HYPERTEACH Marine Optics and Remote Sensing
Computer Lesson 1: The colour of water
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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 matter[1] (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

You will require `Jupyter Notebook` to run this code. We highly recommend that you install the latest Anaconda Python distribution for your operating system. Anaconda Python distributions include Jupyter Notebook.

Instructions for downloading and using the Jupyter Notebook on which this lesson is based can be found at:
https://gitlab.com/benloveday/oc_forward_model

Lesson outline

[1] 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 via empirical relationships.

In this lesson students will use a python-based forward optical model to simulate spectral remote sensing reflectance as function of the input constituents: phytoplankton pigments represented by the chlorophyll-a 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 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 1.0: Load the oc_forward_model jupyter notebook and run with Run_model.ipynb to give the Graphical User Interface (GUI) shown in Figure 1.

This GUI has a left hand panel with the user inputs and a right hand panel with the model outputs. Zoom in/out at the browser level until you see the full left and right panels at the same time as in Figure 1.

In the left hand panel (from top to bottom):

- The horizontal sliders for CHL, NAP and CDOM443 are the main input controls, where the user sets the concentration of these input constituents.
- The plot underneath shows the values of these three sliders graphically (red dots) as well as the TSM (grey dot) which is calculated by the model from NAP and CHL.
- 3 checkboxes for showing in the right hand panel reflectance graph: a) sample Rrs spectra (precalculated and supplied with the model for use in this lesson); b) user-defined Rrs spectra (which can be prepared by the user and saved in

the directory /oc_forward_model/forward_model/Rrs_samples); c) the most recently-saved user Rrs spectrum (updated when Save spectra button is pressed).

- Save spectra button, which will save the current Rrs spectrum for display when the checkbox “Show saved Rrs spectrum” is checked.

In the right hand panel (from bottom to top):

- Backscatter coefficient (bb) spectra with components from pure water molecules (bbw), phytoplankton (bbph) and non-algal particles (bbpNAP) and the total of these 3 components. These are calculated from the input CHL and NAP according to the Inherent Optical Model described in Appendix A.
- Absorption coefficient (a) spectra with components from pure water molecules (aw), phytoplankton (aph), CDOM (aCDOM) and non-algal particles (aNAP) and the total of these 4 components. These are calculated from the input CHL, CDOM and NAP according to the Inherent Optical Model described in Appendix A.
- Remote sensing reflectance (Rrs) spectrum from the currently-selected input constituents as modelled from absorption and backscatter by the approximate reflectance model given in Appendix A.

While the current lesson can mainly be carried out using only the GUI, it is educative to see the details of the model, which are contained in the following 3 files, which are part of the downloaded package:

- Components.py contains the formulae implementing the IOP model according to the data from IOP_model.ini and IOPs.txt
- IOP_model.ini contains parameters used in the IOP model, including mass-specific NAP absorption, logarithmic spectral slope of NAP and CDOM absorption, etc.
- IOPs.txt contains tabulated data for pure water absorption and the non-linear coefficients for the [Bricaud et al, 1995] model of phytoplankton absorption.

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 sliders in top left of the GUI in Figure 1), called the “input triplet” in this lesson. The values can be changed by dragging on the slider left/right.

In the right panel middle/lower 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 panel upper plot on the screen the remote sensing reflectance is plotted against wavelength (the student can zoom into the plot by using the simple buttons which appear just below when mousing over a plot, or can modify the y-axis range by modifying the code main.py). The black curve corresponds to the input triplet.

