Remote sensing of Sun-induced fluorescence.
Part 2: from FLH to chl, $\Phi_f$ and beyond.

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How do current chl-based $\Phi_f$ satellite algorithms work?

Measured by ocean color satellites (FLH)

What we want

Modeled

Estimated based on $a_\phi$ or $K_d$ algorithm and known relationships

$L_{uf}$ $\phi_f^{app}$ $E_{PAR}$ $Q_a^*$ $\frac{1}{\alpha_f + K_dPAR}$


In its simplest form

After a few assumptions a surprisingly compact form is obtained.

\[ \phi_f^{\text{app}} = 0.68 \cdot 1.19 \cdot \frac{FLH_{nLw}}{Chl^{0.684}} \]

Where \( FLH_{nLw} \) is the FLH measured on the normalized water leaving radiance spectrum.

$FLH_{nLw}$ looks like chlorophyll
A detour to look at Chl from FLH

\[ Chl = \left[ 0.81 \cdot \frac{FLH_{nLw}}{\phi_f^{app}} \right] \frac{1}{0.684} \]
$\text{FLH}_\text{Lwn} \text{ vs chlorophyll}$

$\log_{10} \text{nFLH} \ (\text{mW cm}^{-2} \text{ sr}^{-1} \mu \text{ m}^{-1})$

$\log_{10} [\text{Chl}] \ (\text{mg m}^{-3})$

Not promising... but perhaps good enough in coastal waters
Coastal waters
Two challenges in Lunenburg Bay (Nova-Scotia, Canada)

Not much variability in the chlorophyll concentration (Factor ~ 4-5)

Surface chlorophyll at LMB1 buoy, May 25 - Nov. 22, 2004

Algorithmes using band ratios do not work

Phytoplankton absorption is small compared to CDOM absorption
Measurements

- AOPs
  - $E_d(0^+)$
  - $R_L(0.65)$
  - $L_u(0.65)$
  - $E_d(2.75)$

Forward and inverse models

- Minimize the difference between model and measurements
  - $K_d(\ )$ $K_d^{\text{mod}}(\ )$
  - $R_L(\ )$ $R_L^{\text{mod}}(\ )$

By changing the amplitudes and shapes of the IOPs

To obtain

- $a$, $a_{\text{CDOM}}$, $b_b$

Validation

- Range of variability

Radiative transfer simulations

Creation of look up tables

Simplified optical models

- $R_L^{\text{mod}} = R_{Lb}^{\text{mod}} + R_{Lf}^{\text{mod}}$
- $K_d^{\text{mod}}$

Analytical fluorescence model

- $R_L^{\text{mod}}(0.65,a,b_b,s)$
- $R_{Lb}^{\text{mod}}(0.65,a,b_b,s)$
- $K_d^{\text{mod}}(a,b_b,s)$

IOPs

- Scattering (ac-9)
- Backscattering (Hydroscat-6)
- Phytoplankton absorption
- CDOM absorption

Range of variability
Summer 2001 at one buoy
Validation in 2004 for three buoys

Similar results in Saanich inlet

Coastal waters only

Similar or slightly better than a blue to green ratio algorithm

E. Devred is pursing this work...
The quantum yield of fluorescence
Quantum yields vs depth

Describing irradiance vs quantum yield function

\[
\Phi_{\text{app}} = \left( q_I e^{\frac{E^o}{E_T}} \right) \left( f_{\text{min}} A + f_{\text{max}} [1 \quad A] \right)
\]

\[
A = e^{\frac{E^o}{E_k}}
\]

Comparison of QY descriptions

From Part 1:

\[
\phi_f^{\text{app}} = \phi_f \left( \frac{PS \, \bar{a}_{PSII} + PS \, \bar{a}_{PSI} + PP \, \bar{a}_{PSII} + PP \, \bar{a}_{PSI}}{PS \, \bar{a}_{PSII} + PS \, \bar{a}_{PSI} + PP \, \bar{a}_{PSII} + PP \, \bar{a}_{PSI}} \right)
\]

\[
= \frac{k_f}{k_f + Ak_p + k_H + Zk_{NPQ} + Ck_{qI}} \left( \frac{PS \, \bar{a}_{PSII} + PS \, \bar{a}_{PSI} + PP \, \bar{a}_{PSII} + PP \, \bar{a}_{PSI}}{PS \, \bar{a}_{PSII} + PS \, \bar{a}_{PSI} + PP \, \bar{a}_{PSII} + PP \, \bar{a}_{PSI}} \right)
\]

