HYPERTEACH Marine Optics and Remote Sensing Computer Lesson 1: The colour of water¹ By Kevin Ruddick

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Presented at the IOCCG Summer School, Villefranche
Topic: "Ocean colour remote sensing of turbid waters"

Aim of Lesson

To learn how the colour of water is affected by its constituents and hence how optical remote sensing can be used to estimate concentrations of chlorophyll-a (CHL) and total suspended particulate matter² (TSM) and related parameters. This computer lesson illustrates points made in the corresponding lecture, e.g. regarding CHL detection limit in turbid waters with multispectral data.

Disclaimer

This ocean colour model gives a first order understanding of variability of ocean colour as function of chlorophyll a concentration, non-algae particle concentration and Coloured Dissolved Organic Matter absorption. It is based on an approximate reflectance model assuming no bottom reflectance, no inelastic scattering, vertically homogeneity and a fixed model for specific inherent optical properties. It is intended for educational purposes only and should not be used for ocean colour data processing or for research grade ocean colour publications. For the latter full radiative transfer simulations should be made, e.g. using HYDROLIGHT water), 6SV (atmosphere) or similar models.

Background information

Software

Access to a PC with Excel is required to carry out the lesson.

Lesson outline

In this lesson students will use an Excel-based forward optical model to simulate spectral remote sensing reflectance as function of the input constituents: phytoplankton pigments represented by the chlorophyll-a

¹ This exercise is based largely on course material developed during the HYPERTEACH project (2005). The corresponding Excel file was designed with the help of Barbara Van Mol.

² Total suspended matter (TSM), also called Suspended Particulate Matter (SPM), is the mass sum of non-algal particulate matter (NAP) and algal particulate matter, the mass of which can be estimated from chlorophyll *a* (CHL) content.

concentration (CHL), non-algal particle concentration (NAP), and coloured dissolved organic matter absorption (CDOM).

Part 1: Basic optical modelling

The lecture and Annex A describe a simple forward model which gives spectral reflectance as output for different input concentrations of non-algae particles (NAP), CHL and CDOM. In this model the total suspended particulate matter concentration (TSM) is obtained by adding the weight concentration of NAP and of algae particles, where the latter is estimated from CHL. Put simply, considering that reflectance is approximately proportional to backscatter divided by absorption:

- Increasing NAP will increase backscatter throughout the spectrum and hence tend to increase reflectance throughout the spectrum. However, since particles also absorb light, especially in the blue, the increased absorption may tend to reduce reflectance at least for certain parts of the spectrum.
- Increasing CHL will increase absorption for the blue spectral range 400-500nm, especially around 440nm and also for the narrow red spectral range 660-680nm and hence tend to reduce reflectance for these ranges. If TSM is composed mainly of non-algae particles, backscatter will change little for different CHL. However, if most suspended particles are algae particles then increasing CHL will increase also the total backscatter as well as absorption and, hence, possibly increase reflectance at least for spectral ranges where the increased backscatter is more important than the increased absorption.
- Increasing CDOM will increase absorption, especially for blue wavelengths, and hence reduce blue reflectance.

Action: Load the Excel workbook entitled "MORS-OCMODEL-v3.1.xls"³. This contains 6 sheets as follows:

INPUT: This is the sheet where you enter input concentrations and see the resulting absorption and backscatter coefficients and remote sensing reflectance spectra.

README: This sheet gives some background documentation and a warning regarding use of the model with remote sensing data

SampleRRS: This sheet contains some saved reflectance spectra which are used for learning how to fit input constituents to reflectance spectra

PARAMETERS: This sheet contains default parameters used by the model, which are set according to the optical theory and assumptions described in Annex A. These parameters should not be modified.

³ This workbook uses macros. You may need to enable or relax Macro security in order to get it to work. Also the screen display may appear different according to the number of pixels in your display. Plots can be resized and axes can be modified using standard Excel/Windows editing tools. Make a write-protected backup of this file before any modifications so you can easily return to it.

CALCULATIONS: This sheet contains all the calculations of absorption and backscatter coefficients and reflectance for wavelengths from 400nm to 800nm every 2nm. This sheet should not be modified, but is interesting for students wanting to see in more detail how the model works.

AEROSOLcorr: This sheet is used in a different exercise (investigating performance of aerosol correction algorithms in turbid waters) and is not needed in the current exercise.

During this lesson the student will change inputs for Chlorophyll concentration (CHL), non-algae particle concentration (NAP) and coloured dissolved organic matter (CDOM) absorption at 443nm (the three cells marked in orange), called the "input triplet" in this lesson. These inputs are shown also in the left hand column plots of the screen (see Figure 1.1) entitled "Input constituents" together with the resulting Total Suspended Matter (TSM). The values can be changed by using the up/down buttons.

