Limnol. Oceanogr.: Methods 3, 2005

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

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Web Appendix 1

Baseline correction of FLH

Hydrolight simulations—Five series of simulations using Hydrolight (a numerical modeling package using invariant imbedding methods to solve the radiative transfer equation, Sequoia Scientific Inc., Version 4.2), four with chlorophyll fluorescence (differing by their quantum yield) and one without, were performed to study the baseline algorithm used by MODIS in case 1 waters. In these simulations, the statistical model of Morel and Maritorena (2001) was followed as closely as possible. The underwater light field was computed for chlorophyll concentrations of 0.03, 0.05, 0.1, 0.3, 0.5, 1.0, 3.0, 5.0, 10.0, and 15.0 mg m^{-3}. The parameterization for scattering and the backscattering fraction is according to Morel and Maritorena (2001). To obtain the appropriate backscattering fraction, we used Fournier-Forand phase functions (Fournier and Forand 1994). The absorption coefficients measured by Pope and Fry (1997) were used for pure water. Absorption by dissolved matter and phytoplankton were modeled following Appendix B in Morel and Maritorena (2001), except that the background a_{gilvin} was set to 0 m^{-1} when the chlorophyll concentration was 0 mg m^{-3}. Scattering and absorption were specified as constant with depth and water depth was infinite. All Hydrolight series were calculated at the MODIS wavebands and additional wavebands, including 709 nm, a medium resolution imaging spectroradiometer (MERIS) band. MERIS uses 665 and 709 nm for the baseline correction and 681 nm for the fluorescence measurement (Anonymous 2002). All simulations included Raman emission parameterized following Morel et al. (2002) and Bartlett et al. (1998) (i.e., spectral dependency λ^{-5} and Raman scattering coefficient of 2.6×10^{-4} m^{-1} at 488 nm). In all cases, Radtran with Hydrolight's default parameters was used to calculate the incident irradiance for the equator and a sun zenith angle of 31°; this is consistent with the equatorial crossing time of MODIS on the autumnal equinox. The quantum yield of fluorescence was set to 0.005, 0.01, 0.03, and 0.05.

Results and discussion—The choice of the 665 nm waveband for the lower bound of the baseline leads partly to the underestimate for the MODIS algorithm. Assuming a Gaussian fluorescence emission with a width at half-maximum of 25 nm centered at 683 nm, the baseline is 0.2878 of the signal at 678 nm. This factor is accounted for in the MODIS C_f parameter and is included in the *CFE* algorithm (Letelier pers. comm. unref.). The trends with chlorophyll and quantum yield, however, are not accounted for, and originate from the relative amplitude of the backscattered upwelling radiance emission to fluorescence emission and the increasing concavity of the backscattered emission as chlorophyll increases around 676 nm (Fig. 5, right panel).

The simulations in this study were conducted for just above the sea surface. Additional biases that may originate in the use of the atmospheric aerosol scattered radiance plus water leaving radiance (top of atmosphere minus Rayleigh scattered photons) to obtain *FLH* have not been investigated. The observed negative radiances in the MODIS *FLH* before the addition of a constant (Abbott and Letelier 1999) did not occur in our simulation and are attributable to the shape of the atmospheric radiance (Letelier pers. comm. unref.). Nevertheless, even at the sea surface, baseline-corrected fluorescence is not a direct measure of the fluorescence emission. The fraction of the total fluorescence emission it measures varies with chlorophyll concentration.

The addition of a small baseline value, FLH_o, of 1.26×10^{-5} W m^{-2} nm^{-1} sr^{-1} to the measured upwelling radiance eliminated much of the trend with chlorophyll concentration (Fig. 5, inset). This, however, cannot be applied directly to the *FLH* measurement without further correction accounting for scattering in the atmosphere.

The use of the baseline method to retrieve fluorescence emission has been examined in the past mostly with the objective of obtaining chlorophyll concentration. Fisher and Kronfeld (1990), using 645 and 725 nm for the baseline and 685 nm for the measurement, found a slight overestimate of the upwelling radiance due to fluorescence at chlorophyll

concentrations below ~20 mg m^{-3} and an underestimate above 20 mg m^{-3}. This is different from our simulation (Fig. 5), which shows an increasing underestimate of the fluorescence radiance below the surface with decreasing chlorophyll concentrations in case 1 waters, especially at lower quantum yields. Our results are more in line with those of Gower et al. (1999), which suggest that, in the MERIS configuration, the fluorescence radiance measurement would be underestimated by approximately 30% at 15.4 mg chl m^{-3}. Gower et al. (1999) did not verify this relationship for a range of chlorophyll concentrations but suggest it should be nearly constant. The different results are likely the result of varying modeling approaches for the incident irradiance, the inherent optical properties of the water, the parameterization of Raman scattering, the quantum yield of fluorescence or the wavebands used. Application of the results from Fig. 5 to the data requires an iterative scheme or a precalculated look-up table (e.g., Fell et al. 2000) as the quantum yield must be known to correct the *FLH*. This was not attempted here. Further work will be necessary to completely account for this effect in case 1 waters and possibly extend it to the top of the atmosphere (corrected for molecular scattering) measurement of *FLH* (Abbott and Letelier 1999). At this point, however, given the potential underestimation of fluorescence radiance by *FLH* in low chlorophyll waters, it is not surprising to find CFE or our algorithm returning lower quantum yields in regions with lower chlorophyll concentration. This artifact could account for more than half of the increasing trend observed in φ_{est} versus MODIS chlorophyll in Fig. 9 and Fig. 13.