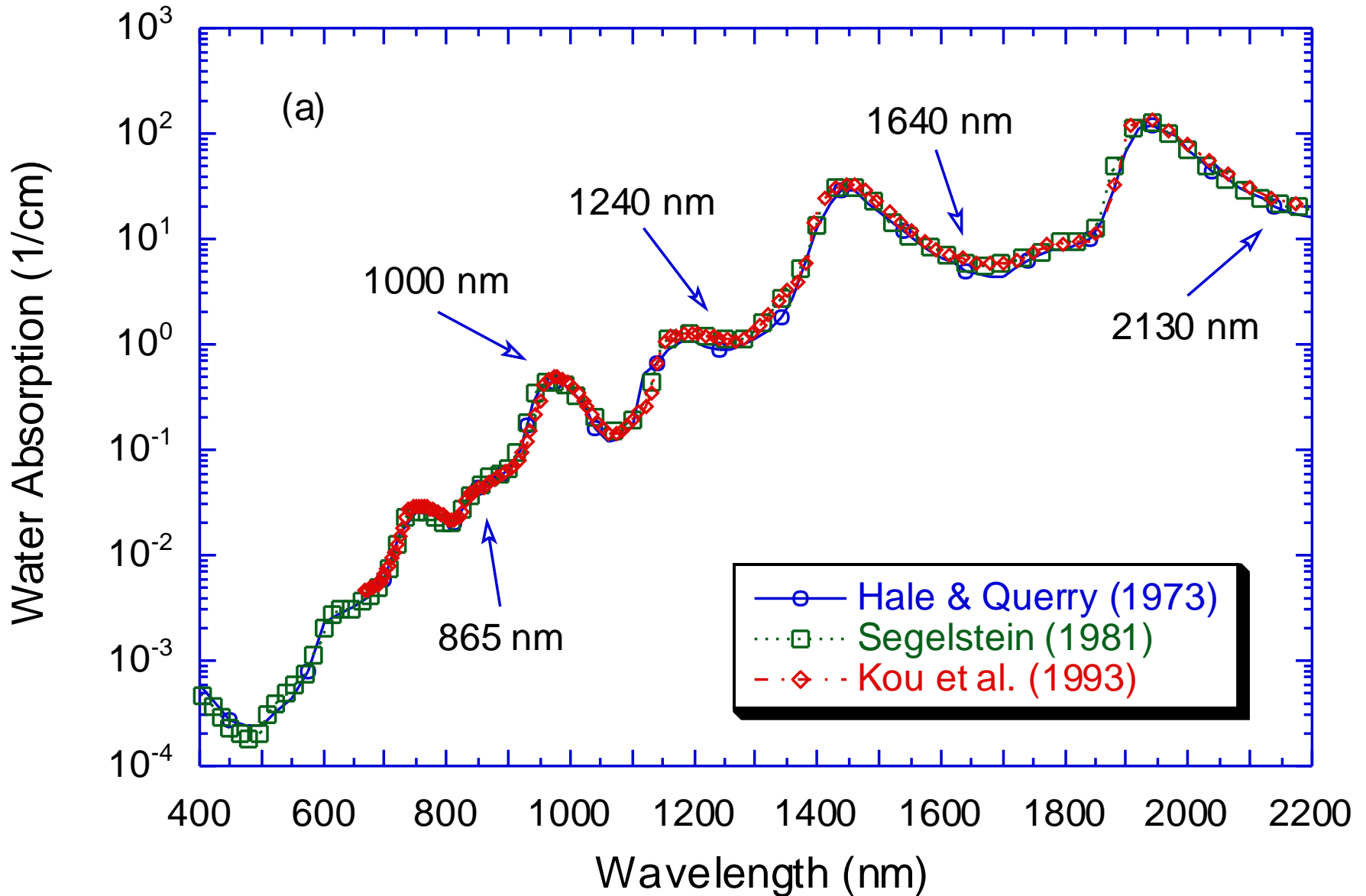
Lee, Z-P., K. Carder, R. Arnone, & M-X. He, Determination of primary spectral bands for remote sensing of aquatic environments, *sensors*, 7, 3428-3441, 2007.

Atmospheric Transmission Considerations



- Trace gases like water vapor, oxygen, ozone & others produce many absorption features in atmospheric transmittance
- Option 1: Avoid in ocean biology sensor design or
- Option 2: Make corrections in data processing (requires accurate estimates of concentrations & vertical distributions).

