

A software tool for simulation and analysis of optical in-situ spectra

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Abstract – Optical data collected from ships serve as reference measurements for remote sensing of oceans, coastal and inland waters. They are usually a set of different types of spectra. A comfortable WINDOWS based software tool has been developed for forward and inverse calculations of major types, namely, upwelling radiance, downwelling irradiance, remote sensing reflectance, specular reflectance at the surface, irradiance reflectance below the surface, and bulk absorption of the water body. The calculations can be adapted easily to regional specifics, because all input data are taken from files in ASCII format. Main applications of the tool are data analysis of optical in-situ spectra from different sources, data generation for remote sensing simulations and sensitivity studies in different types of waters, and visualisation of spectral changes upon altered parameters.

I. INTRODUCTION

Development and validation of algorithms for the interpretation of remote sensing data from oceans, coastal and inland waters is based on in-situ measurements of concentrations of water constituents which absorb or scatter light (mainly phytoplankton, suspended matter, Gelbstoff) as well as on optical in-situ data which build the link between water constituents and remotely sensed signals. While airborne and spaceborne sensors measure just one data type, the upwelling radiance, optical data collected from ships are usually a set of different types of spectra, and they have in general a higher spectral resolution. Major types of optical in-situ spectra are downwelling irradiance above and below the water surface, radiance and irradiance reflectance above and below the surface, absorption, scattering, backscattering and diffuse attenuation. WASI (= water colour simulator), a WINDOWS based software tool, has been developed for forward and inverse calculations of several of these spectra. The experimental basis of the algorithms are data from Lake Constance (Bodensee) [1] [2].

II. IMPLEMENTED ALGORITHMS

The radiative transfer equation for an absorbing and scattering medium like water cannot be solved analytically, hence observables which depend on the radiation field (apparent optical properties) can be calculated only approximately. From a numerical point of view, any desired accuracy can be achieved by using converging methods like Monte Carlo, matrix operator, successive order of scattering, finite elements, etc. In practice, however, accuracy is determined by the knowledge of concentration, vertical distribution and optical properties of the water constituents. As far as these unavoidable errors are large compared to numerical errors, the use of less accurate methods is justified. The calculations of WASI use analytic approximations based on parameters which can be measured relatively easy. Advantages of analytic equations are that inversion is relatively simple, altered input data sets are included quickly, and computing is fast.

A. Absorption

The absorption of the water body, a , is the sum of absorption by pure water, a_w , and absorption by water constituents:

$$a(\lambda) = a_w(\lambda) + a_y(\lambda_0) \cdot \exp[-S \cdot (\lambda - \lambda_0)] + \sum_{i=1}^6 C_i \cdot a_i^*(\lambda). \quad (1)$$

λ denotes wavelength. Absorption of a single water constituent is calculated as the product of concentration and specific absorption coefficient. In WASI specific absorption spectra a_i^* of 6 phytoplankton classes [3] and of Gelbstoff are implemented. The C_i are the concentrations of these classes in units of chlorophyll-a concentration ($\mu\text{g/l}$). As usual [4] [5], Gelbstoff concentration is expressed as absorption a_y at a reference wavelength λ_0 , and the wavelength dependency of Gelbstoff absorption as an exponential function with spectral slope S .

B. Subsurface irradiance reflectance

The subsurface irradiance reflectance $R(\lambda)$ is expressed according to Gordon et al. [6] as function of absorption a and backscattering b_b of the water body:

$$R(\lambda) = f \cdot \frac{b_b(\lambda)}{a(\lambda) + b_b(\lambda)}. \quad (2)$$

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The factor of proportionality has a default value of $f=0.33$. It can be fitted during inversion.

b_b is the sum of backscattering by pure water and suspended particles. In WASI the following parameterisation is chosen:

$$b_b(\lambda) = b_{b,W}(\lambda) + C_L \cdot b_{b,L}^* + C_S \cdot b_{b,S}^* \cdot \left(\frac{\lambda}{\lambda_S} \right)^n.$$

Morel's [7] empirical relation $b_{b,W}(\lambda) = b_1 \cdot (\lambda/500)^{-4.32}$ is used for pure water, with $b_1 = 0.00111 \text{ m}^{-1}$ for fresh water and $b_1 = 0.00144 \text{ m}^{-1}$ for oceanic water with 35–38 ‰ salinity.

For suspended matter a distinction between large and small particles is made. The backscattering of large particles is modeled as the product of concentration C_L and a wavelength-independent specific backscattering coefficient $b_{b,L}^*$ with a default value of $0.0086 \text{ m}^2 \text{ g}^{-1}$. The backscattering of small particles is calculated as the product of concentration C_S , specific backscattering coefficient $b_{b,S}^*$ and a normalised spectrum $(\lambda/\lambda_S)^n$. The Angström exponent n , which determines the spectral shape, depends on particle size distribution.

