

Remote Sensing of the Eutrophic State of Coastal Waters via Phytoplankton Functional Groups

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Abstract – It is unlikely that we will be able to remotely sense coastal or oceanic water chemistry comprehensively from on-orbit passive or active sensors. Inferences currently are made on nitrates using sea surface temperature as a surrogate. Passive microwave sensors monitor conductivity as a surrogate for surface salinity. Suspended sediments, of course, are detectable by scattering. While Raman laser spectroscopy can diagnose constituent chemicals, issues of detection sensitivity and also eye safety are concerns especially in coastal regions. However, it might be that we don't have to pursue this challenging objective. We are primarily concerned from a marine management perspective with situations where coastal waters become degraded and the biology is disrupted. In such circumstances, the forcing on the relative mix of phytoplankton functional groups [PFGs] may well provide the important signature that identifies the impact that coastal water chemistry [or water temperature] is having on the biological systems. A number of case studies have shown that it is feasible to identify PFGs using both multi-spectral and hyperspectral remote sensing based primarily on the spectral absorption of the individual plankton species. As a general observation, it appears that as water quality degrades with an increase in concentration of pollutants, in particular, excess nutrients such as phosphates and nitrates from agricultural run-off and sewer outfalls, the diatom population decreases and flagellate population increases. If it is possible to demonstrate that the technology does deliver with acceptable accuracy the important trends over time in PFG composition then it certainly should be feasible to go back in time for at least a decade to examine temporal trends in the mix of PFGs.

Keywords: Phytoplankton functional groups water quality

1. STATEMENT OF THE PROBLEM

The change over time of the composition of phytoplankton species in a water body has been linked to climate change and anthropogenic forcing such as eutrophication. Achieving reliable methods of observing such changes on a global scale using remote sensing observation from orbiting satellite sensors is accordingly a desirable goal. In this paper we revisit the formulation of the RTE for an assemblage of PFGs in a water body and consider the tractability of approaches to the solution.

2. PHYSICAL AND CHEMICAL FORCING

There is a considerable literature that has tracked the changes in phytoplankton communities over time in many of the world's oceans and in some cases going back thousands for years using benthic sediment analyses.

These changes are important since evidence increasingly suggest that their response may be indicators of the impact (i) of global warming [eg SST] (ii) of CO₂-linked ocean acidification,

and (ii) of oceanic and particularly coastal pollution on the abundance, spatial distribution primary productivity and species composition of phytoplankton assemblages.

It is certainly true that the traditional methods of *in situ* sampling of the oceans followed by laboratory analyses [eg HPLC and flow cytometry] as well as underway methods [eg continuous plankton recorders] are well established and reliable methods that have elucidated trends in response to physical and chemical forcing [see Moore et al 2009 for recent review of current instrumentation]. In more recent times, since we have had earth observing environmental satellites, the incidence, spatial extent and duration of red tides, coccolithophore and trichodesmium blooms have been documented globally.

In Australian waters, it has been difficult in the past to obtain data sets that comprise in-water chemical analyses, pigment analyses [eg HPLC], plankton populations analysed by functional groups, and spectral absorption and scattering data on the various plankton that enable trend in PFG composition to be evaluated in a comprehensive manner. NCRIS Integrated Marine Observing System's [IMOS] investment has put in place (i) a sustained observing program of national reference stations and (ii) repeat coastal cruise programs that collect and analyse water samples for chemical and biological constituents and that routinely deploy continuous plankton recorders [CPR]. The prospect of acquiring data sets to test the hypothesis is very encouraging.

3. SOME RECENT DEVELOPMENTS

It is of note that the IOCCG established a Working Group to prepare a monograph on the PFG topic indicating that not only is the field maturing but also that the methods being applied are delivering some interesting data sets covering seasonal and regional variability through to interannual global variability.

It is also interesting that a number of major outbreaks of blooms [eg of the coast of China during the Beijing Olympics] and in the Arabian Sea, off the SW coast of India, would appear to be linked to coastal water quality degradation and in the latter case reflect a significant decadal shift in PFGs from diatoms to flagellates (S Matondkar, *private comm.*)

Finally, it is worth noting that in 2010 Ocean Optics XX Conference in Anchorage scheduled a Short Course on PFGs. The Short Course was the most popular of those on offer attracting 30 registrants indicating that the field is having some impact on the marine research community. It is evident that the field has progressed significantly in a few short years with indications that phytoplankton size distributions and discrimination of plankton populations into PFGs is being achieved. It is also apparent that good quality digital libraries of

pigment spectral absorption are becoming assembled but are not as yet comprehensive or widely available. Further, the community needs to continue to undertake validation campaigns evaluating the algorithms they apply and to provide indications of the accuracy of the retrieved products.

