Inherent Optical Properties (IOPs)

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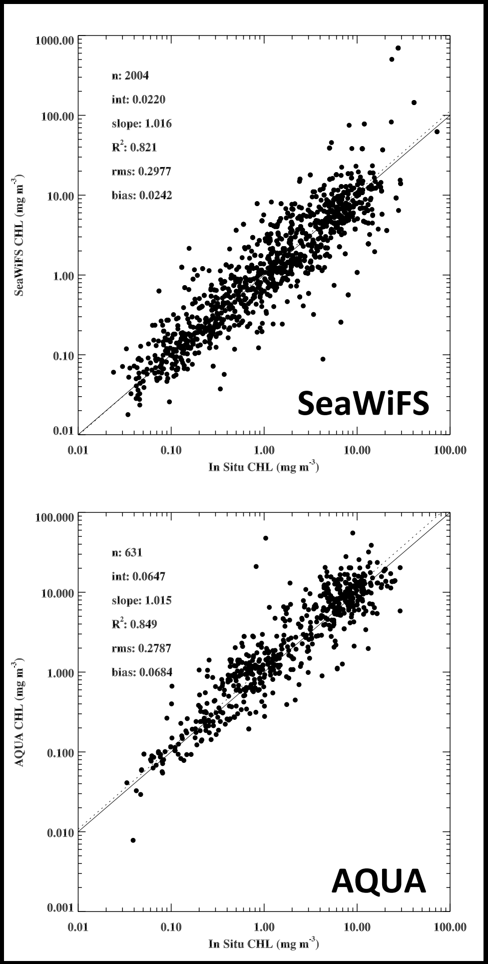
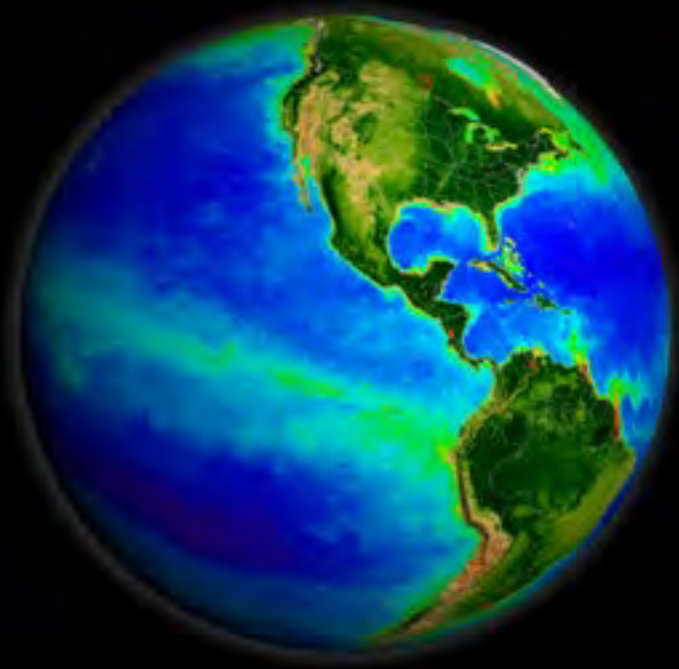
Why look at IOPs?

Chl is the historical OC product

- Routinely measured at sea
- Primary Production
- Proxy for phytoplankton biomass
- Easy to empirically derive from reflectance (Rrs ratio → Chl)

