

New algorithms for MODIS sun-induced chlorophyll fluorescence and a comparison with present data products

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Web Appendix 2

Interpretation of the quantum yield of sun-induced chlorophyll fluorescence quantum yield

We have defined the quantum yield of fluorescence *in vivo*, φ , as the ratio of photons fluoresced by chlorophyll *a* over the whole fluorescence band to the photons absorbed by all cellular pigments. This is the definition typically used for sun-induced fluorescence studies (e.g., Babin et al. 1996*b*; Ostrowska et al. 1997; Maritorena et al. 2000; Morrison 2003). This definition has important implications for the interpretation of the retrieved yields, especially in terms of photosynthetic capabilities.

Even if retrieved perfectly, φ is not directly interpretable in terms of photosynthetic and nonphotosynthetic rate processes. This is because a variable fraction of photons is absorbed by the fluorescing photosystem II (Johnsen et al. 1997). The quantum yield retrieved by our approach will therefore be related to φ_{PSII} , the quantum yield of fluorescence used in models of photosynthesis and electron transport and interpretable in terms of rate constants as

$$\varphi = \varphi_{PSII} \cdot \frac{\int_{PAR} a_{PSII}(\lambda) \cdot \overset{\circ}{E}(\lambda) \cdot d\lambda}{\int_{PAR} a_{\phi}(\lambda) \cdot \overset{\circ}{E}(\lambda) \cdot d\lambda} \quad (22)$$

where a_{PSII} (m^{-1}) represents the absorption by photosynthetic pigments in the PSII antenna and core and a_{ϕ} is the total absorption by phytoplankton, which also includes absorption by photoprotective pigments (Bidigare et al. 1990; Jeffrey et al. 1997) and the photosynthetic pigment associated with PSI. To relate φ to φ_{PSII} , the spectral optical cross-section of PSII and the spectral total optical cross-section have to be measured (e.g., Sosik and Mitchell 1995). Variability on the

order of 2 to 8 have been observed *in situ* for the ratio of photosynthetic to nonphotosynthetic pigment absorption (e.g., Bidigare et al. 1992; Babin et al. 1996*a*; Allali et al. 1997) and on the order of about 2 for PSII to total absorption (e.g., Sosik and Mitchell 1995) but the ranges could be larger (*see, for example*, Johnsen et al. 1997; Lutz et al. 1998, 2001).

In a study of vertical profiles of φ in the Baltic Sea, Ostrowska et al. (1997) found that the yield was not correlated with incident PAR, correlated weakly with temperature and chlorophyll concentration, and correlated best with \bar{a}_{ϕ}^* . The quantum yield was decreasing with increasing \bar{a}_{ϕ}^* from $\varphi \approx 0.012$ at $\bar{a}_{\phi}^* = 0.005 \text{ m}^2 \text{ mg chl}^{-1}$ to $\varphi \approx 0.005$ at $\bar{a}_{\phi}^* = 0.025 \text{ m}^2 \text{ mg chl}^{-1}$. This is consistent with an increase in the fraction of absorption by nonphotosynthetic pigments decreasing the yield and is another possible explanation of the increasing φ_{est} with increasing chlorophyll concentration (*see also* Eq. 15 in Babin et al. 1996*b*) observed in the top panels of Fig. 9 and Fig. 13, since \bar{a}_{ϕ}^* generally decreases with increasing chlorophyll *a* concentration (Bricaud et al. 1995; Ciotti et al. 2002).

The implication is that variability in the pigment composition is probably as much a determinant of φ as are the rate constants for photochemistry and heat dissipation (e.g., Gilmore and Govindjee 1999). Any interpretation of the yields in terms of photosynthetic or nonphotochemical capacities should take these changes into account (e.g., Maritorena et al. 2000). For example, the increase with depth of the ratio of absorption by photosynthetic to nonphotosynthetic pigments should be reflected in an increase in the quantum yield sun-induced chlorophyll fluorescence. However, this does not imply a decrease in nonphotochemical quenching or in the photochemical quantum yield.