Water Absorption



**Results from SWIR
Atmospheric
Correction for
turbid ocean
waters: US east
coast**

**MODIS-Aqua
True Color Image**

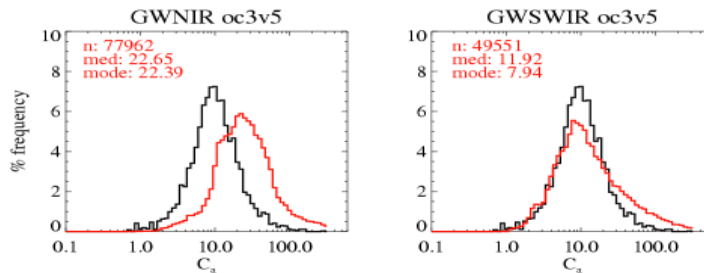
U.S. East Coastal

**April 6,
2004**



SWIR-based Corrections: Impact on Chlorophyll Retrievals

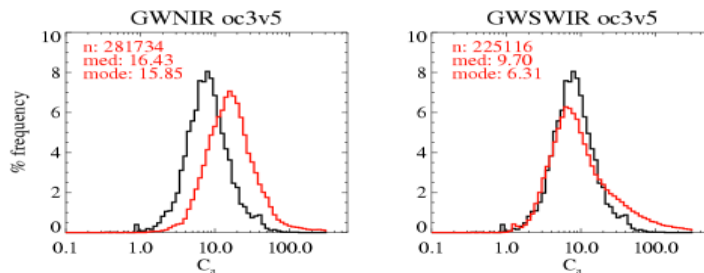
Upper Bay, ALL in situ = n: 3663, med: 10.52, mode: 10.00
color legend: in situ MODIS-Aqua



**Chlorophyll
(mode)**

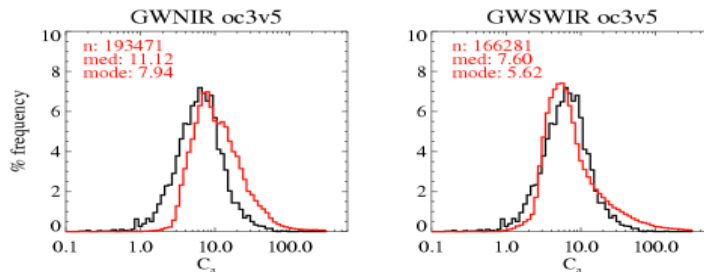
Field: 10 mg/m³
w/o SWIR: 22 mg/m³
w/ SWIR: 8 mg/m³

Mid Bay, ALL in situ = n: 5814, med: 8.43, mode: 7.94
color legend: in situ MODIS-Aqua

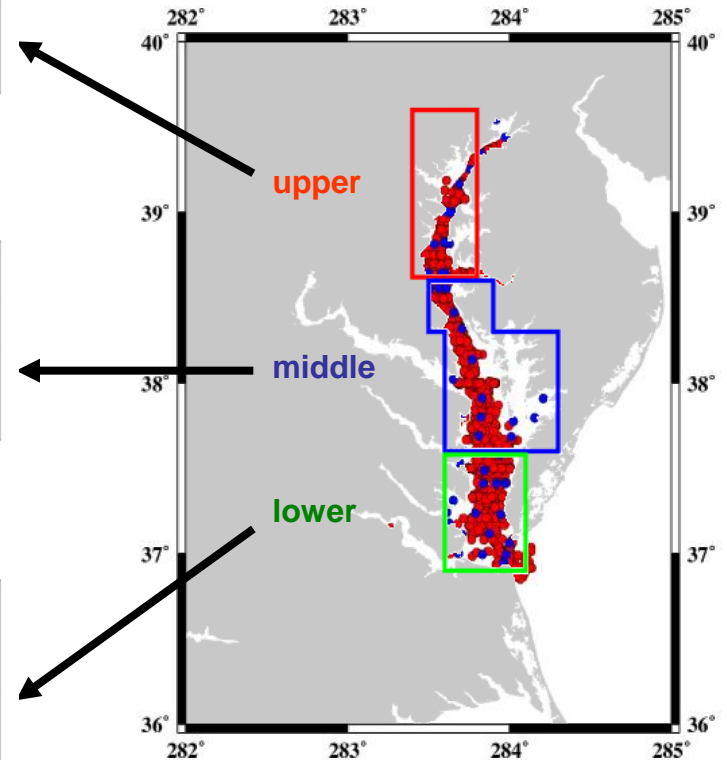


Field: 8 mg/m³
w/o SWIR: 16 mg/m³
w/ SWIR: 6 mg/m³

Lower Bay, ALL in situ = n: 7204, med: 6.50, mode: 6.31
color legend: in situ MODIS-Aqua