Chl is the OC product with the most complete validation

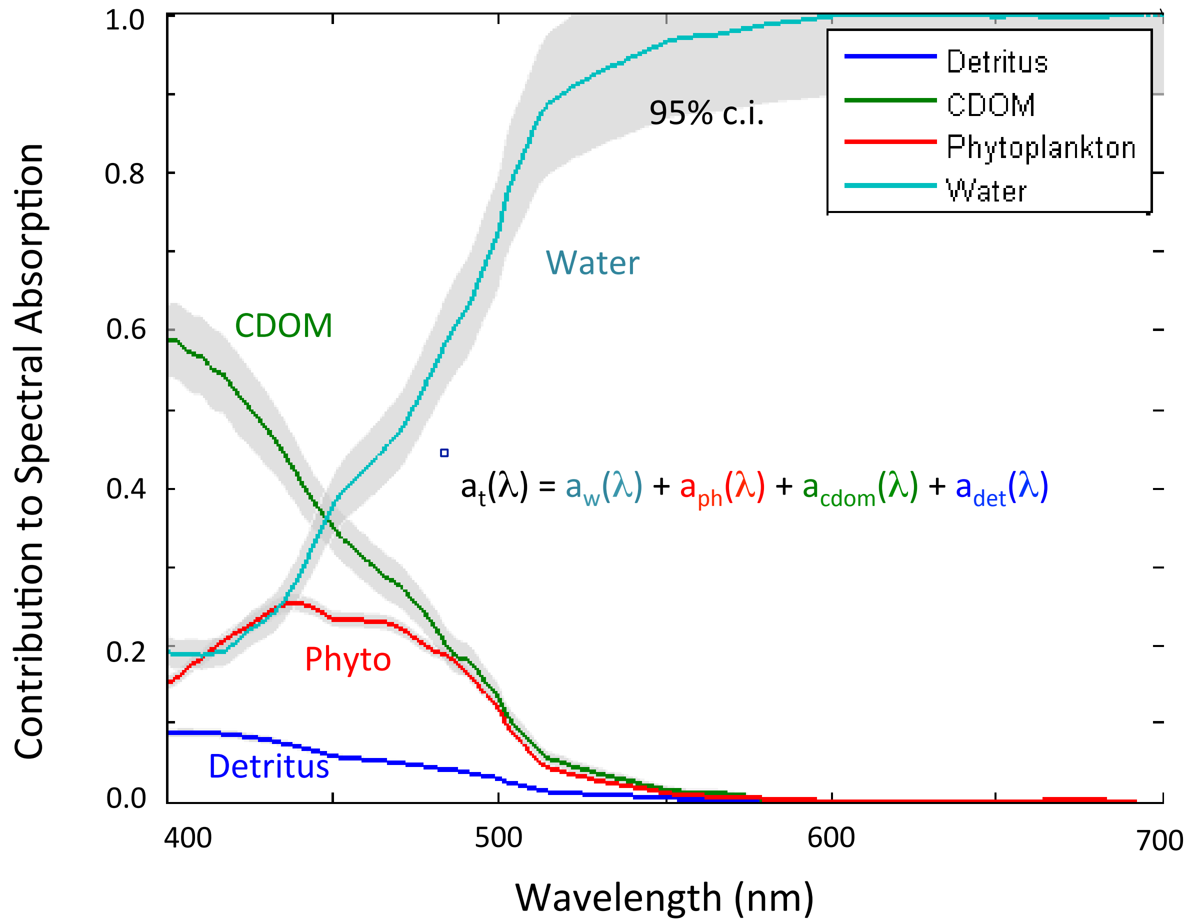




Several issues with Chl:

- The C/Chl ratio is not constant
- Chl is not directly related to reflectance
- Phytoplankton (≈Chl) is only one of the components that determine the ocean color signal

Mean Absorption Component Spectra
(Open Ocean, consistently sampled and processed)



Global surface measurements (I8/I9, A20/A22, P16N/P16S, P18, BATS; N = 371)
US Global Ocean Carbon & Repeat Hydrography Cruises.

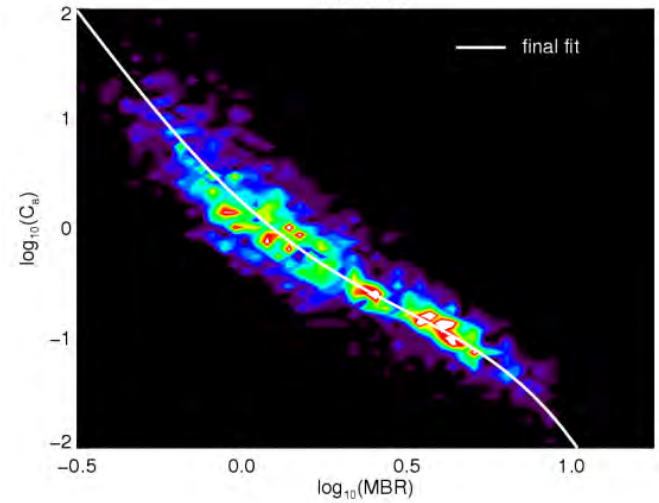
CDOM absorption frequently dominates absorption in the blue

Chl and the band ratio algorithm

MODIS operational Chl: Maximum Band Ratio algorithm (MBR)