C. Downwelling irradiance

The downwelling irradiance $E_d(\lambda)$ is approximated as sum of four "light sources" sun, blue sky, aerosols and clouds according to the empirical model of Gege [1] [8]:

$$E_d(\lambda) = E_0(\lambda) \cdot \left[\alpha \cdot t_A(\lambda) + \beta \cdot \left(\frac{\lambda}{\lambda_R} \right)^{-4.09} + \gamma \cdot \left(\frac{\lambda}{\lambda_M} \right)^\nu + \delta \cdot t_C(\lambda) \right]. \quad (3)$$

E_0 is the extraterrestrial solar irradiance. The transmission spectra $t_A(\lambda)$, $(\lambda/\lambda_R)^{-4.09}$, $(\lambda/\lambda_M)^\nu$ and $t_C(\lambda)$, which spectrally characterise the light sources, are assumed to be constant over time, and differences between individual $E_d(\lambda)$ spectra are attributed only to differences in their weights α , β , γ , δ , and eventually to the Angström exponent ν of the aerosols. The model fits to measured spectra $E_d(\lambda)$ highly accurate with an average rms error of 0.1 % [1].

D. Specular reflectance

As the water surface is frequently wind-roughened, radiance from any point in the sky can in principle be reflected by waves into an above-water sensor. Hence the radiance $L_u^*(\lambda)$ that is reflected at the surface into the sensor is parameterised analogously to $E_d(\lambda)$ as a sum of the four above-mentioned light sources:

$$L_u^*(\lambda) = E_0(\lambda) \cdot \left[\alpha^* \cdot t_A(\lambda) + \beta^* \cdot \left(\frac{\lambda}{\lambda_R} \right)^{-4.09} + \gamma^* \cdot \left(\frac{\lambda}{\lambda_M} \right)^\nu + \delta^* \cdot t_C(\lambda) \right].$$

The parameters of $L_u^*(\lambda)$ are the weights α^* , β^* , γ^* , δ^* ; for aerosol scattering the same Angström exponent ν is used as for $E_d(\lambda)$.

The reflectance spectrum of light specularly reflected at the water surface into the sensor ("specular reflectance") is:

$$R_{surf}(\lambda) = \rho^+ \cdot \frac{L_u^*(\lambda)}{E_d(\lambda)}. \quad (4)$$

The reflection factor ρ^+ can, in principle, be calculated using the Fresnel equations. In practice it is not known accurately due to the unknown orientation of individual waves. Only when these statistical effects are smoothed out by averaging a large area (length scale in the order of several hundred meters) or a long time interval (more than several seconds) the surface reflections can be calculated as a mean if the wind speed is known [9]. In WASI ρ^+ is a free parameter.

E. Upwelling radiance

All information about water constituents that can be obtained by remote sensing is contained in the water leaving radiance. For measurements above the water surface this signal is contaminated with radiation reflected at the water surface. The sum of both components is the upwelling radiance L_u . It is calculated as follows:

$$L_u(\lambda) = \frac{S}{Q} \cdot R(\lambda) \cdot E_d(\lambda) + \rho^+ \cdot L_u^*(\lambda). \quad (5)$$

Due to refraction and reflection at the water-air interface the radiance upwelling in the water is weakened at the surface. This radiance reduction factor s has a value around 0.54. The factor Q , the ratio of upwelling irradiance to upwelling radiance in the water, is a measure of light field isotropy; it typically ranges from 3 to 6 sr.

The radiance upwelling in the water can be calculated using eq. (5) and setting $s=1$ and $\rho^+=0$.

F. Remote sensing reflectance

Because the dependence of L_u on the illumination is strongly reduced when it is normalised to the downwelling irradiance, data analysis is frequently based on the ratio $R_{rs} = L_u / E_d$, called remote sensing reflectance. From eqs. (4) and (5) follows:

$$R_{rs}(\lambda) = \frac{S}{Q} \cdot R(\lambda) + R_{surf}(\lambda). \quad (6)$$

Note that R_{rs} and R_{surf} have the dimension sr^{-1} , while R is dimensionless.

III. GENERAL FEATURES

WASI has a WINDOWS-typical graphical user interface. It is written in Borland Delphi 5.0. The software consists of an executable file (WASI.EXE), an initialisation file (WASI.INI) and 19 data files. The initialisation file comprises all parameter values, user

settings and information about the data files (paths, file names, header lines, columns with x- and y-values). The data files include basis spectra required for the calculations ($a_w(\lambda)$, $a_i^*(\lambda)$, $E_0(\lambda)$, $t_A(\lambda)$, $t_C(\lambda)$) as well as default spectra representing measurements ($a(\lambda)$, $R(\lambda)$, $E_d(\lambda)$, $R_{surf}(\lambda)$, $L_u(\lambda)$, $R_{rs}(\lambda)$). Visualisation and saving is possible for all these spectra, as well as for the basis spectra calculated using analytic equations (Gelbstoff absorption, backscattering of pure water and of small particles, Rayleigh and aerosol scattering in the atmosphere), for provisional results of interest (total absorption of phytoplankton, total absorption of water constituents, calculated $R(\lambda)$) and for fit curves. WASI.INI and the data files are in ASCII format in order to be easily readable and changeable.