Field: 6 mg/m³
w/o SWIR: 8 mg/m³
w/ SWIR: 6 mg/m³



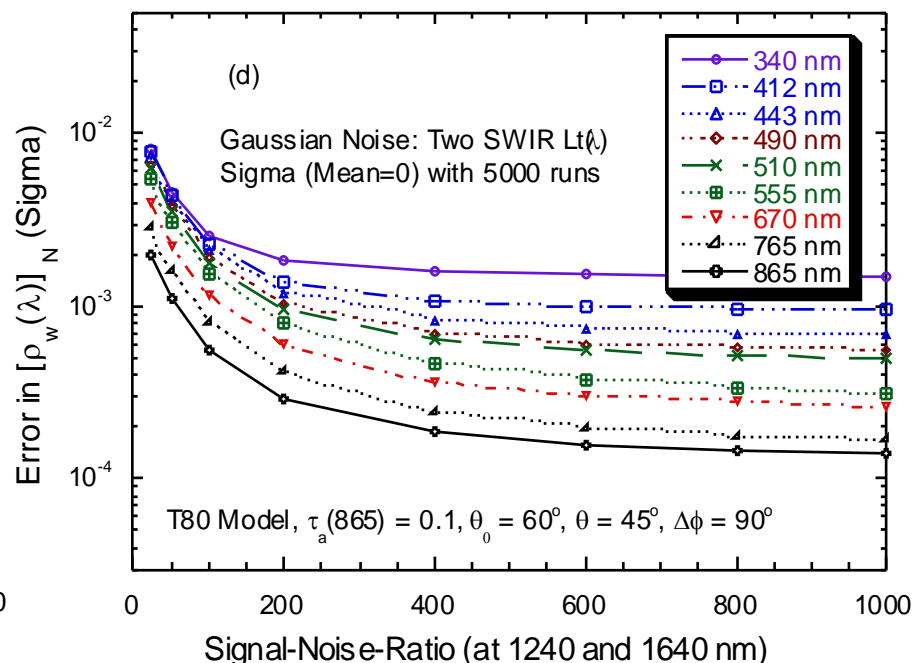
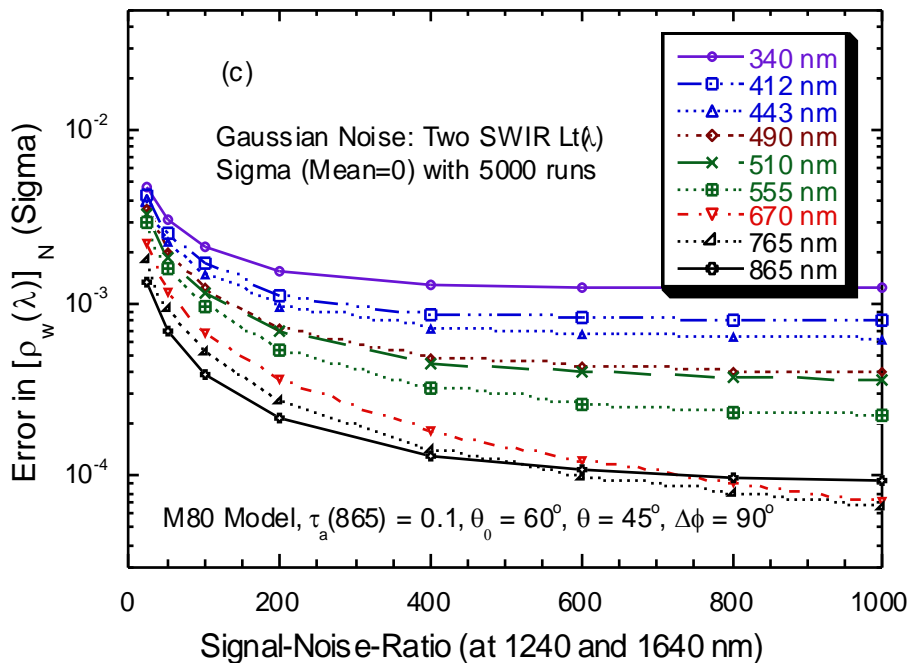
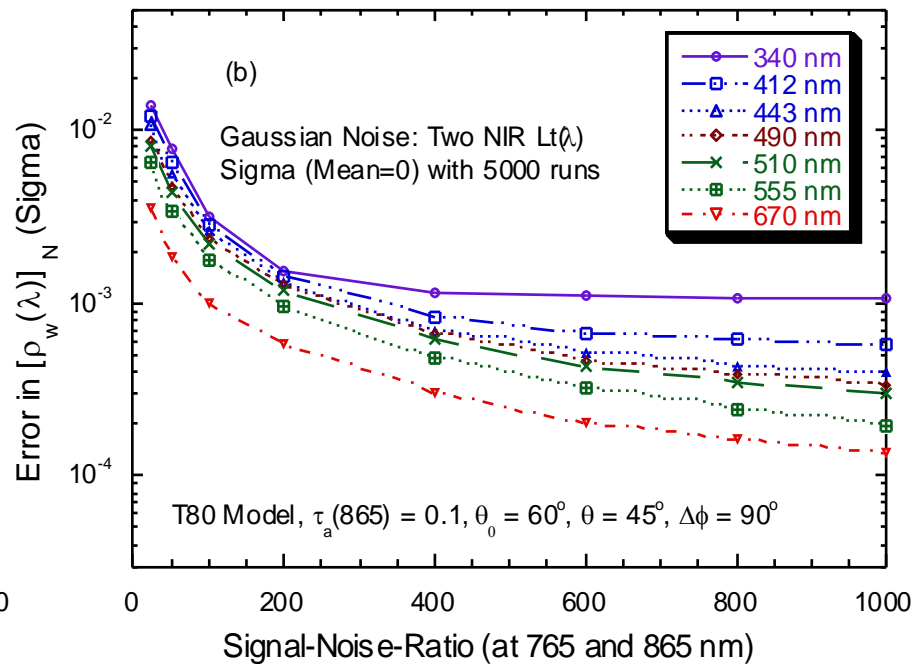
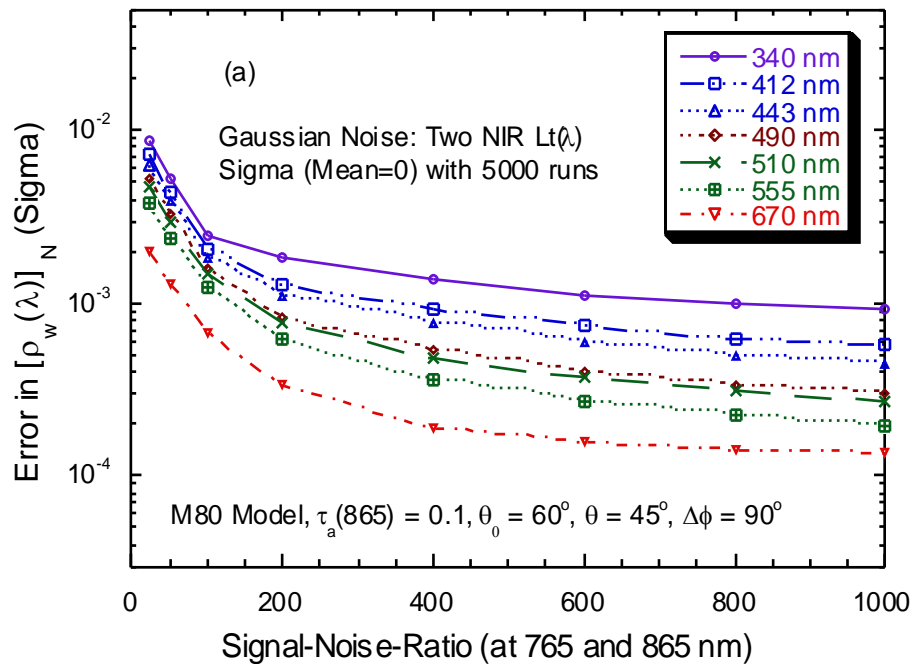
Chesapeake Bay