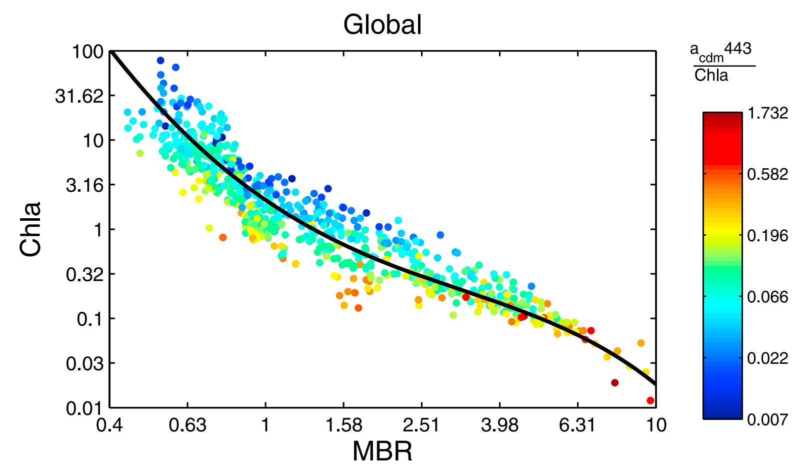
$$X = \log_{10}\left(\frac{Rrs(443)>Rrs(490)}{Rrs(547)}\right)$$

$$Chl = 10^{\wedge}(a_0 + a_1 * X + a_2 * X^{\wedge 2} + a_3 * X^{\wedge 3} + a_4 * X^{\wedge 4})$$



Chl retrievals from MBR algorithm are biased by other optically active components. CDOM in particular

In waters with high CDM MBR algorithm will overestimate Chl



From Szeto et al. JGR [2011]

Siegel et al. [2005]
Morel & Gentili [2009]
Loisel et al. [2010]
Szeto et al. JGR [2011] analysis of NOMAD data
Sauer et al. [2012] for MODIS

Semi-analytic OC models can account for CDOM and Chl

For example, the GSM model (Garver & Siegel, 1997; Maritorena et al., 2002) simultaneously retrieves three relevant properties: Chl, CDM [$a_{cdom}(443)+a_{det}(443)$] & BBP [$b_{bp}(443)$]

$$R_{rs}(\lambda) = \frac{t}{n_w^2} \sum_{i=1}^{2} g_i \left(\frac{b_{bw}(\lambda) + b_{bp}(\lambda)}{a_w(\lambda) + a_{\phi}(\lambda) + a_{cdm}(\lambda) + b_{bw}(\lambda) + b_{bp}(\lambda)} \right)^i$$

Gordon et al. (1988)

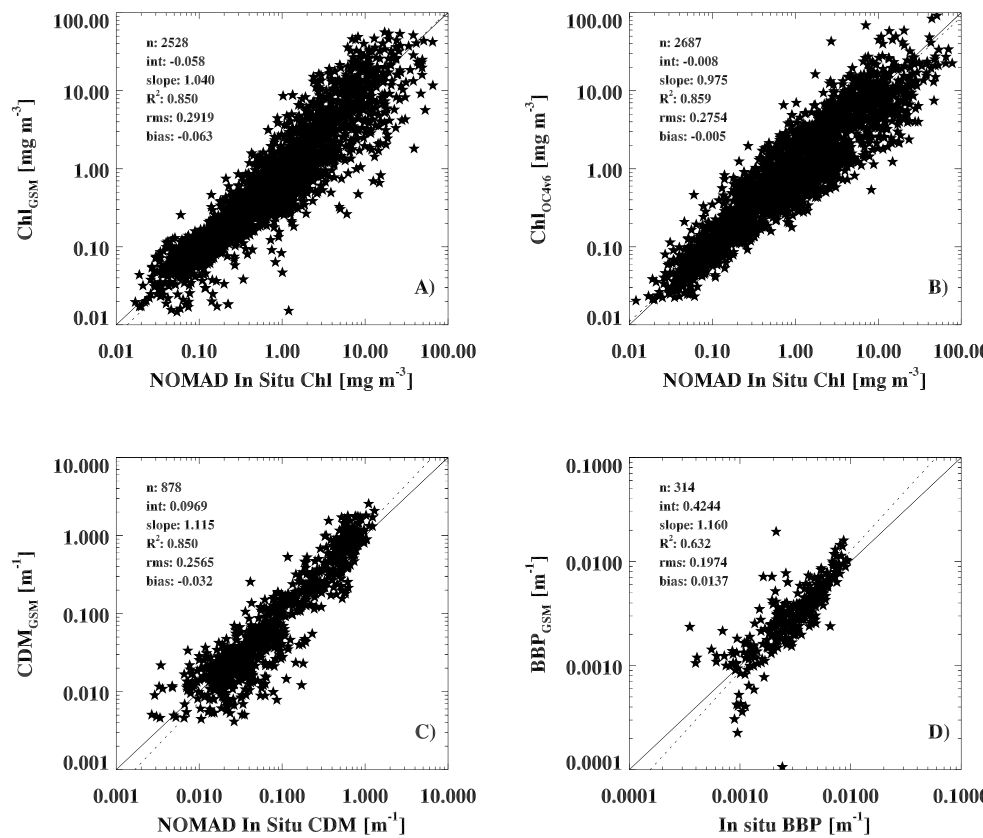
$a_{ph}(\lambda) = Chl\ a_{ph}^*(\lambda)$

$a_{cdm}(\lambda) = a_{cdm}(443)\ \exp(-S(\lambda - 443))$

$b_{bp}(\lambda) = b_{bp}(443)\ (\lambda/443)^{-\eta}$

Non-water components of absorption and scattering are expressed as known shape functions with unknown magnitudes which are retrieved through non-linear least-squares fitting.