From Morrison:

\[
\phi_f = \left( q_I e^{-\frac{\phi}{E_T}} \right) \left( \phi_f^{\text{min}} A + \phi_f^{\text{max}} [1 - A] \right)
\]

\[
A = e^{\frac{\phi}{E_k}}
\]
Comparison of QY descriptions

From Part 1:

\[
\frac{f_{app}}{f} = \frac{PSa_{PSII}}{PSa_{PSII} + PSa_{PSI} + PPa_{PSII} + PPa_{PSI}} \\
= \frac{k_f}{k_f + Ak_p + k_H + Zk_{NPQ} + Ck_{ql}} \left( \frac{PSa_{PSII}}{PSa_{PSII} + PSa_{PSI} + PPa_{PSII} + PPa_{PSI}} \right)
\]

From Morrison:

\[
f = \left( q_I e^{\frac{\hat{E}}{E_T}} \right) \left( f_{\text{min}} A + f_{\text{max}} \begin{bmatrix} 1 & A \end{bmatrix} \right)
\]

\[
A = e^{\frac{\hat{E}}{E_k}}
\]

Morrison described the variability in the inherent quantum yield not in the apparent quantum yield of fluorescence.
Interpreting variability in $\Phi_f$
Phytoplankton photocompensation from space-based fluorescence measurements

J. Ruairidh Morrison¹ and Deborah S. Goodwin²
Phytoplankton photocompensation from space-based fluorescence measurements

J. Ruairidh Morrison\textsuperscript{1} and Deborah S. Goodwin\textsuperscript{2}

\[ f = \left( A_I e^{\frac{\bar{\bar{E}}}{E_T}} \right) \left( f_{\text{min}} A + \left[ f_{\text{max}} \right] \right) \]

Assume \( \bar{\bar{E}} \gg E_k \) leads to \( A = 0 \)
Assume \( q_I \) is constant = 0.35

\[ A = e^{\frac{\bar{\bar{E}}}{E_k}} \]
Phytoplankton photocompensation from space-based fluorescence measurements

J. Ruairidh Morrison¹ and Deborah S. Goodwin²

\[ \phi_f = 0.032 e^{-\frac{E}{E_T}} \]
This allows them to retrieve $E_T$.

$E_T$ varies with growth irradiance.
Satellite-detected fluorescence reveals global physiology of ocean
Similar results, a different hypothesized cause

When the eddy slows (period increases) quenching is reduced by nutrient stress and this leads to an increase in $\Phi_f$.

One current hypothesis: reduced qI quenching or downregulation under nutrient stress accounts for most of the variability?


Satellite-detected fluorescence reveals global physiology of ocean phytoplankton

M. J. Behrenfeld\textsuperscript{1}, T. K. Westberry\textsuperscript{1}, E. S. Boss\textsuperscript{2}, R. T. O’Malley\textsuperscript{1}, D. A. Siegel\textsuperscript{3}, J. D. Wiggert\textsuperscript{4}, B. A. Franz\textsuperscript{5}, C. R. McClain\textsuperscript{5}, G. C. Feldman\textsuperscript{5}, S. C. Doney\textsuperscript{6}, J. K. Moore\textsuperscript{7}, G. Dall’Olmo\textsuperscript{1}, A. J. Milligan\textsuperscript{1}, I. Lima\textsuperscript{6}, and N. Mahowald\textsuperscript{8}
Satellite-detected fluorescence reveals global physiology of ocean phytoplankton


\[ \text{app} = \frac{k_f}{k_f + A k_p + k_H + Z k_{NPQ} + C k_{qI}} \left( \frac{PS \overline{a}_{PSII} + PS \overline{a}_{PSI} + PP \overline{a}_{PSII} + PP \overline{a}_{PSI}}{PP \overline{a}_{PSII} + PP \overline{a}_{PSI}} \right) \]