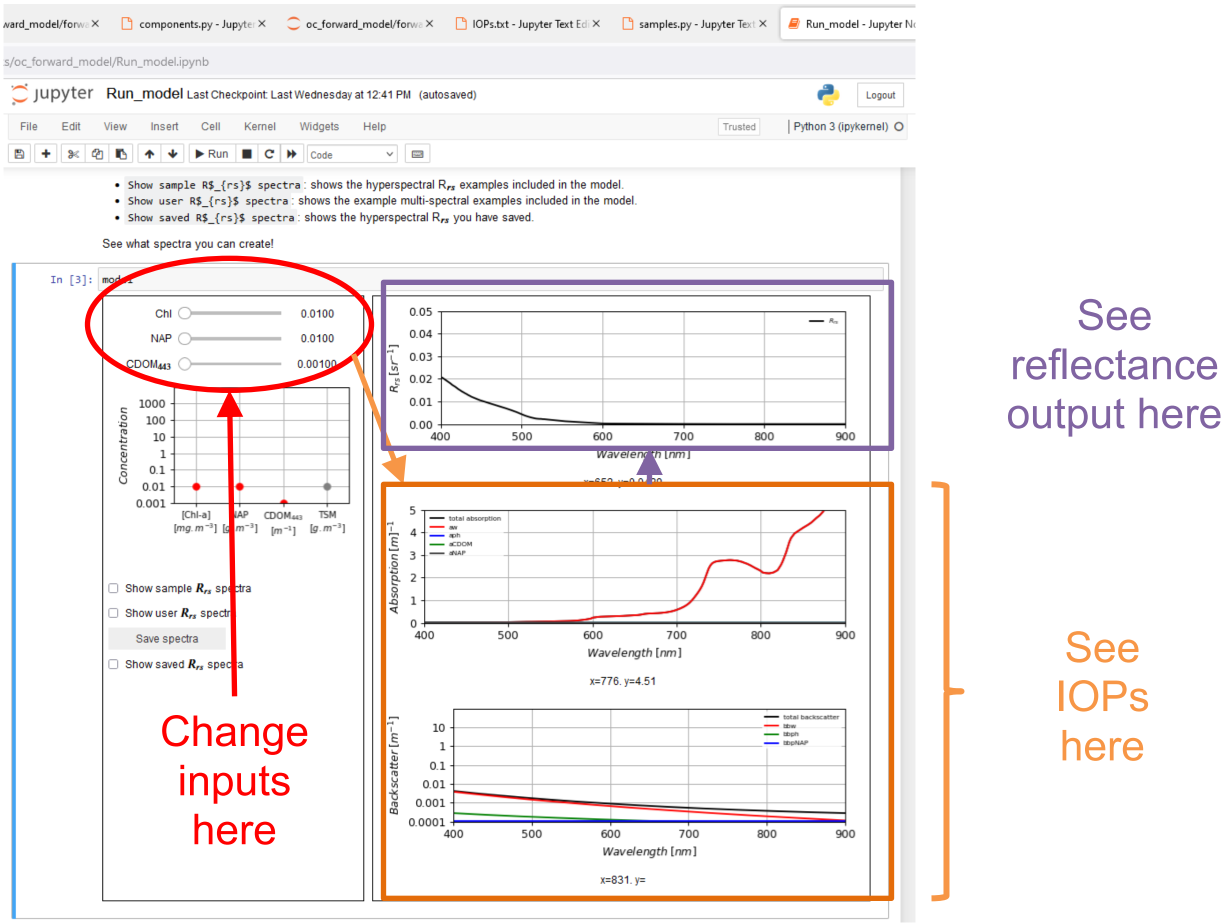

Figure 1. *Screen shot of the jupyter notebook where students change input and see results graphically.*

Action 1.1: 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). See that the total absorption coefficient is almost identical to the pure water absorption coefficient, aw, (centre-right plot) – in fact, since the lines are plotted on top of each other, you may need to increase NAP to 50 g/m3 or increase CHL to 15 mg/m3 to see the difference between total absorption and aw for 600-700nm or for 660-680nm respectively. Resetting to the minimal input parameters CHL=0.01 mg/m3, NAP=0.01 g/m3, CDOM=0.001 /m, see also that the total backscatter coefficient is mainly from pure water, bbw, and partly from phytoplankton, bbph for the range 400-600nm (for the range 600-900nm all three components are at very low values). The reflectance (thick black line on the upper right plot) 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

bottom left panel and plot the saved spectrum (behind as grey dashed line) by clicking the “show saved” checkbox in the same window.
Now vary the three input parameters, by dragging the sliders or by entering numerical values in the boxes just to right of the sliders, and see how the reflectance changes and why (via the absorption and backscatter coefficients).

Question 1.1: *For low CHL and CDOM, 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 1.2: 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/m^3. *[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 1.3: Reset all three components to low values. check “show sample Rrs spectra” to see four pregenerated reflectance spectra and uncheck “show saved Rrs spectrum” – see Figure 3. Now try to find the input concentrations that correspond to these pregenerated reflectance spectra in the plot by fitting the thick black curve in the reflectance plots to the other coloured curves.