Validation statistics for Chl_{GSM} with in situ data are as good as for Chl_{MBR} and almost as good with satellite data.



Comparison of MBR Chl and GSM Chl and influence of CDOM

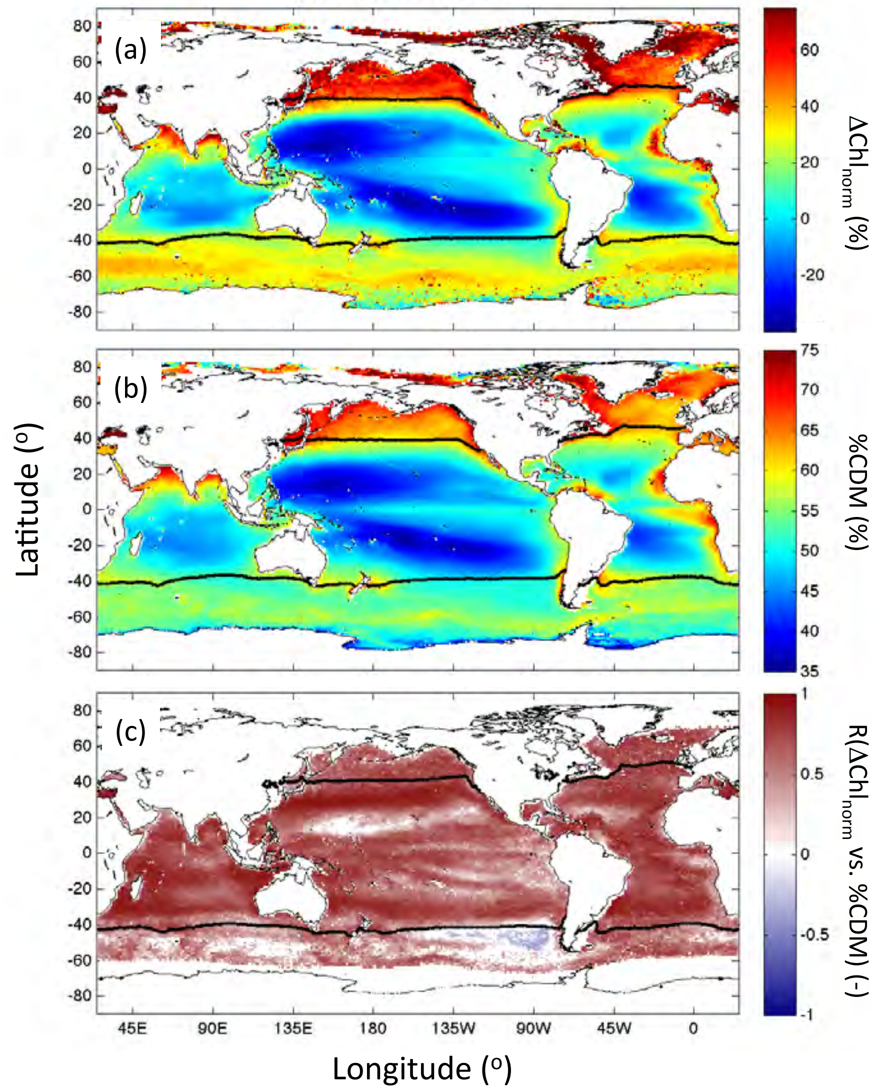
Relative difference

$\Delta Chl_{norm} = 100*(Chl_{MBR}-Chl_{GSM})/Chl_{GSM}$

Contribution of CDM to absorption

%CDM = 100*CDM/(CDM+APH)