In the text they also discuss how iron stress could decrease qI and increase the PSII photosynthetic absorption cross-section (in high macronutrient regions).
Satellite-detected fluorescence reveals global physiology of ocean phytoplankton

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\[
\frac{\text{app}}{f} = \frac{k_f}{k_f + Ak_p + k_H + Zk_{\text{NPQ}} + Ck_{\text{qI}}} \\
\frac{PS}{PP} \left( \frac{\overline{a}_{\text{PSII}}}{\overline{a}_{\text{PSI}}} + \frac{PS}{PP} \frac{\overline{a}_{\text{PSII}}}{\overline{a}_{\text{PSI}}} + \frac{PP}{PP} \frac{\overline{a}_{\text{PSII}}}{\overline{a}_{\text{PSI}}} \right)
\]

In summary, according to them, whatever the process, iron stress is expected to increase the apparent quantum yield of fluorescence.
Observed quantum yield did not show clear relationship with macronutrient concentration
Satellite-detected fluorescence reveals global physiology of ocean phytoplankton

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Two general hypotheses

1. Growth irradiance is responsible for much of the variability in the quantum yield of Sun-induced fluorescence - Morisson and Goodwin

2. Nutrient limitation is responsible for much of the limitation in the quantum yield of Sun-induced fluorescence
   a. Macro-Nutrient - Schallenberget al. (effect on qI), Letelier and Abbott (effect on PQ)
   b. Iron - Behrenfeld and others
Others possible?
Physiology vs ecology: species composition another possibility?

3 species, 6 growth irradiances

**T. oceanica**

**T. weissflogii**

**T. pseudonana**
Three general hypotheses

1. Growth irradiance is responsible for much of the variability in the quantum yield of Sun-induced fluorescence (Morisson and others)

2. Nutrient limitation is responsible for much of the limitation in the quantum yield of Sun-induced fluorescence
   a. Macro-Nutrient (Schallenberg, Letelier and others)
   b. Iron (Behrenfeld and others)

3. Species composition
Four general hypotheses

1. Growth irradiance is responsible for much of the variability in the quantum yield of Sun-induced fluorescence (Morisson and others)

2. Nutrient limitation is responsible for much of the limitation in the quantum yield of Sun-induced fluorescence
   a. Macro-nutrient (Schallenberg, Letelier and others)
   b. Iron (Behrenfeld and others)

3. Species composition

4. We are not measuring the quantum yield of fluorescence...
   a. Biases prevent us from observing real global distributions
How do current chl-based \( \phi_f \) satellite algorithms work?

Measured by ocean color satellites

What we want

Modeled

Retrieved by OC algorithm

Estimated based on \( a_\phi \) or \( K_d \) algorithm and known relationships


Errors in \( a_\phi \) (or chl) estimated by ocean color algorithms thus propagate directly to estimates of \( \phi_f \).

An overestimate of \( a_\phi \) leads to an underestimate of the quantum yield.
Parameterization “errors”

\[ a = a^* \times Chla \]
Parameterization “errors”

Current algorithms are likely biased across Chla gradient because of such parameterization errors (error likely also in $Q_a^*$ vs Chla and $K_{dPAR}$ vs Chla).

\[
\frac{a_{phy}}{a_{phy}} = 0.81 \times \frac{FLH_{Lwn}}{Chl^{0.684}}
\]

The exact exponent matters over three orders of magnitudes.
FLH is a biased estimate of fluorescence

Biases in $\alpha_\phi$: main source and potential corrections

The absorption by colored dissolved organic matter (CDOM) appears to be the largest bias in the estimate of phytoplankton absorption from space using empirical algorithms.

Two approaches to resolve this issue...

