GLAM Bio-Lith RT: A tool for Remote Sensing Reflectance Simulation and Water Components Concentration Retrieval in Glacial Lakes

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Appendix

A Modeling of the Remote Sensing Reflectance Below the Surface for Shallow Water

As shown in section 2, the remote sensing reflectance **below** the surface for **shallow water** is modeled as follows:

$$R_{rs}^{sh-}(\lambda) = R_{rs}^{-}(\lambda)\left[1 - A_{rs,1}e^{-z_B(K_d(\lambda)+k_{uW}(\lambda))}\right] + A_{rs,2}R_{rs}^{b}(\lambda)e^{-z_B(K_d(\lambda)+k_{uB}(\lambda))} \tag{A.0.0.1}$$

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where on the right-hand side the first term is the remote sensing reflectance of a water slab with thickness z_B, and the second term is the remote sensing reflectance of the lakes's bottom seen at the lake surface within the water column. $A_{rs,1} = 1.1576$ and $A_{rs,2} = 1.0389$ are fixed empirical constant defined in [7]. $R^b_{rs}(\lambda)$ is the lake bottom reflectance and is calculated as follows:

$$R^b_{rs}(\lambda) = \sum_{n=0}^{N-1} f_n B_n a_n(\lambda) \tag{A.0.0.2}$$

In A.0.0.2, six types of bottom surfaces are considered. Hence six albedos (irradiance reflectance of a surface is called albedo) $a_n(\lambda)$ are considered at the same time. The surface albedos spectra are provided for six different types of bottom. f_n is the areal fraction of bottom surface type n, and $\sum_{n=0}^{N-1} f_n = 1$. B_n is the proportion of radiation that is reflected to the sensor. [4] and so do we consider all the surface types as Lambertian surfaces (isotropic reflection) hence $B_n = 1/\pi = 0.318$ sr^{-1} for all n.

K_d, k_{uW}, and k_{uB} measure the radiation attenuation within the water slab (attenuation for downwelling irradiance, upwelling radiance reflected in the water, and upwelling radiance reflected by the bottom respectively) and they are computed as below:

$$K_d(\lambda) = k_0 \frac{a(\lambda) + b_b(\lambda)}{cos\Theta'_{sun}} \tag{A.0.0.3}$$

$$k_{uW}(\lambda) = \frac{a(\lambda) + b_b(\lambda)}{cos\Theta'_V} \left[1 + \omega_b(\lambda)\right]^{3.5421} \left[1 - \frac{0.2786}{cos\Theta'_{sun}}\right] \tag{A.0.0.4}$$

$$k_{uB}(\lambda) = \frac{a(\lambda) + b_b(\lambda)}{cos\Theta'_V} \left[1 + \omega_b(\lambda)\right]^{2.2658} \left[1 - \frac{0.0577}{cos\Theta'_{sun}}\right] \tag{A.0.0.5}$$

k_0 depends on the scattering phase function. It usually set equal to 1.0395 for case-1 water and equal to 1.0546 for case-2 water ([4] default).

The remote sensing reflectance **above** the water surface can be model in different ways, the following one is set by default in [4] and used here:

$$R_{rs}(\lambda) = \frac{(1-\sigma)\left(1-\sigma^-_L\right)}{n^2_W} \cdot \frac{R^-_{rs}(\lambda)}{1 - \rho_u Q R^-_{rs}(\lambda)} + R^{surf}_{rs}(\lambda) \tag{A.0.0.6}$$

On the right-hand side, the first term measures the reflection in the water, the second at the surface. $n_W = 1.33$ is the water index of refraction. $Q = 5$ sr is defined in the previous sections. σ is the reflection factor for the downwlling irradiance above the water surface. It is set equal to 0.03 by default. σ^-_L is the reflection factor for the upwelling radiance below the water surface. It is computed as follows:

$$\sigma^-_L(\Theta_v) = \rho_L(\Theta_v) = \frac{1}{2} \left| \frac{sin^2(\Theta_v - \Theta'_v)}{sin^2(\Theta_v + \Theta'_v)} + \frac{tan^2(\Theta_v - \Theta'_v)}{tan^2(\Theta_v + \Theta'_v)} \right| \tag{A.0.0.7}$$

where the viewing angles are related by the Snell's law:

$$n_W sin\Theta_v^{'} = n_{air} sin\Theta_v \tag{A.0.0.8}$$

ρ_u is the reflection factor for the upwelling irradiance below the water surface. It is set equal to 0.54 by default. $R_{rs}^{-}(\lambda)$ is the remote sensing reflectance below the surface for deep water described previously. If shallow water is considered, $R_{rs}^{-}(\lambda)$ is replaced with $R_{rs}^{sh-}(\lambda)$, which is described above as well.