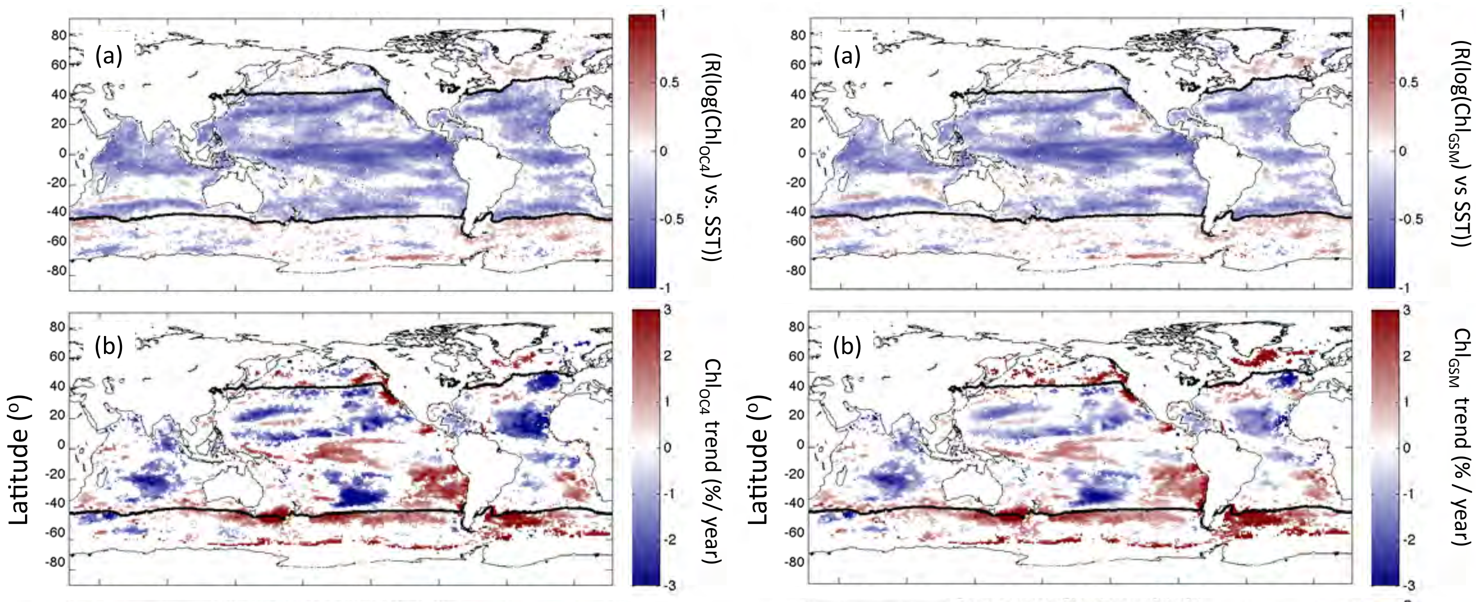
r between ΔChl_{norm} and %CDM



Siegel et al., in Press RSE

MBR Algo

GSM Algo



Correlation
Chl vs SST

Mission Trend

Regional-scale correlation between Chl and SST in the Tropical ocean is almost identical

Mission trends show same spatial patterns but different magnitudes

Siegel et al., in Press RSE

So…

It’s worth looking at IOPs for the purpose of correcting the Chl estimates from empirical ratio algorithms (or generate a Chl estimate from the IOPs)

Another good reason to look at IOPs is because they provide links to biogeochemistry

Phytoplankton absorption:

- Pigment composition
- Community structure
- Physiology

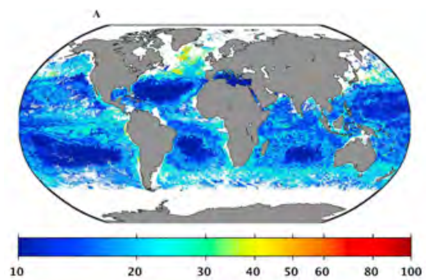
CDM (non-algal) absorption:

- Photochemistry
- Correct empirical Chl retrievals

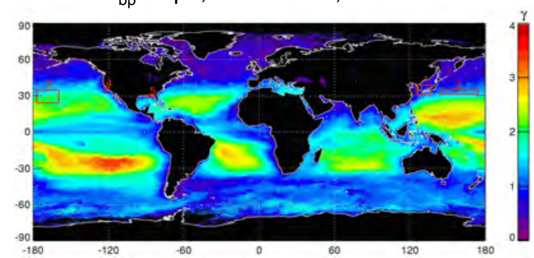
Particulate backscattering:

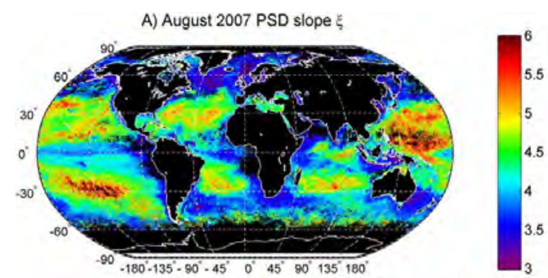
- Particle Size Distribution (size index)
- Primary Production
- POC, PIC