In the centre two plots the absorption and backscatter coefficients corresponding to this input choice are shown as components and as the total of all components.

In the right hand plot on the screen the remote sensing reflectance is plotted against wavelength (where appropriate the student can use the standard Excel Format-axis function to change the linear y-axis to a logarithmic y-axis to show the large range of reflectances that can be encountered). The black curve corresponds to the input triplet.

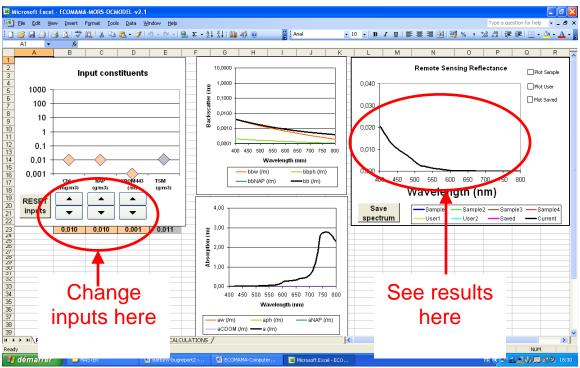


Figure 1.1. Screen shot of the Excel workbook "INPUT" worksheet where students change input and see results graphically.

Action: Set low values for all three input parameters: CHL=0.01 mg/m3, NAP=0.01 g/m3, CDOM=0.001 /m (as in Figure 1.1). This can be done by pressing the "RESET INPUTS" button. See that the total absorption coefficient is almost identical to the pure water absorption coefficient, aw, (bottom-centre plot) and that the total backscatter coefficient is mainly from pure water, bbw, and partly from phytoplankton, bbph. The reflectance (thick black line on the right hand plots) shows a peak in the blue (400nm) with rapid decrease to below 0.0025 in the green (520nm). This is very clear blue water. Save this spectrum by clicking the "Save Spectrum" button in the reflectance chart window and plot the saved spectrum (behind in mauve) by clicking the "plot saved" checkbox in the same window.

Now vary the three input parameters and see how the reflectance changes and why (via the absorption and backscatter coefficients).

Question 1.1: How does increasing non-algae particle concentration (NAP),e.g. to 1.0 then to 10.0 then to 100.0 g/m3 affect: a) absorption, b) backscatter and c) reflectance?

Action: Reset all three components to low values and now investigate how reflectance changes as CHL is increased to 1.0 then to 30.0 mg/m³. [in reality CDOM would generally increases simultaneously when CHL increases because of generation of CDOM by degradation of marine phytoplankton but that it is not modelled explicitly here - CDOM must be increased manually by the user]

Question 1.2: For low NAP and CDOM how does an increase in CHL affect the wavelength of maximum reflectance? How will this be seen in terms of the colour perceived by a human observer?

Action: Reset all three components to low values. Click "plot sample" to see four pregenerated reflectance spectra. Now try to find the input concentrations that correspond to these pregenerated reflectance spectra in the right hand plot by fitting the thick black curve in the reflectance plots to the other coloured curves.

Question 1.3: What CHL, NAP and CDOM combination gives a reflectance spectrum similar to that of the blue curve (low reflectance blue water)?

Hint 1: The blue curve has very low red (600nm) reflectance and so has low NAP concentration.

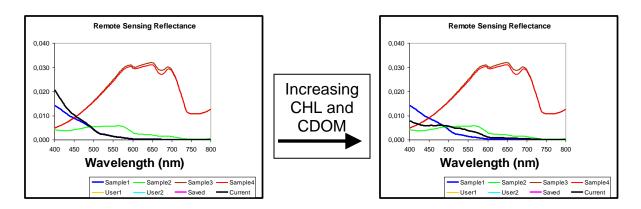


Figure 1.2. The blue, green, red and brown curves are pregenerated and do not change. The black curve will change according to the inputs for CHL, NAP and CDOM. Here low values are given for all three inputs (CHL=0.01 mg/m3, NAP=0.01 g/m3, CDOM=0.001 /m) in the left hand plot. Increasing CHL from 0.01 to 1.0 mg/m3 and CDOM from 0.001 /m to 0.01 /m changes the black curve, increasing reflectance for 450-550nm as shown in the right hand plot.

Hint 2: CDOM affects blue reflectance most but has less effect on green and red wavelengths. So set NAP and CDOM to low values and try to fit the spectrum at 500-550nm by varying CHL (see Figure 1.2). Then fit the spectrum at 400-450nm by varying CDOM absorption.

Question 1.4: What CHL, NAP and CDOM combination gives a reflectance spectrum similar to that of the green curve (medium reflectance green water)?

Hint 1: Red (600nm) reflectance is now moderate. This can be achieved either by very high CHL or by moderate NAP concentrations. Try both to fit the spectrum for 550-720nm. Then vary CDOM to achieve a good fit in the region 400-450nm.