$R_{rs}^{surf}(\lambda)$ is the reflection at the surface, also called specular reflectance, and is modeled as follows:

$$R_{rs}^{surf}(\lambda) = \rho_L \frac{L_s(\lambda)}{E_d(\lambda)} \tag{A.0.0.9}$$

If the wavelength-independent model is selected A.0.0.9 is replaced by:

$$R_{rs}^{surf} = \frac{\rho_L}{\pi} \tag{A.0.0.10}$$

ρ_L is called the Fresnel reflectance and is given by A.0.0.7. $L_s(\lambda)$ and $E_d(\lambda)$ are the sky radiance and the downwelling irradiance above the water surface, respectively. In our software, we modeled these two quantities as in [4]. For the sake of completeness, they are reproduced here with a brief explanation.

The downwelling irradiance $E_d(\lambda)$ is modeled as follows:

$$E_d(\lambda) = f_{dd} E_{dd}(\lambda) + f_{ds} E_{ds}(\lambda) \tag{A.0.0.11}$$

$E_{dd}(\lambda)$ is the direct component of $E_d(\lambda)$. It represents the sun disk in the sky as photon source. $E_{ds}(\lambda)$ is the component of $E_d(\lambda)$ scattered from the sky and is the sum of two components:

$$E_{ds}(\lambda) = E_{dsr}(\lambda) + E_{dsa}(\lambda) \tag{A.0.0.12}$$

$E_{dsr}(\lambda)$ measures the Rayleigh scattering. $E_{dsa}(\lambda)$ measures the aerosol scattering. f_{dd} and f_{ds} are correction factors that correct the intensities of the light sources according to the illumination conditions. They allow simulation and measurements analysis at non-standerd illumination conditions [4]. $E_{dd}(\lambda)$, $E_{dsr}(\lambda)$, and $E_{dsa}(\lambda)$ are calculated in the following way:

$$E_{dd}(\lambda) = E_0(\lambda) T_r(\lambda) T_{aa}(\lambda) T_{as}(\lambda) T_{oz}(\lambda) T_o(\lambda) T_{wv}(\lambda) cos\Theta_{sun} \tag{A.0.0.13}$$

$$E_{dsr}(\lambda) = \frac{1}{2} E_0(\lambda) \left(1 - T_r^{0.95}(\lambda)\right) T_{aa}(\lambda) T_{as}(\lambda) T_{oz}(\lambda) T_o(\lambda) T_{wv}(\lambda) cos\Theta_{sun} \tag{A.0.0.14}$$

$$E_{dsa}(\lambda) = E_0(\lambda) T_r^{1.5}(\lambda) T_{aa}(\lambda) \left(1 - T_{as}(\lambda)\right) T_{oz}(\lambda) T_o(\lambda) T_{wv}(\lambda) cos\Theta_{sun} F_a \tag{A.0.0.15}$$

$cos\Theta_{sun}$ is the solar zenith angle. $E_0(\lambda)$ is the solar irradiance coming from the sun. It is corrected for orbital eccentricity and sun-earth distance. It is imported from the database. F_a is the aerosol forward scattering probability and is modeled as follows:

$$F_a = 1 - 0.5e^{[(B_1+B_2cos\Theta_{sun})cos\Theta]} \tag{A.0.0.16}$$

where:

$$B_1 = B_3\left[1.459 + B_3\left(0.1595 + 0.4129B_3\right)\right] \tag{A.0.0.17}$$

$$B_2 = B_3\left[0.0783 + B_3\left(-0.3824 - 0.5874B_3\right)\right] \tag{A.0.0.18}$$

$$B_3 = -0.1417\alpha + 0.82 \tag{A.0.0.19}$$

where α is the Angstrom exponent and ranges from 0.2 to 2 [4].