Phytoplankton size; Mouw & Yoder, 2010



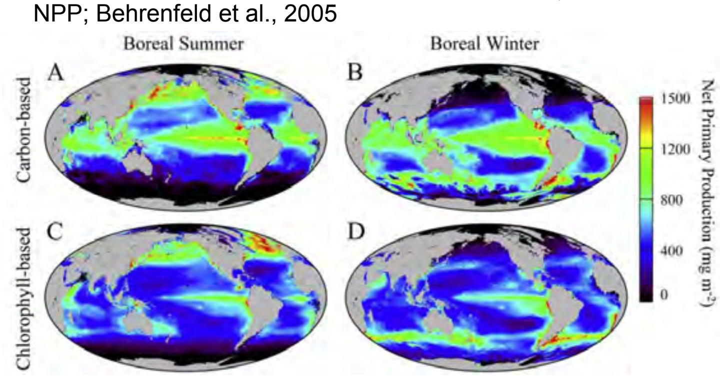
b_{bp} slope; Loisel et al., 2006





PSD; Kostadinov et al., 2009

NPP; Behrenfeld et al., 2005



Where are we at with IOP algorithms and products?

Several IOP products are available through the NASA OBPG ocean color web:

- $a_{cdm}(443)$, $a_{ph}(443)$, $b_{bp}(443)$ from different models
- IOPs are not "standard" products, they are "evaluation" products

Several workshops and evaluation exercises for IOP products and algorithms:

SeaBAM, 1996

OCBAM, 2005

IOCCG, 2005

NASA IOP Workshops, 2008, 2010

ESA CCI, 2013

The NASA OBPG IOP algorithms Workshops (2008, 2010)

- Goal was mostly to look under the hood of 7 IOP algorithms to interpret their differences and assess their suitability for global application
- Since SA algorithms are all based on the same fundamental relationship between Rrs and IOPs, the differences among them come from their overall design
  - Assumptions
  - Parameterization of the absorption and backscattering components
  - Inversion or optimization approach
- Seven IOP algorithms were tested against the NOMAD in situ data set and some satellite data
- NASA OBPG developed the generalized IOP (GIOP) model software which allows the user to choose the parameterization and inversion method of a SA ocean color model.

Generalized ocean color inversion model for retrieving marine inherent optical properties

P. Jeremy Werdell,[1,2,*] Bryan A. Franz,[1] Sean W. Bailey,[1,3] Gene C. Feldman,[1]
Emmanuel Boss,[2] Vittorio E. Brando,[4] Mark Dowell,[5] Takafumi Hirata,[6]
Samantha J. Lavender,[7] ZhongPing Lee,[8] Hubert Loisel,[9]
Stéphane Maritorena,[10] Fréderic Mélin,[5] Timothy S. Moore,[11]
Timothy J. Smyth,[12] David Antoine,[13] Emmanuel Devred,[14]
Odile Hembise Fanton d'Andon,[15] and Antoine Mangin[15]

(In Press, Applied Optics)

ESA OC-CCI round-robin

Aim is to establish an objective methodology for OC algorithm selection based on performance and suitability for use in climate-change studies.

Table 2: Model output variables.

Model	Output variable									Reference
	$K_d(489)$	C	$a(\lambda)$	$a_{ph}(\lambda)$	$a_{dg}(\lambda)$	$b_b(\lambda)$	γ	S_{dg}	$a_{ph}(555)/a_{ph}(443)$	
A	$\times^{*}$	$\times^{\$}$	×	×	×	×	×	×	×	Smyth et al. (2006)
B	$\times^{*}$	$\times^{\$}$	×	×	×	×	×	×	×	Smyth et al. (2006)
C	$\times^{*}$	×	×	×	×	×	×	×	×	Devred et al. (2011)
D	$\times^{*}$	×	×	×	×	×	×	×	×	Lee et al. (2002)
E	$\times^{*}$	$\times^{\$}$	×	×	×	×	×	×	×	Lee et al. (2009)
F	$\times^{*}$	$\times^{\$}$	×	×	×	×	×	×	×	Lee et al. (1998, 1999)
G	$\times^{*}$	×	×	×	×	×	×	×	×	Maritorena et al. (2002)
H	$\times^{*}$	×	×	×	×	×	×	×	×	Maritorena et al. (2002)
I	$\times^{*}$	×	×	×	×	×	×	×	×	Franz and Werdell (2010)
J	$\times^{*}$		×	×	×	×	×	×	×	see#
K	$\times^{*}$	×	×	×	×	×	×	×	×	Doerffer and Schiller (2000)
L		×								O'Reilly et al. (2000)
M		×								O'Reilly et al. (2000)
N		×								O'Reilly et al. (2000)
O		×								Morel et al. (2007)
P		×								Hu et al. (2012)
Q	×									NASA (2009)