1) Empirical corrections (e.g. $\phi$-correction)
2) Semi-analytical approaches (e.g. GSM or QAA algorithms)

Both approaches also allow an estimate of CDOM absorption

Fluorescence vs chlorophyll OC2M

Scaled theoretical line (Huot et al. 2005)

$nFLH$ is the fluorescence line height on nLw:

\[
nFLH = \frac{L_{uf}}{E_{PAR}} \mu f \times Q_{d}^a \times \frac{1}{a_f + K_{dPAR}}
\]
Correction for “average” effect of PAR.

\[ \mu \ iPAR^{-1} \]

\[ \sim \varphi_f \]

Effect of irradiance

Behrenfeld et al. 2009
\(E_{\text{dPAR}}^{-1}\)

Best fit to median points

\[
\text{chl} = \frac{nFLH}{\hat{\gamma}_{\text{median}}}
\]

\(E_{\text{dPAR}} \, (\mu \text{ mol m}^{-2} \text{ s}^{-1})\)
Further dependence on chlorophyll

\[ chl = \frac{nFLH}{\hat{y}_{\text{median}}} \]

Median trends vary with chlorophyll concentration

We can represent those trends for all [chl] with a “median surface”.
One step further...

Let's divide the results from the previous graph...

by the « median surface »
...and plot the results as a function of CDOM absorption

CDOM is not only causing an increased attenuation of irradiance
Most likely it is causing a bias in the estimates of chlorophyll - OC2M is biased by CDOM no surprise there!
What happens if we correct OC2M for CDOM using the $\Phi$-correction?
Before (MARD=0.887)

After (MARD=0.815)
Effect of CDOM

(Φ-corrected OC2M)

Before

After
Other algorithms

- B) OC3M
  - $\text{MARD} = 0.826$

- C) $\phi$-corrected OC3M
  - $\text{MARD} = 0.808$

- D) GSM
  - $\text{MARD} = 0.792$

- E) QAA
  - $\text{MARD} = 0.889$
CDOM is a different story

Φ corrected –OC2M

Φ corrected –OC3M

GSM

QAA
Summing up so far...

$E_{d\text{PAR}}$ has a significant effect of $nFLH$ which depends on the trophic level.

\(\Phi\)-correction allows the best retrieval of CDOM trends and improves chl empirical algorithms significantly.

GSM performs very well for chl, less well for CDOM.
New algorithm for the quantum yield of fluorescence.

Objective: Removing the variability in nFLH arising from phytoplankton absorption, CDOM absorption and $E_{d\text{PAR}}$ to observe variability caused by other factors.


\[
nFLH \approx \frac{L_{uf}}{\bar{E}_{\text{PAR}}} \propto \varphi_f(\hat{E}_{\text{PAR}}, \text{chl}) \cdot \alpha_{\varphi} \cdot Q^* \cdot \frac{1}{a_f + K_{d\text{PAR}}}
\]

The LUT “replaces” the magenta lines in current algorithms.
The $\chi_{\text{fluo}}$ index

$$\chi_{\text{fluo}} = \frac{FLH_{nLw}}{FLH_{\text{LUT}}}$$
Composite March 2007

\(X_{flu} (MBR)\)

\(\Phi\)-corrected OC3M

\(E_{dFAR}\)

Sea Surface Temperature
Algorithms comparison (March 2007)

Behrenfeld et al. 2009, ($\Phi_{\text{sat}}$; equation A-12)

$$\phi_f^{\text{app}} = 0.68 \cdot 1.19 \cdot \frac{FLH_{nLw}}{Chl^{0.684}}$$
The new algorithm - Conclusions

Upside:

Accounts for most of the variability in ocean color affecting $nFLH$ that is not due to physiology or species composition (globally).

Easy to tune the LUT for regional application; no need to know in situ optical properties.

Independent of absolute calibration of the satellite (as long as it is stable).

Downside:

The $\chi_{flu}$ index provides only relative values of the quantum yield.
Where do we go now?

Enhanced abilities to interpret Sun-induced fluorescence fields observed from space could provide unprecedented information about phytoplankton physiology at global scales.

- **The four testable hypotheses highlighted before provide good ground for future work.**
  - Nutrient enrichment experiments coupled with measurements of Sun-induced fluorescence along (well chosen) transects could provide strong evidence into the nutrient-iron limitation hypothesis.
  - These experiments complemented with species composition (HPLC, flowcytometry) and average growth irradiance within the mixed layer should help identify the variable that explains the most variance.
  - Natural and anthropogenic iron enrichment areas are being studied at the moment and may help confirm the iron stress hypothesis.
  - The proposed algorithm just presented should reduce biases in current algorithms