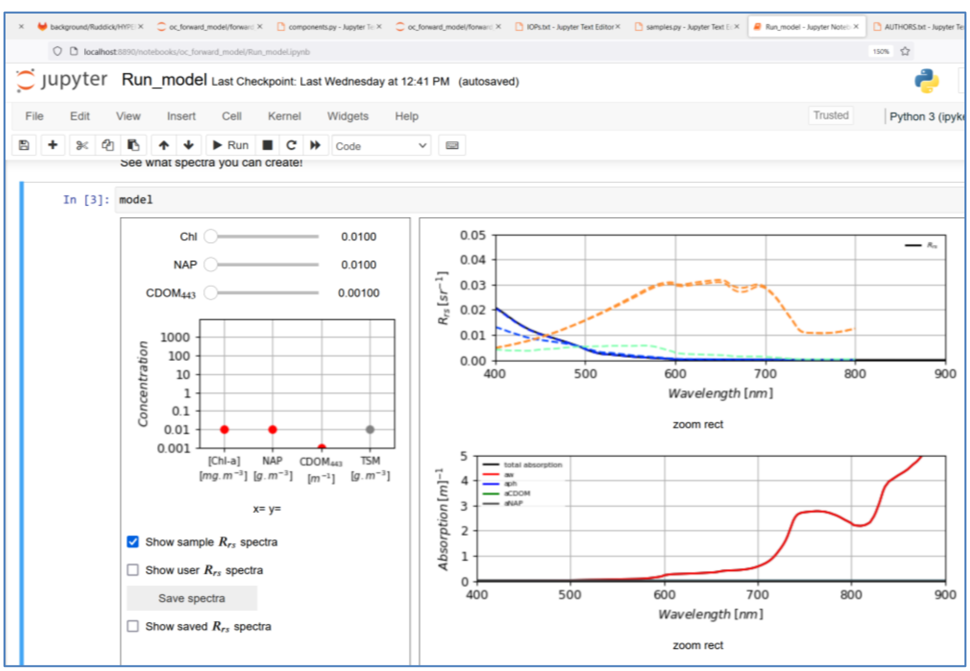

Figure 2. *Screen shot of the jupyter notebook showing the 4 pre-generated reflectance spectra (dashed lines, upper right plot).*

***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 with Rrs(400nm)=0.013 has very low red (600nm) reflectance and so has low NAP concentration.
Hint 2: At 400nm and 500nm CDOM has significant effect, but some CHL absorption is needed to fit well for the region 435-450nm.

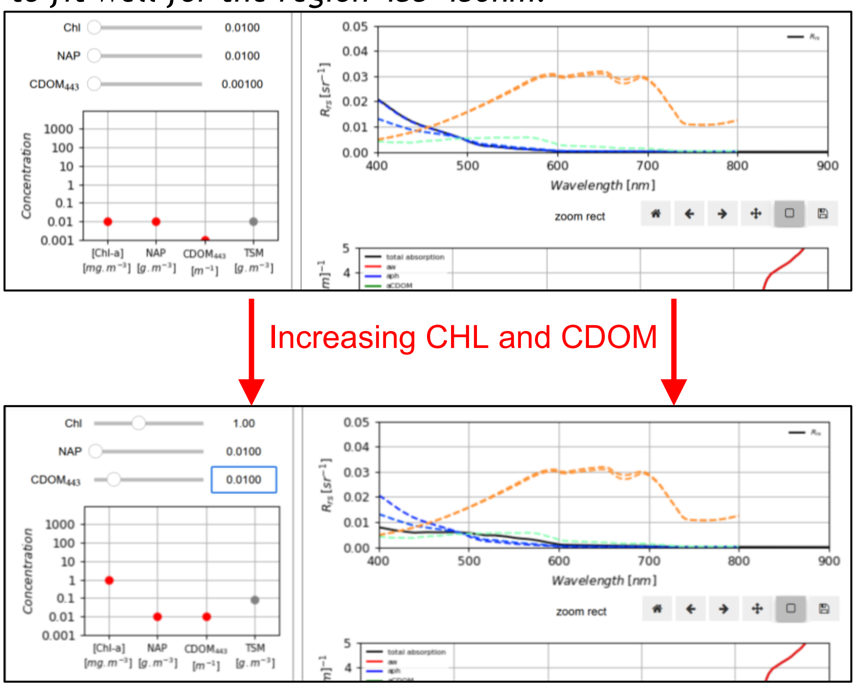

Figure 3 The dashed Rrs *curves are pregenerated and do not change. The black* Rrs *curve will change according to the inputs for CHL, NAP and CDOM. Here low values are given for all three inputs (CHL=0.01 mg/m3, NAP=0.01 g/m3, CDOM=0.001 /m) in the* top *plot. Increasing CHL from 0.01 to 1.0 mg/m3 and CDOM from 0.001 /m to 0.01 /m changes the black curve, increasing reflectance for* 490-600nm and decreasing reflectance for 400-490nm *as shown in the* bottom *plot.*