29 variables

11 semi-analytical algorithms (IOPs, Chl, Kd(490))

6 empirical algorithms (Chl)

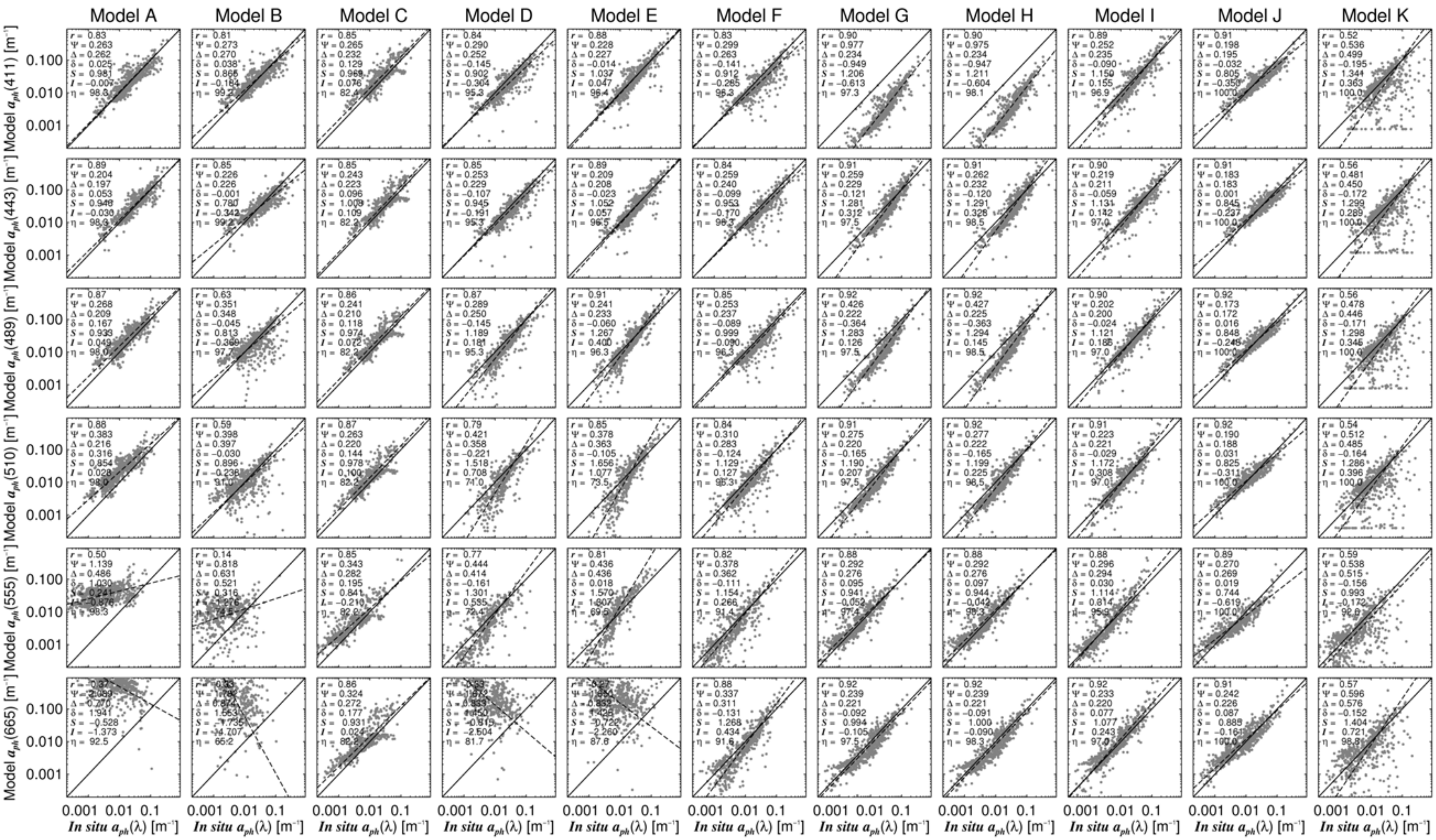
- Tested with the NOMAD in situ data set
- Developed an objective classification designed to rank the quantitative performance of the models based on various univariate statistics.