Unpublished, OBPG

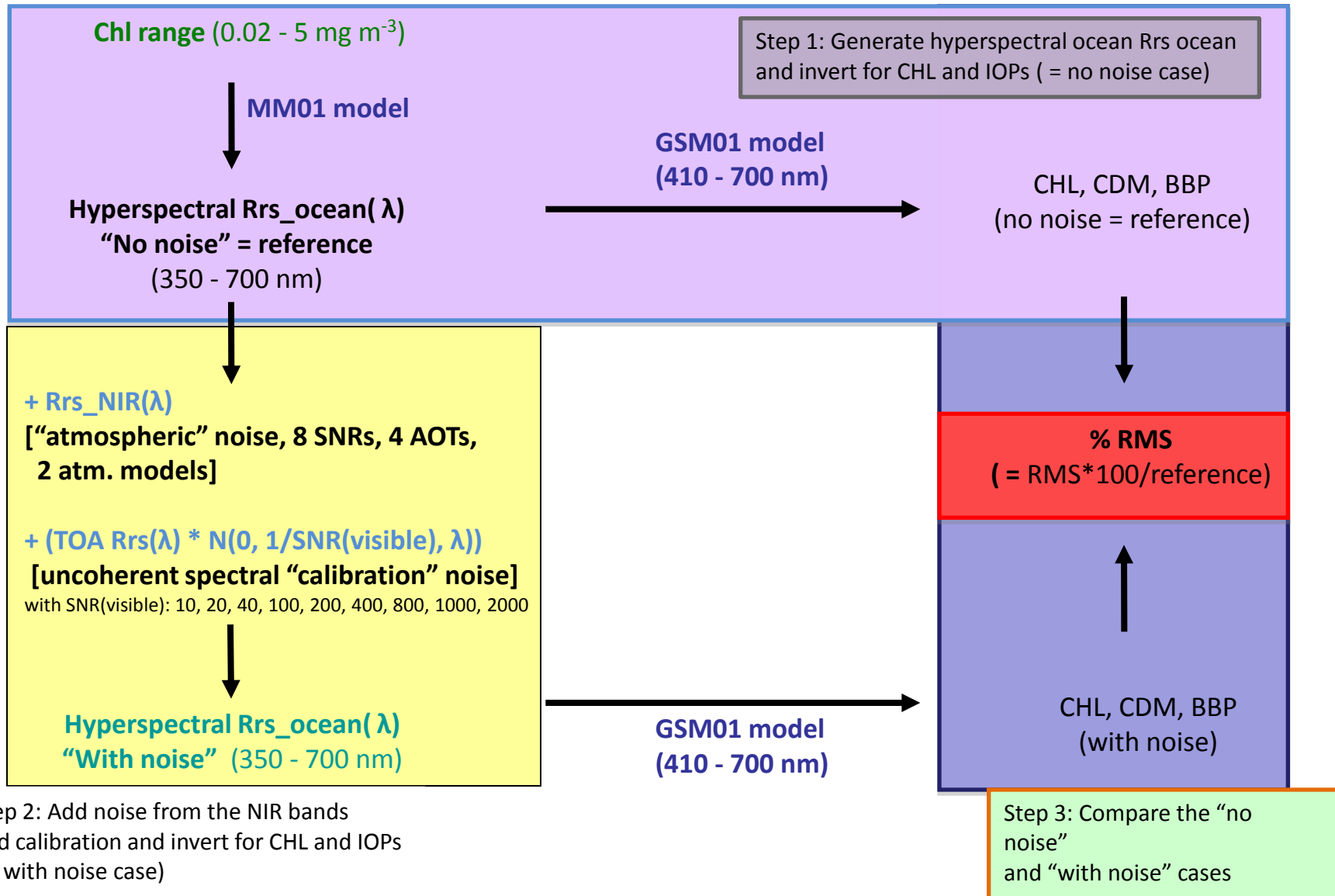
**Ocean Radiometer
Measurement Requirements:
Signal-to-Noise Ratios**