Hint 3: 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. Then fit the spectrum at 400-450nm by varying CDOM absorption (see Figure 3*).*

***Question 1.4**: What CHL, NAP and CDOM combination gives a reflectance spectrum similar to that of the green curve with Rrs(590nm)=0.004 (medium reflectance green water)?*

Hint 1: Red (600nm) reflectance is now moderate. This can be achieved either by very high CHL or by low/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 upper orange curve (high reflectance, turbid red/brown water) with Rrs(670nm)=0.0288?*

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 lower orange curve different from the upper orange curve ? Which CHL, NAP and CDOM combination gives a reflectance spectrum similar to that of the upper orange curve (high reflectance, turbid red/brown water) with Rrs(670nm)=0.0272?*

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 using and modifying this simple model.

Action 2.0: 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 2.1: Now reset inputs to low default values, uncheck "show sample Rrs spectra" and check the "show user Rrs" checkbox in the left panel. This loads a spectrum reduced to multispectral data (central wavelengths[2] of Landsat-8 visible bands). Try fitting this spectrum as before.

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

Action 2.2: Now swap to Sentinel-2 central wavelengths by overwriting the file "Rrs_user_01.txt" in the directory oc_forward_model/forward_model/Rrs_samples by the file "Rrs_S2_01.txt" from the same directory and resetting the user spectrum by rerunning the jupyter notebook steps "model = forward_model.ForwardModel()" and "model".

Question 2.2: *How does this help constrain the retrieval?*

Action 2.3: Make a back-up of the original file in the directory oc_forward_model/forward_model/Rrs_samples (save in a different place) and set challenge reflectance spectra for other students to match by saving spectra and copying the file *** to **"Rrs_user_01.txt" in the directory oc_forward_model/forward_model/Rrs_samples**.

Action 2.4: (for the truly adventurous) After making a backup of the original files, now try modifying also some of the default parameters such as the logarithmic spectral slope of CDOM absorption (SCDOM) set in the file IOP_model.ini and resetting the model plots as in Action 2.2. In reality this parameter is not known

[2] The data shown here is from hyperspectral reflectance spectra subsampled at the central wavelengths of Landsat-8. This is similar but not identical to the reflectance that would be measured by the spectral response function of each Landsat-8 band because the latter are quite broad and would require a spectral convolution of radiance.

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. Landsat-8 central wavelengths, 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 happens if the central wavelengths of Landsat-8 and Sentinel-2 are replaced by a more realistic spectral convolution over the wide spectral bands of these instruments?*

Question 2.6*: Does the Sentinel-3/OLCI band set improve retrievals with respect to the Sentinel-2 central wavelengths?*

Question 2.7*: What if random sensor noise is added to the reflectance spectrum in the case of the Landsat-8 or Sentinel-2 central wavelengths.*

Question 2.8*: What if an aerosol correction error, e.g. of the smooth spectral shape given by the "L2-WFR/RMSD" curve from Fig9.middle of [Vanhellemont and Ruddick, 2021; https://doi.org/10.1016/j.rse.2021.112284] is added to the Sentinel-2 reflectance sample given here? 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_w, phytoplankton, a_{ph}, non-algae particles, a_{NAP}, and coloured dissolved organic matter, a_{CDOM}, as follows:

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

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

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

  where $A(\lambda)$ and $B(\lambda)$ are empirical spectral values tabulated by (Bricaud et al. 1995)
- $a_{NAP}(\lambda)$ is modelled as a linear function of the concentration of non algae particles, X, with spectral variation given by (Babin et al. 2003):

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

  using a logarithmic spectral slope of $S_{NAP}=0.0123nm^{-1}$, and specific absorption of $a^*_{NAP}(443nm)=0.041m^2g^{-1}$
- and $a_{CDOM}(\lambda)$ is modelled with respect to the CDOM absorption at 443nm, $Y=a_{CDOM}(443nm)$, as an exponentially decreasing function of wavelength according to the measurements of (Babin et al. 2003):

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

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

b) Backscatter

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

$$b_b(\lambda) = b_{bw}(\lambda) + b_{bph}(\lambda) + b_{bNAP}(\lambda) \tag{5}$$

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

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

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

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

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

- $b_{bNAP}(\lambda)$ 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):

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

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

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

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:

$$T = X + 0.07C \tag{12}$$

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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Morel, A. and S. Maritorena (2001). "Bio-optical properties of oceanic waters: a reappraisal." Journal of Geophysical Research **106**(C4): 7163-7180.