$T_r(\lambda)$, $T_{aa}(\lambda)$, $T_{as}(\lambda)$, $T_{oz}(\lambda)$, $T_o(\lambda)$, and $T_{wv}(\lambda)$ are the transmittance of the atmosphere after Rayleigh scattering, aerosol absorption, aerosol scattering, ozone absorption, oxygen absorption, and water vapour absorption respectively. Their equations follow:

$$T_r(\lambda) = e^{\frac{-M'}{115.640\lambda^4 - 1.335\lambda^2}} \tag{A.0.0.20}$$

$$T_{aa}(\lambda) = e^{-(1-\omega_a)\tau_a(\lambda)M} \tag{A.0.0.21}$$

$$T_{as}(\lambda) = e^{-\omega_a\tau_a(\lambda)M} \tag{A.0.0.22}$$

$$T_{oz}(\lambda) = e^{-a_{oz}(\lambda)H_{oz}M_{oz}} \tag{A.0.0.23}$$

$$T_o(\lambda) = e^{\frac{-1.41a_o(\lambda)M'}{\left[1+118.3a_0(\lambda)M'\right]^{0.45}}} \tag{A.0.0.24}$$

$$T_{wv}(\lambda) = e^{\frac{-0.2385a_{wv}(\lambda)\cdot WV\cdot M}{[1+20.07a_{wv}(\lambda)\cdot WV\cdot M]^{0.45}}} \tag{A.0.0.25}$$

M' is the atmospheric path length corrected for nonstandard atmospheric pressure P:

$$M' = \frac{M \cdot P}{1013.25} \tag{A.0.0.26}$$

M is the atmospheric path length:

$$M = \frac{1}{cos\Theta_{sun} + a\left(90^{\circ} + b - \Theta_{sun}\right)^{-c}} \tag{A.0.0.27}$$

where $a = 0.50572$, $b = 6.079975^{\circ}$, and $c = 1.253$ [4].

M_{oz} is the ozone atmospheric path length:

$$M_{oz} = \frac{1.0035}{\left(cos^2\Theta_{sun} + 0.007\right)^{0.5}} \tag{A.0.0.28}$$

ω_a is the aerosol single scattering albedo:

$$\omega_a = \left(-0.0032AM + 0.972\right) e^{3.06 \cdot 10^{-4} RH} \tag{A.0.0.29}$$

where AM is the air mass type, and RH is the relative humidity. AM ranges from 1 (for open-ocean aerosols) to 10 (continental water aerosols). RH ranges from 46 to 91%.

$\tau_a(\lambda)$ is the aerosol optical thickness:

$$\tau_a(\lambda) = \beta\left(\frac{\lambda}{\lambda_a}\right)^{-\alpha} \tag{A.0.0.30}$$

α is the Angstrom exponent defined above. $\lambda_a = 550$ nm is the reference wavelength [4]. β is the turbidity coefficient and is modeled as follows:

$$\beta = \tau_a(550) = 3.91\frac{H_a}{V} \tag{A.0.0.31}$$

where V is the horizontal visibility ranging from 8 to 24 km, and H_a is the aerosol scale height which is set equal to 1 km.

WV is the water vapor concentration and ranges from 0 to 5 cm.

$a_{oz}(\lambda)$, $a_o(\lambda)$, and $a_{wv}(\lambda)$ are the absorption spectra of ozone, oxygen, and water vapour respectively and they are imported from file.

The sky radiance $L_s(\lambda)$ is parameterized as follows:

$$L_s(\lambda) = g_{dd}E_{dd}(\lambda) + g_{dsr}E_{dsr}(\lambda) + g_{dsa}E_{dsa}(\lambda) \tag{A.0.0.32}$$

where the downwelling irradiances are given above, and $g_{dd} = 0.02$, $g_{dsr} = \frac{1}{\pi}$, and $g_{dsa} = \frac{1}{\pi}$ are the irradiances intensities in sr^{-1}.

As stated above the RT model used in GLAM BioLith–RT is the same used in [4, 7]. Thus more details are available in those references.

B GLAM BioLith-RT: software implementation and features

GLAM BioLith-RT is entirely coded in `Matlab` and available at https://github.com/nsidc/HMA_GLAM_BioLith-RT_5. All the detailed information on how to run the code are given in the `Readme.txt` file provided with the code. All the input spectra to run the simulations are taken from the database in the folder DATA available in WASI4 package http://www.ioccg.org/data/software.html. For the constrained optimization framework the `Matlab` function `fmincon` is used. For the Bayesian inversion framework, the `MCMC toolbox` developed for Matlab available at http://helios.fmi.fi/ lainema/mcmc/ is used.