The Ocean Colour Climate Change Initiative: A round-robin comparison on in-water bio-optical algorithms

Robert J.W. Brewin[a,b,*], Shubha Sathyendranath[a,b], Dagmar Müller[c], Carsten Brockmann[d], Pierre-Yves Deschamps[e], Emmanuel Devred[f], Roland Doerffer[c], Norman Fomferra[d], Bryan Franz[g], Mike Grant[a], Steve Groom[a], Andrew Horseman[a], Chuanmin Hu[h], Hajo Krasemann[c], ZhongPing Lee[i], Stéphane Maritorena[j], Frédéric Mélin[k], Marco Peters[d], Trevor Platt[a], Peter Regner[l], Tim Smyth[a], Francois Steinmetz[e], John Swinton[m], Jeremy Werdell[g], George N. White III[n]

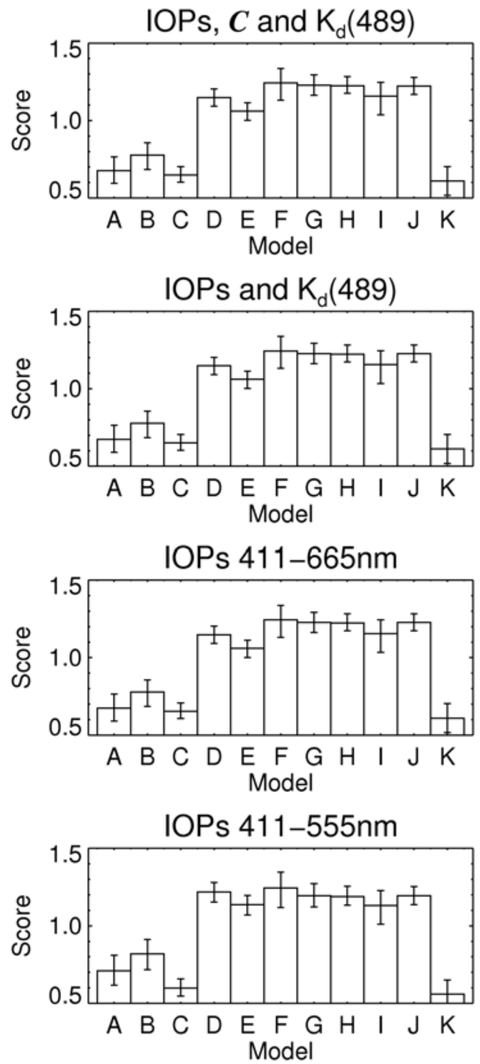
(In Press, RSE)

ESA OC-CCI



Brewin et al.,RSE In Press

OC-CCI and NASA IOP Workshops Main Conclusions



Brewin et al.,RSE In Press

- No perfect algorithm that does it all at all wavelengths
- The performance of each model varies depending on product and wavelength
- Most semi-analytic models perform well in predicting total absorption, $a_t(\lambda)$, and total backscattering, $b_b(\lambda)$
- Performance is generally degraded when decomposing a_t into a_{ph} and a_{cdm}
- Difficult to rank the performance of the algorithms, as many of the models have overlapping error bars.

Issues with the in situ data:

- No independent data set for model testing
- Time and space biases
- Mesotrophic waters are over-represented
- Need measurement uncertainty quantification (closure issues)

Summary

- IOPs are important for ocean biogeochemistry studies
- IOPs are not “Standard” (= operational) products, they are “Evaluation” products
- It’s probably time for some of them to become “Standard” products
- No “perfect” IOP algorithm or model
- There is room for improvement in terms of products and spectral accuracy
- Need more diverse and high quality in situ data

Can we improve the IOP models?

$$Rrs(\lambda) = \frac{t}{n_w^2} \frac{f(\lambda)}{Q(\lambda)} \left(\frac{b_{bw}(\lambda) + b_{bp}(\lambda)}{a_w(\lambda) + a_{ph}(\lambda) + a_{cdm}(\lambda) + b_{bw}(\lambda) + b_{bp}(\lambda)} \right)$$

$a_{ph}(\lambda) = A(\lambda)\ Chl^{B(\lambda)}$ $a_{cdm}(\lambda) = a_{cdm}(443) \exp(-S(\lambda - 443))$ $b_{bp}(\lambda) = b_{bp}(443)\ (\lambda / 443)^{-\eta}$

- Replace some constant parameters by dynamic expressions (e.g. t/n_w^2, f/Q, S, η).
- Improve phytoplankton absorption parameterization through better, bigger, more diverse data sets

Challenges:

Highly non-linear

Dynamic parameterization is not always obvious

Still some empiricism

What is best?

- High accuracy at 1 λ vs a lower but consistent accuracy at all λs?
- High accuracy for some products but lower accuracy for some others?
- High accuracy retrievals but poor spatial and temporal coverage (filtering)
- ....