The next two Questions, 1.5 and 1.6, illustrate a critical problem of CHL retrieval in turbid waters

Question 1.5: What CHL, NAP and CDOM combination gives a reflectance spectrum similar to that of the brown curve (high reflectance, turbid red/brown water)?

Hint 1: Red and even near infrared (700-800nm) is now significant suggesting a very high particle concentration. Reset all concentrations to low values then vary NAP to fit the near infrared spectrum.

Hint 2: Next vary CDOM to fit the blue spectrum (400-450nm). Finally adjust CHL.

Question 1.6: In the previous exercise where do you see the biggest impact of a change in CHL? How is the red curve different from the brown curve? Which CHL,

NAP and CDOM combination gives a reflectance spectrum similar to that of the red curve (high reflectance, turbid red/brown water)?

Hint 1: Vary NAP then CDOM then CHL as previously.

Part 2: Advanced optical modelling

For students wishing to become experts in aquatic optics much, much more can be learnt from this simple model.

Action: Play with the input concentrations until you are so familiar that you can a) estimate the concentrations just by looking at the reflectance spectrum and b) understand how the component absorption and backscatter coefficients are affecting the reflectance spectrum. In some cases the reflectance spectrum may not vary even if you multiply one of the inputs by ten. In reality this means that the colour of water is not sensitive to that parameter for that combination of the other parameters. As a consequence remote sensing of the insensitive parameter will not be feasible.

Action: Now reset inputs to low default values and click the "Plot User" checkbox in the reflectance plot area. This loads a spectum reduced to multispectral data (SeaWiFS visible bands). Unclick the "PlotSample" checkbox. Try fitting this spectrum as before.

Question 2.1: What information, if any, is lost? Do you find a single perfect solution?

Action: Add the MERIS/OLCI 709nm band by copying from cell SampleRRS:F171 to G171.

Question 2.2: How does this help constrain the retrieval?

Action: Make a back-up of the original worksheet (save at a different name) and set challenge reflectance spectra for other students to match by saving spectra and pasting values from the SampleRRS sheet cells B16:B216 to the same sheet cells H16:H216 and clicking "plot user (which is then plotted as the blue curve).

Action: (for the truly adventurous) After making a backup of the original worksheet, now try modifying also some of the default parameters such as the logarithmic spectral slope of CDOM absorption (SCDOM) set in cell B23 of the PARAMETERS sheet. In reality this parameter is not known precisely but measurements show that it may take values between about 0.014 nm⁻¹ and 0.022 nm⁻¹.

Question 2.3: If SCDOM were also considered unknown and set as a fourth variable input parameter, would it be possible to estimate it by fitting the

reflectance spectrum as before? Would there be a unique solution for the four input parameters or is it possible that different combinations give equally acceptable solutions: a) in the hyperspectral case? b) in the multispectral, e.g. SeaWiFS bands, case?

Question 2.4: In Question 1.1 you noticed that increasing NAP beyond 10.0 g/m3 made no difference to the blue reflectance, which reached a "saturation" value. So what optical parameters determine that saturation value?

Question 2.5: What if the reflectance spectrum is reduced a) to the Landsat-8 band set? B) to the Sentinel-2 band set (and assuming negligible sensor noise)

Question 2.6: What if random sensor noise is added to the Sentinel-2 bandset? How does this affect the estimated concentrations after spectral fitting?

Annex A. The simple "HYPERTEACH" model of water colour

This annex describes the simple HYPERTEACH ocean colour model, which takes as input the chlorophyll-a concentration, C, the concentration of non algae particles, X, and the CDOM absorption at 443nm, Y. From these three variables, using the theory of aquatic optics and certain simplifying assumption, the remote sensing reflectance spectrum, R_{rs} , is calculated. By playing with the computer version of this model, students can vary continuously, C, X and Y and observe the consequent variation of R_{rs} , thus understanding how the composition of water affects its colour.

a) Absorption

The total absorption coefficient is decomposed into components representing the absorption coefficients respectively of: pure water (molecules), $a_{\scriptscriptstyle w}$, phytoplankton, $a_{\scriptscriptstyle ph}$, non-algae particles, $a_{\scriptscriptstyle NAP}$, and coloured dissolved organic matter, $a_{\scriptscriptstyle CDOM}$, as follows:

$$a(\lambda) = a_w(\lambda) + a_{ph}(\lambda) + a_{NAP}(\lambda) + a_{CDOM}(\lambda) \tag{1}$$

where λ represents wavelength. Each of these components is in turn modelled as follows:

- The tabulated data for $a_{w}(\lambda)$ of (Buiteveld et al. 1994) is used
- $a_{ph}(\lambda)$ is modelled as an increasing, slightly non-linear function of chlorophyll-a concentration, C

$$a_{ph}(\lambda) = A(\lambda)C^{1-B(\lambda)}$$
 (2)

where $A(\lambda)$ and $B(\lambda)$ are empirical spectral values tabulated by (Bricaud et al. 1995)

• $a_{\scriptscriptstyle NAP}(\lambda)$ is modelled as a linear function of the concentration of non algae particles, X, with spectral variation given by (Babin et al. 2003):

$$a_{NAP}(\lambda) = Xa_{NAP}^*(443nm)e^{-S_{NAP}(\lambda - 443nm)}$$
 (3)

using a logarithmic spectral slope of $S_{N\!AP}=0.0123nm^{-1}$, and specific absorption of $a_{N\!AP}^*\left(443nm\right)=0.041m^2g^{-1}$

• and $a_{\text{CDOM}}\left(\lambda\right)$ is modelled with respect to the CDOM absorption at 443nm, $Y=a_{\text{CDOM}}\left(443nm\right)$, as an exponentially decreasing function of wavelength according to the measurements of (Babin et al. 2003):

$$a_{CDOM}(\lambda) = Ye^{-S_{CDOM}(\lambda - 443nm)} \tag{4}$$

using a logarithmic spectral slope of $S_{\rm CDOM} = 0.0176 nm^{-1}$.

b) Backscatter

The total backscatter coefficient is similarly decomposed into components representing the backscatter coefficients respectively of: pure water (molecules), b_{bw} , phytoplankton, b_{bnh} , and non-algae particles, b_{bNAP} , as follows:

$$b_{b}(\lambda) = b_{bw}(\lambda) + b_{bnh}(\lambda) + b_{bNAP}(\lambda) \tag{5}$$

where λ represents wavelength. Each of these components is in turn modelled as follows:

• $b_{bw}(\lambda)$ is modelled according to (Morel 1974):

$$b_{bw}(\lambda) = 0.5*0.00288*\left(\frac{\lambda}{500nm}\right)^{-4.32}$$
 (6)

• $b_{bph}(\lambda)$ is modelled using the formulation of (Morel and Maritorena 2001):

$$b_{b\phi}(\lambda) = \left\{0.002 + 0.01*\left[0.50 - 0.25\log_{10}C\right]\right\} * \left(\frac{\lambda}{550}\right)^{\nu} 0.416 C^{0.766}$$
 (7)

• $b_{bNAP}(\lambda)$ is modelled as a linear function of the concentration of non algae particles, X, with power law spectral variation (Morel and Prieur 1977), specific scattering taken from (Babin et al. 2003) and assuming a scattering to backscattering ratio of 0.02 from Petzold (Mobley 1994):

$$b_{bNAP}(\lambda) = 0.02 * 0.51 m^2 g^{-1} * X * \left(\frac{\lambda}{555 nm}\right)^{-n}$$
 (8)

For the purposes of this lesson the power law exponent is taken as n=0, giving the simpler wavelength-independent formulation:

$$b_{bNAP}(\lambda) = 0.02 * 0.51 m^2 g^{-1} * X$$
 (9)

c) Reflectance

Finally the remote sensing reflectance, R_{rs} , is defined as:

$$R_{rs}(\lambda) = \frac{L_w^{0+}}{E_d^{0+}} \tag{10}$$

where L_w^{0+} is the above water water-leaving radiance (corrected for air-water interface reflection) and E_d^{0+} is the above water downwelling irradiance (Babin et al. 2003). This reflectance can be modelled as:

$$R_{rs}(\lambda) = \frac{\Re f'}{Q} \frac{b_b(\lambda)}{a(\lambda) + b_b(\lambda)} \tag{11}$$

According to optical theory the factor $\gamma' = \Re f'/Q$ may vary by a few tens of percent as function of sun and viewing angles, waves (and hence wind speed), particle type, etc. However, for the purposes of this lesson it will taken as a constant: $\gamma' = 0.53*0.13 = 0.069$.

Although not imposed directly as an input variable, the total suspended matter (in g/m3), T, is calculated from the inputs for non-algae particle concentration (in g/m3) and chlorophyll-a concentration (in mg/m3) via:

$$T = X + 0.07C (12)$$

d) Implementation

Thus, the model can be summarized in the following steps:

- 1. User inputs C, X and Y. T is calculated as an auxiliary variable.
- 2. Spectral absorption and backscatter coefficients a and b_b are calculated from C, X and Y.
- 3. Remote sensing reflectance R_{rs} is calculated from a and b_b .

This model has been prepared as an Excel spreadsheet, which students will familiarise with in the IOCCG Summer School session on "Ocean Colour Remote Sensing in turbid, coastal waters".

References

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