In the GLAM BioLith-RT package, the user finds several data sets, functions, and scripts to compute the quantities of interest. The most important are the following:

- script `main.m` for:
  - $R_{rs}(\lambda)$ simulation via the function `AOP_Rrs.m` given the input select by the user
  - Water component concentrations retrieval given the observed and the simulated $R_{rs}(\lambda)$: constrained optimization framework via the function `InvModelBioLithRT_Copt.m` and Bayesian inversion framework via the function `InvModelBioLithRT_Bopt.m`
- function `AOP_Rrs.m` for $R_{rs}(\lambda)$ simulation
- function `InvModelBioLithRT_Copt.m`: objective function for the constrained optimization to concentrations retrieval
- function `InvModelBioLithRT_Bopt.m`: objective function for the Bayesian inversion to concentrations retrieval

It is up to the user whether to use the software only for $R_{rs}(\lambda)$ simulation (forward modeling mode only) or to retrieve water component concentrations (inverse modeling mode). The inverse modeling mode is the default option. To switch only to the forward modeling mode, the instructions are given below.

Inverse modeling mode: inputs

Following is the list of the input for the inverse modeling mode:

- Observed remote sensing reflectance at different wavelengths. The wavelength range allowed is from 400 to 700 nm (visible). Within the allowed range, the user can enter any wavelength desired
- Case water selection. The user can choose to work with either case–1 or case–2 water
- View (camera) and Sun angle relative to the zenith, in degrees
- Water component concentrations (assumed to be constant for the depth of the water slab): phytoplankton (ph), colored dissolved organic matter (CDOM) and suspended particle matter (SPM)
- Suspended particle matter grain size (default 33.6 μm)
- Selection between deep water or shallow water (when the bottom contribution is not negligible)

- Bottom depth and the areal fraction of bottom surface, when shallow water is selected
- Quantities related to the remote sensing reflectance above the water surface: irradiance intensities, intensities of light sources, Angstrom exponent, atmospheric pressure, relative humidity, scale height for ozone, scale height of the precipitable water in the atmosphere.

The default input to run the Bayesian inversion are: number of parameters to be tuned, the tuned parameters first guess to start the MCMC sampling process, prior distributions for the fit parameters, likelihood function, initial error variance, number of simulations for the MCMC, and the algorithm to perform the MCMC sampling. More inputs are available, and the default settings can be changed, detailed information are available at http://helios.fmi.fi/ lainema/mcmc/mcmcrun.html.

The wavelength is the predictor/control variable. By default the fit parameters are the water component concentrations and all the other parameters listed are considered as fixed in the optimization problem. However, the user can change the fit and fixed parameters according to the knowledge that he/she has about the water system of interest. That is, to obtain accurate results in the inverse modeling the uncertainty on the true values of the fixed parameters should be as low as possible. In the following section, a sensitivity analysis is presented to show how the inverse modeling results are sensitive to the uncertainty in the true value of the fixed parameters. The accuracy of the retrieval decreases as the uncertainty in the true value of the fixed parameters increases.

Inverse modeling mode: default outputs

Following is the list of the default outputs for the inverse modeling mode:

- Simulated spectral remote sensing reflectance (Rrs0) given the water component concentrations estimated by the user
- Objective function value (Res0) computed with Rrs0 versus the observed remote sensing reflectance Rrs_obs
- Retrieved concentrations and corresponding objective function value computed via the constrained optimization framework
- Simulated R_{rs} (Rrs_fit) given the retrieved water component concentrations via the constrained optimization framework
- Retrieved concentrations probability distributions computed via the Bayesian inversion framework
- Simulated R_{rs} (Rrs_B) given the mean value of the retrieved water component concentrations probability distributions
- Plot Rrs0, Rrs_fit, Rrs_B and Rrd_obs versus wavelengths

Forward modeling mode: for spectral remote sensing reflectance simulations

If the user is only interested in spectral remote sensing reflectance simulations, then the option to use the forward mode only should be selected. How to switch to forward mode only is explained in detail in the `Readme.txt`. The inputs for the forward modeling mode are the same as for the inverse modeling mode except for the wavelengths range of interest that in this case needs to be specified. The wavelength range allowed is from 400 to 700 nm (visible). Within the allowed range, the user can enter any wavelength desired. The outputs are the simulated spectral remote sensing reflectance Rrs0 and its plot versus the wavelengths.

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