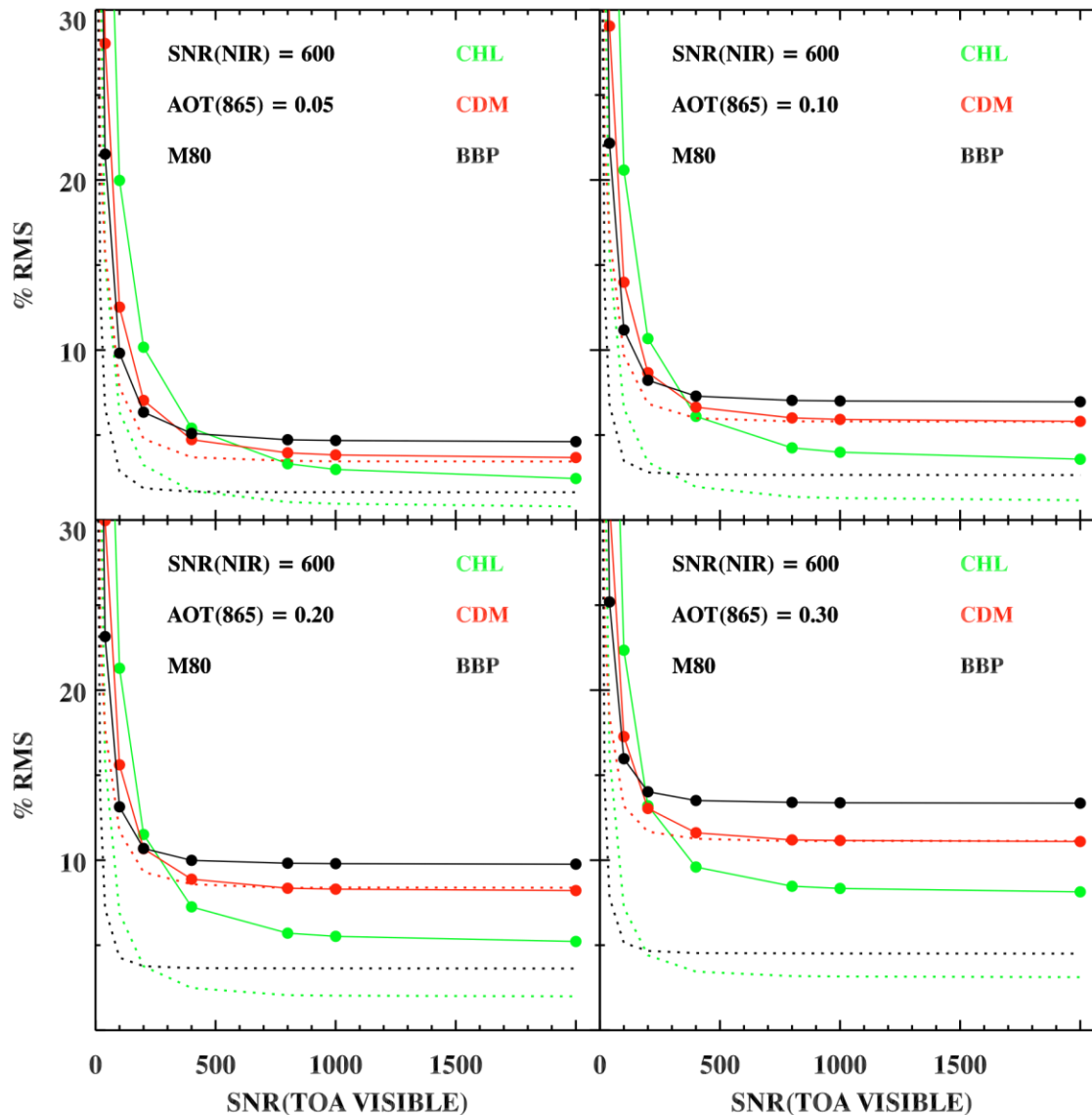
Simulations for NIR and SWIR SNR Requirements