Morel, A. and L. Prieur (1977). "Analysis of variations in ocean color." Limnology and Oceanography **22**(4): 709-722.

Answers

Answer 1.1: *Increasing non-algae particle concentration increases absorption for the blue spectral region (you may need to zoom in to see this), and for the green region if sufficiently high. Backscatter increases at all wavelengths, giving an increase in reflectance at all wavelengths at first, but when the increased blue absorption takes effect the blue reflectance increases no further while the green and red reflectances continue to increase rapidly at first, then more and more slowly as maximum reflectance is reached.*

Answer 1.2: *For low NAP and CDOM, and for CHL=1 mg/m^3, the reflectance spectrum has a maximum at 400nm and a local maximum at about 460nm. If CHL increases further to CHL=30 mg/m3 the reflectance at 400nm decreases, because phytoplankton absorb strongly in the blue, but the reflectance maxima around 490nm and 570nm increase because the total absorption is lower there. As CHL increases the water colour goes from blue to green.*

Answer 1.3: *Input of CHL=0.1 mg/m^3, NAP=0.01 g/m^3 and CDOM=0.004 /m were used to generate the "blue curve" reflectance spectrum.*

Answer 1.4: *Input of CHL=10.0 mg/m^3, NAP=0.01 g/m^3 and CDOM=0.04 /m were used to generate the "green curve" reflectance spectrum. [however, you may have found a different solution that fits quite well too]*

Answer 1.5: *Input of CHL=12.6 mg/m^3, NAP=50.1 g/m^3 and CDOM=1.58 /m was used to generate the "brown curve" reflectance spectrum.*

Answer 1.6: *When the brown curve in question 1.5 is well-fitted variation of CHL has little effect on the reflectance spectrum. It is only near 670nm that a difference can be seen when varying CHL. This implies that the blue and green spectral regions are not useful in algorithms for CHL retrieval in such high NAP and CDOM waters. The red curve is lower reflectance (so lower backscatter OR higher absorption) and has a clearer local minimum at 670nm (so has higher CHL). CHL=19.9 mg/m^3, NAP=50.1 g/m^3 and CDOM=1.58 /m was used to generate the red curve.*

Answer 2.1: *This is a broad question with no simple, unique answer. However, an example of what is lost with the Landsat-8 bands is that the local minimum near 670nm for high CHL can no longer be distinguished because neighbouring bands are spectrally too far away. As a consequence different triplet values (especially with different CHL) seem to fit reasonably well, indicating that the solution is less well-constrained than when the same spectrum was fitted previously in Question 1.6, but with hyperspectral data.*

Answer 2.2: *The Sentinel-2 705nm band helps constrain better the CHL solution for this problem. The presence of such is band, in addition to a band somewhere in the range 665-670nm, is very advantageous for CHL retrieval in turbid waters.*

Answer 2.3*: This question and other similar questions relating to uniqueness of solutions are being considered by various research groups internationally but no clear answer has been provided yet. It is suspected that if we have too many "unknown" variables to retrieve then there could be multiple solutions that are equally possible. i.e. optical remote sensing cannot give a single answer but gives potentially more than one answer which is completely coherent with the available data. In such cases extra data, e.g. from in situ measurements or from knowledge of parameters such as SCDOM (which can then be accepted as fixed), is needed to determine which solution corresponds to the reality. An interesting discussion of possible multiple solutions to the optical remote sensing problem is given by [Sydor, Applied Optics, vol 43, no 10, 2004]. The problem of possible existence of multiple solutions is much more severe when less spectral information is available (e.g. Landsat-8 bands instead of hyperspectral). In the extreme case of very limited spectral information (e.g. AVHRR bands 1 and 2) there is no way of distinguishing between non-algae and algae particles.*

Answer 2.4*: There is an interesting discussion of this "reflectance saturation" phenomenon in [Luo, Y., Doxaran, D., Ruddick, K., Shen, F., Gentili, B., Yan, L. and H. Huang (2018). Saturation of water reflectance in extremely turbid media based on field measurements, satellite data and bio-optical modelling. Optics Express, 26, 10435-10451.* https://doi.org/10.1364/OE.26.010435*]*

Answers 2.5, 2.6, 2.7 and 2.8*: We don't give all the answers!*