4. THE FORWARD MODEL

Let us focus initially on the very simple system comprising a single phytoplankton immersed in a large volume of sea water. For the moment we will neglect any consideration of the interaction of photons with the water and the air-water interface and we also neglect, for the moment, any inelastic scattering processes such as Raman scattering. So, as this narrow parallel beam of photons of wavelength λ enters the water column, it happens that some photons interact with the phytoplankton. We would expect the following as an outcome:

- i. Some photons would “miss” the phytoplankton and continue to greater depths.
- ii. A number of photons would scatter from the phytoplankton and some proportion of these photons would actually backscatter [b_{bp}] and exit toward the water surface.
- iii. A further number would enter the phytoplankton structure and might be absorbed by the pigment [a_{phi}].

The water reflectance of this system can be modelled as a function of absorption coefficient [a] and backscattering coefficient [b_b], providing a means to estimate the concentration of phytoplankton using remote sensing.

A widely used expression of the sub-surface remote sensing reflectance, r_{rs} , defined as the ratio of upwelling radiance [$L_u(O)$] to downwelling irradiance [$E_d(O)$], just below the water surface (Sathyendranath et al. 2004) is,

$$r_{rs} = \frac{f' b_b}{Q a + b_b}, \quad \dots 1$$

where, the value of $f'Q$ is dependent on the bidirectional nature of the water column and solar-sensor viewing geometry, whereby, the values are commonly taken from Look-Up-Tables previously generated using numerical simulations of radiative transfer.

The total absorption of the water column is commonly expressed as the sum of pure water absorption [a_w], the absorption of coloured dissolved organic matter [a_{cdom}] and phytoplankton [a_{phi}] that may be present,

$$a = a_w + a_{cdom} + a_{phi}. \quad \dots 2$$

Similarly, the total backscattering can be expressed as the sum of pure water backscattering [b_{bw}] and from particles [b_{bp}],

$$b_b = b_{bw} + b_{bp}. \quad \dots 3$$

If we now allow the addition of a different phytoplankton species j to be present in the water column and close by the original species i , so it also intercepts the beam of photons then we have:

$$a = a_w + a_{cdom} + a_{phi,i} + a_{phi,j} \quad \dots 4$$

and

$$b_b = b_{bw} + b_{bp,i} + b_{bp,j}. \quad \dots 5$$

If we generalise to a number of n different phytoplankton species and include their concentrations C_n [assume low concentration so there are no obscuration / packing issues] we could formulate eqn. 1 more generally as:

$$r_{rs} = \frac{f'}{Q} \frac{b_{bw}}{a_w + a_{cdom} + b_{bw}} \frac{\sum_n C_n b_{bp,n}}{\sum_n C_n [a_{phi,n} + b_{bp,n}]} \quad \dots 6$$

There are a number of improvements that can be made to eqn. 6 including deriving path elongation terms using a numerical radiative transfer solver such as Hydrolight, following Lee et al. (2004) (Mobely and Sundman 2001). However, increasing model sophistication will require the full spectral phase function for PFGs to be known rather than just the backscatter.

Inversion of equation (6) could be performed by a successive iteration technique, such as Levenberg-Marquardt. However, increasing the number of PFGs introduces extra degrees of freedom. Multispectral or even hyperspectral data is therefore desirable to keep the problem well-conditioned. Nevertheless, the possibility for multiple contradictory solutions within the bounds of image and environmental noise exists, representing the fundamental limitation on imagery information content. Regularisation methods have been used when multiple solutions are produced in order to identify the most probable solution.

Look-up-tables, built using a forward model such as equation 6, are an alternative inversion technique and with a suitable adaptive construction can facilitate sensitivity analysis and uncertainty propagation by simple brute-force ensemble inversion over multiple degrees of freedom (Hedley et al. 2009).

Clearly, various possibilities of differing sophistication exist for the construction of a physics-based inversion approach for PFG studies. The current limiting factor is determining IOP contributions of each PFG.

If we were remotely sensing a marine system, we would probably be using some selected wavelengths, such as with multispectral satellite sensor observations. We might decide, because of the spectral properties of pigments and the large array of pigments, that to assist in discriminating pigments we should resort to hyperspectral sensing.