- **Noise Model:** Gaussian noise (mean = 0) is used for the simulations. The standard deviation (STD) of the Gaussian distribution is the noise level (i.e., related to the SNR values).
- **Atmospheric Correction:** Atmospheric correction simulations using two NIR bands (Gordon and Wang, 1994) and using various SWIR bands (Wang, 2007) have been carried out including noise in the corresponding NIR and SWIR bands.
- **Aerosol Property:** Simulations were carried out for a typical Marine aerosol model (M80) and a Tropospheric model (T80 = M80 without the large size fraction) for aerosol optical thicknesses (at 865 nm) of 0.05, 0.1, 0.2, and 0.3.
- **SNR Simulations:** For each case, atmospheric correction for 5000 noise realizations with a given SNR value was carried out. This produces the uncertainty in the derived normalized water-leaving reflectance from UV to red (or NIR). The uncertainty includes errors from both the correction algorithm and the added Gaussian noise in the NIR and SWIR bands.
- **Example Results:** Plots (a) and (b) are results for the NIR with the M80 and T80 models, while plots (c) and (d) are for the SWIR SNR simulations. The error in the normalized water-leaving reflectance, $[\rho_w(\lambda)]_N$, is actually the standard deviation of the derived $[\rho_w(\lambda)]_N$ over the 5000 realizations.
- **Conclusion:** Atmospheric correction and bio-optical simulations show that (1) for the NIR bands we require the minimum SNR value of **~600** and (2) for the SWIR bands (1240, 1640 nm, we require the minimum SNR value of **~200**.



Simulations for Visible SNR Requirements





Average ocean retrieval AOT ~ 0.1 , so an SNR ~ 1000 in the visible is an adequate minimum requirement. Fluorescence bands need a higher SNR.

**Ocean Radiometer
Measurement Requirements:
Summary**

Instrument Requirements: Radiometer (refinements under discussion)

- 5 nm resolution 350 to 775 nm (functional group derivative analyses)
- 300 – 1500:1 SNR for 15 nm aggregate bands UV & visible
 - 300:1 for 350 nm @ Ltyp
 - 1125:1 for 360 nm @ Ltyp
 - 1500:1 for bands between 380-665 nm @ Ltyps
- 10 nm fluorescence bands (667, 678, 710, 748 nm band center)
 - 1500:1 SNR for 667, 678, & 710 nm @ Ltyps
- 10 to 40 nm bandwidth aerosol correction bands at 748, 765, 820, 865, 1245, 1640, 2135 nm
 - 600:1 SNR for 748, 765, 820 & 865 nm @ Ltyps
 - 300:1 SNR at 1245 nm, 250 SNR at 1640 nm, 100 SNR at 2135 @ Ltyps
- Stability
 - 0.1% radiometric stability knowledge (mission duration)
 - 0.1% radiometric stability (1 month prelaunch verification)
- 58.3° cross track scanning
- Sensor tilt ($\pm 20^\circ$) for glint avoidance
- Polarization: < 1.0% sensor radiometric sensitivity,
< 0.2% prelaunch characterization accuracy
- < 2% prelaunch radiance calibration accuracy (minimum)
 - Goal: 0.5% prelaunch calibration accuracy
- 1 km spatial resolution @ nadir
- No saturation in UV to NIR bands
- 5 year minimum design lifetime

Other Perform/Test Specs:

Relative spectral response
Straylight
Temperature sensitivity
Response vs. scan
etc.

Ocean Radiometer Performance/Test Specifications Working Group

(not a formal ACE working group)

Gerhard Meister (NASA/GSFC*; OBPG): Chair

Chuck McClain: Co-chair

- Zia Ahmad (NASA/GSFC*; OBPG)
- Bob Barnes (NASA/GSFC*; OBPG)
- Fred Patt (NASA/GSFC*; OBPG)
- Bryan Franz (NASA/GSFC; OBPG)
- Steve Brown (NIST)
- Sean Bailey (NASA/GSFC*; OBPG)
- Jeremy Werdell (NASA/GSFC*; OBPG)
- Wayne Robinson (NASA/GSFC*; OBPG)
- Brian Monosmith (NASA/GSFC)
- Alan Holmes (consultant)
- Rick Stumpf (NOAA/NOS)

Define detailed sensor performance requirements & related test specifications:

- Review SeaWiFS, MODIS, VIIRS specs
- Define test scenarios
- Identify test technology requirements

*contract staff

Ocean Radiometer multi-spectral band specifications:

Band Center	Band- width	Application/Comments	19-Jun-09 Ltyp (Ahmad)	Lmax (Barnes)	SNR (goal)
350	15	Absorbing aerosol detecton	7.460	35.6	300
360	15	CDOM-chlorophyll separation; strong NO2 absorption	7.220	37.6	1125
385	15	CDOM-chlorophyll separation; strong NO2 absorption; avoid precipitous drop in solar spectrum at 400 nm	6.110	38.1	1500
412	15	CDOM-chlorophyll separation; SeaWiFS (20 nm) & MODIS (15 nm) bands; strong NO2 absorption	7.860	60.2	1500
425	15	CDOM-chlorophyll separation, strong NO2 absorption	6.950	58.5	1500
443	15	Chlorophyll-a absorption peak; SeaWiFS (20 nm) & MODIS (10 nm) bands; strong NO2 absorption	7.020	66.4	1500
460	15	Assessory pigments & chlorophyll	6.830	72.4	1500
475	15	Assessory pigments & chlorophyll	6.190	72.2	1500
490	15	SeaWiFS (20 nm) & MODIS (10 nm) bands; chlorophyll band-ratio algorithm	5.310	68.6	1500
510	15	SeaWiFS (20 nm) band; chlorophyll-a band-ratio algorithm; strong O3 absorption	4.580	66.3	1500
532	15	Aerosol lidar transmission band; MODIS (10 nm) band; strong O3 absorption	3.920	65.1	1500
555	15	Bio-optical algorithms (e.g., band- ratio chlorophyll); MODIS-548 nm, SeaWiFS-555 nm; strong O3 absorption	3.390	64.3	1500
583	15	Phycoerythrin, strong O3 absorption	2.810	62.4	1500
617	15	Strong O3 absorption; bounded at 628 nm by water vapor absorption band	2.190	58.2	1500
640	10	Between O3 & water vapor absorption peaks	1.900	56.4	1500
655	15	Chlorophyll a&b, strong O3 absorption, weak water vapor absorption	1.670	53.5	1500

Notes:

Minimum of 26 bands

Units: mW/cm² μm str

Ltyp's based on fits to
MODIS and SeaWiFS
observations

Based on SeaWiFS
observations, Lmax's result
in <0.2% pixels saturated

SNR ratios to SeaWiFS:
412-670 nm (1.5-1.7)
765 nm (1.15), 865 nm (1.5)

Analysis of MODIS ocean
products showed cirrus
contamination to be
insignificant.

Ocean Radiometer multi-spectral band specifications *cont.:* preliminary

665	10	Fluorescence line height baseline, bandwidth constrained by water vapor absorption line & 678 band			
			1.600	53.6	1500
678	10	Fluorescence line height; band center offset from fluorescence peak by O2 absorption line			
			1.450	51.9	1500
710	15	Fluorescence line height baseline; HABS detection; terrestrial "red edge"; straddles water vapor absorption band			
			1.190	48.9	1500
748	10	Atmospheric correction-open ocean; MODIS band, between O2 A-band & water vapor absorption peaks			
			0.930	44.7	600
765	40	Atmospheric correction-open ocean; SeaWiFS band, O2 A-band absorption			
			0.830	43.0	600
820	15	Water vapor concentration/corrections. There are other water vapor absorption features that could be used.			
			0.590	39.3	600
865	40	Atmospheric correction-open ocean; SeaWiFS band (40 nm bandwidth); MODIS band-869 (15 nm bandwidth)			
			0.450	33.3	600
1245	20	Atmospheric correction-turbid water; MODIS band; bandwidth constrained by water vapor & O2 absorption peaks			
			0.088	15.8	300
1640	40	Atmospheric correction-turbid water; MODIS-1640 nm, moved to 1610 to broaden bandpass & improve SNR			
			0.029	8.2	250
2135	50	Aerosol properties, turbid water aerosol correction			
			0.008	2.2	100