5. FURTHER CONSIDERATIONS

If we consider eqn. 6, we know that the size distribution of phytoplankton relative to the wavelength λ , will determine the backscatter efficiency. So, $b_{bp,n}$ in principle, may be modelled using Mie theory. Further, we could adopt a size distribution for phytoplankton species n that is representative of one of the three commonly used [pico, nano or micro] populations. With respect to $a_{phi,n}$ we would need to have access to a library of spectral absorption coefficients [m^{-1}] for the n phytoplankton pigments.

We now consider just the term in eqn. 6 [with Σ in the numerator and denominator] and assume we have a water column with 5 different phytoplankton species present at moderate concentrations and we observe at wavelength λ . We would have, with respect to the unknown quantities, just 5 concentration C_n values and, because we have permitted only 3 size distributions (there are just 3 $b_{bp,n}$ from which to select) and there would be 5 $a_{phi,n}$ spectral selections to choose from; one for each phytoplankton species.

If we know something about the plankton species that are likely to occur, such as in a marine province, we would already know the 5 likely $a_{phi,n}$. So, we would have the one radiometric measurement wavelength λ and 8 unknowns. The concentration C_n are the “real” unknowns we seek whereas the b_b are, as noted, constrained to be one of 3 values based on one of the predetermined size distributions, namely nano, pico and micro.

If we make several observations at a set of wavelengths λ_k , then in this rather oversimplified system we have a very tractable formulation which, in principle, is soluble.

The use of eqn. 6 in estimating the relative contribution (or concentrations) of different phytoplankton species was tested for a simplified case whereby two different phytoplankton species were modelled. In this test, a number of sub-surface remote sensing reflectance spectra were simulated using Hydrolight 5.0 over a range of environmental conditions and varying proportions of average phytoplankton and cyanobacteria. Levenberg-Marquart non-linear optimisation was used to invert the simulated r_{rs} spectra using eqn. 6. Here, the combined absorption of phytoplankton was parameterised as,

$$a_{phi} = C [F a_{avg} + (1-F) a_{cyano}] \quad \dots 7$$

where, C is the total phytoplankton concentration, a_{avg} is the spectral absorption of average phytoplankton (taken from Hydrolight) and a_{cyano} is the spectral absorption of the toxic algae cyanobacteria (Marrable et al., 2010). F is the relative fractional contribution of the 2 species. Fig. 1 shows the model retrieval results of the toxic algae fractional component as compared with the input values to Hydrolight. This example shows encouraging results in separating the different phytoplankton species using such an approach. More detailed simulations, which include more complex cases of using up to 5 different phytoplankton species and 3 different size classes will be considered in ongoing research.

1. CONCLUSIONS

In this paper we have omitted consideration of many important issues that would impact the accuracy of the derived product, namely the composition of the functional groups that make up the phytoplankton community in a water body. Their omission does not imply that they are trivial matters to address. These include atmospheric correction, the air-water interface term, sea surface glint, effects of dense packing of assemblages, and importantly non-elastic processes [eg Raman scattering] (Sathyendranath and Platt 1998) etc. Our aim here has been more to restate the problem and the formalisms and to review the tractability of analytically-based solutions for the concentrations of PFGs.

While we have a significant way to go in this task we are encouraged by the tractability of the problem and the prospect of deriving solutions including associated uncertainties. Next

steps include the creation, using the forward model, of datasets suitable for inversion using one or more solution schemes that will permit an estimation of errors and sensitivity of the solutions to simulated instrumental noise added to the synthetic radiances.

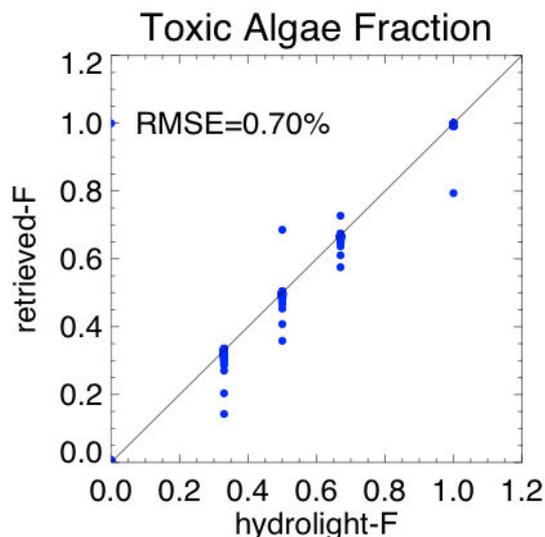


Figure 1: Comparison scatter plot of model retrieved F (eqn. 6) and hydrolight input F.

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