Represents one option for a required function

Notes: Franz MODIS Lmax values show the effects of sensor degradation

Ahmad Ltyp values based on curve fit to Franz MODIS Ltyp's

Units: mW/cm² um str

Lmax (Barnes) assumes albedo of 1.1 with 0 degree incidence angle

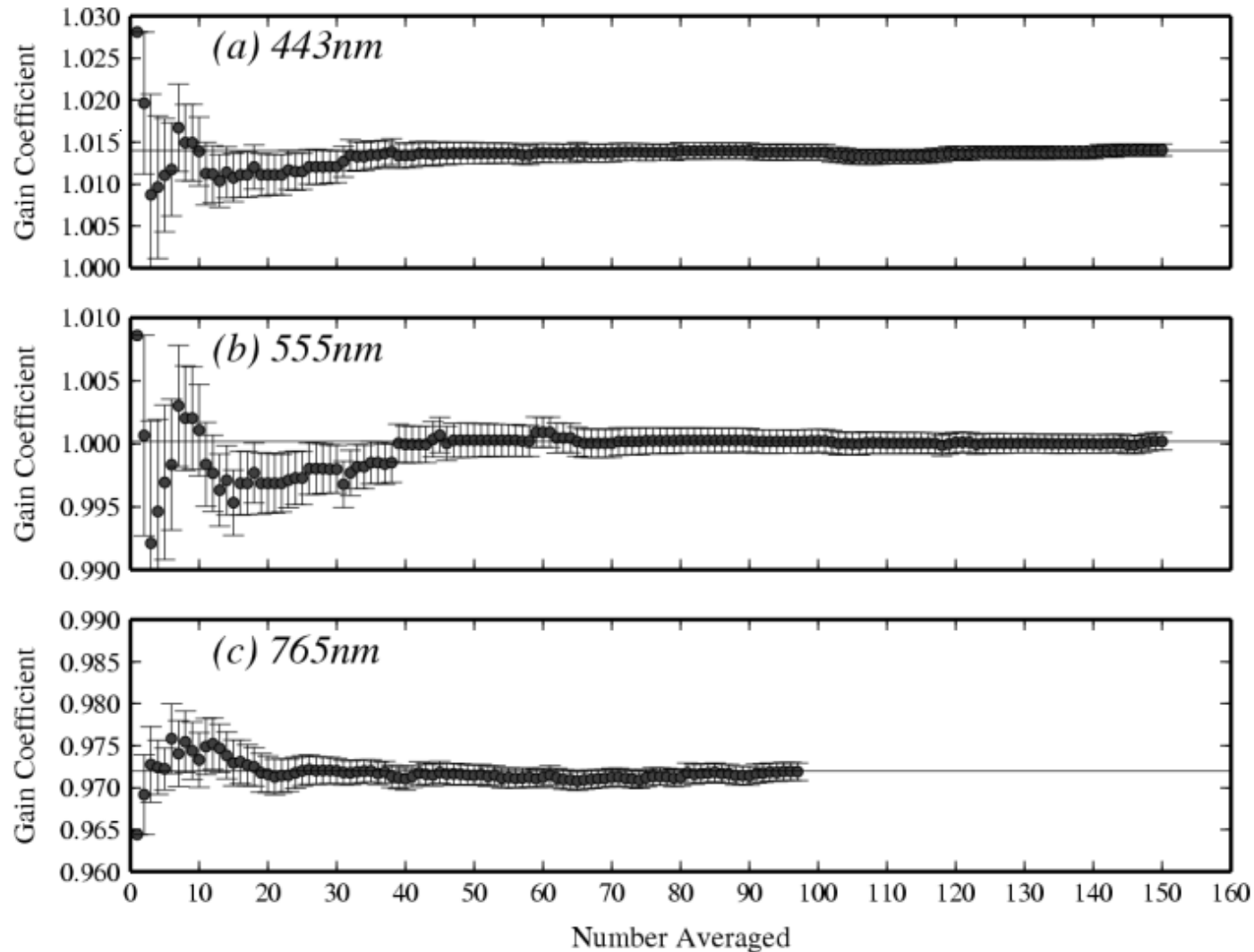
ACE Platform/Mission Support Requirements

- Orbit permitting 2-day global coverage of ocean radiometer data
- Sun-synchronous orbit with equator crossing time between 10:30 & 1:30
- Storage and downlink capacity for full spectral & spatial data
- Comprehensive pre- & post-launch calibration & validation program
 - Monthly lunar imaging at 7° phase angle through Earth sensor observing port
 - Vicarious calibration capability

Vicarious Calibration Gain Convergence

- Only a small % of samples result in a MOBY-satellite “match-ups” for the vicarious calibration.

- For MODIS, took over 2 years to collect enough match-ups to derive gain corrections.



B. A. Franz, S. W. Bailey, P. J. Werdell, and C. R. McClain, "Sensor-independent approach to the vicarious calibration of satellite ocean color radiometry," *Appl. Opt.* 46, 5068-5082 (2007)

Other Requirements

Global data sets from missions, models, or field observations

- **Measurement requirements** (satellite data processing)
 - Ozone concentrations
 - Total water vapor
 - Surface wind velocity
 - Surface barometric pressure
 - NO₂ concentration
 - Vicarious calibration & validation data
 - Full prelaunch characterization
- **Science requirements**
 - Sea surface temperature (SST)
 - Sea surface height (SSH)
 - Photosynthetically available radiation (PAR)
 - UV observations
 - Mixed layer depths (MLD)
 - CO₂
 - pH
 - Ocean circulation fields
 - Aerosol deposition (nutrients)
 - Run-off loading in coastal zone

Summary

- Ocean biology measurement requirements are stringent (calibration, characterization, aerosol correction, bio-optical algorithms, etc.).
- Next generation of sensors must include at least three times the number of multi-spectral ocean bands as SeaWiFS & MODIS.
- GeoCAPE focus on turbid coastal waters accentuates requirements for radiometric accuracy & band selection.
- Requirements for geostationary and LEO are not identical and differences need to be clearly understood.