Calculations can be performed either at equidistant wavelengths for a step width and interval specified by the user, or for specific wavelengths which are read from a file. The latter option is of interest for simulating or analysing data from sensors with non-equidistant spectral channels. The spectral resolution of input and output data can be chosen arbitrarily and independently between the files. The basis spectra provided with the software have different spectral coverage and resolution; they are suited for calculating all types of spectra at least from 390 to 800 nm at a spectral resolution of 1 nm. Both forward and inverse calculations can be performed in a batch mode, which allows to generate or process automatically a large number of spectra.

IV. FORWARD MODELING

Forward modeling is the calculation of a spectrum or a series of spectra according to user-specified parameter settings. Any spectrum from chapter II that is specified by a numbered equation can be calculated. WASI's user interface of the forward model is shown in Fig. 1. The spectrum type is selected from the drop-down list above the "Start" button. Its parameters are listed at the left side, all of them can be changed. Up to three parameters, selected in the "Parameter" drop-down list, can be iterated simultaneously. After pressing the "Start" button the resulting spectra are calculated, displayed and contingently saved.

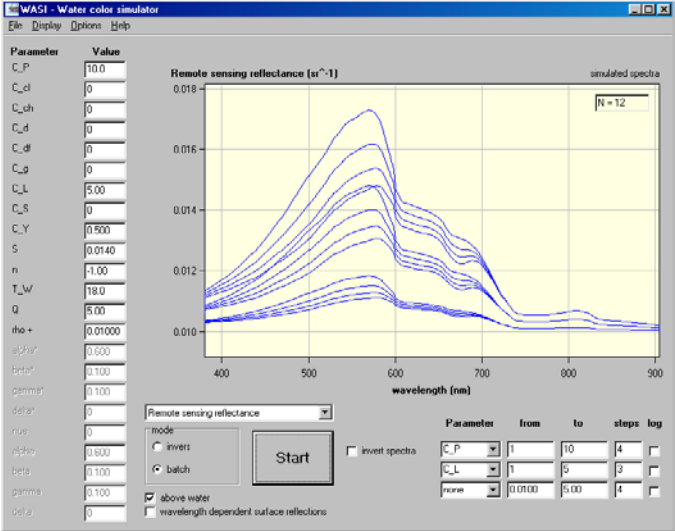


Fig. 1. Forward modeling using WASI.

V. INVERSE MODELING

Inverse modeling is the determination of model parameters for a given spectrum or a series of spectra. A general problem of inversion is that the result may depend on the start values of the fit parameters and on the search strategy of the inversion algorithm. In order to handle this problem, which depends on the fit curve and on the number of fit parameters, the inversion algorithm has been fine-tuned individually for each spectrum. Some fine-tuning can be done by the user; the corresponding user interfaces are shown in Fig. 2. For example, the information from distinct spectral regions can be weighted differently by using a wavelength-dependent weighting factor when minimizing the residual error of the fit curve.

WASI allows to invert the spectra from chapter II, except $R_{surf}(\lambda)$. The user interface of the inverse model is shown in Fig. 3. The plot of Fig. 3 compares a measured remote sensing reflectance

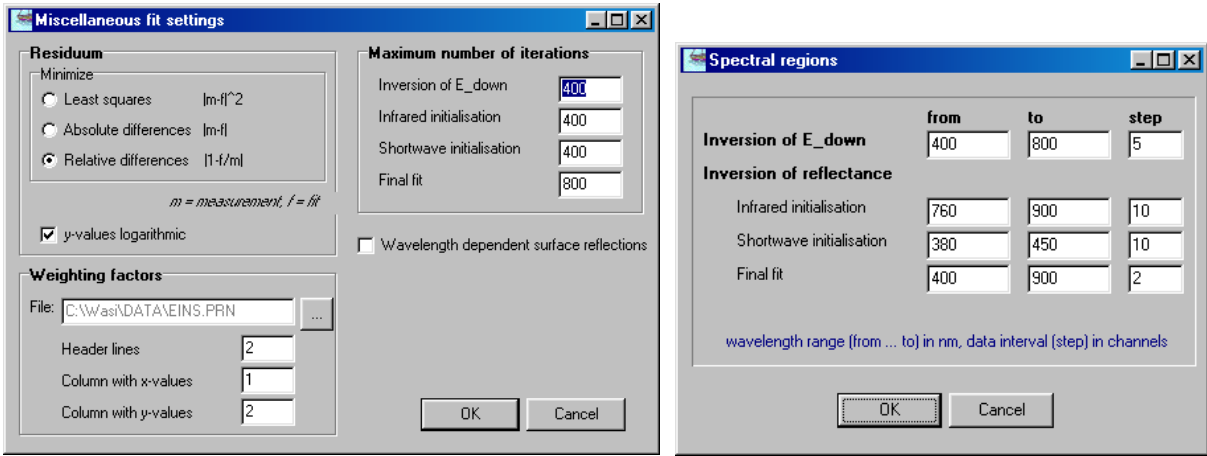


Fig. 2. Popup menus for specifying details of the inversion algorithm.

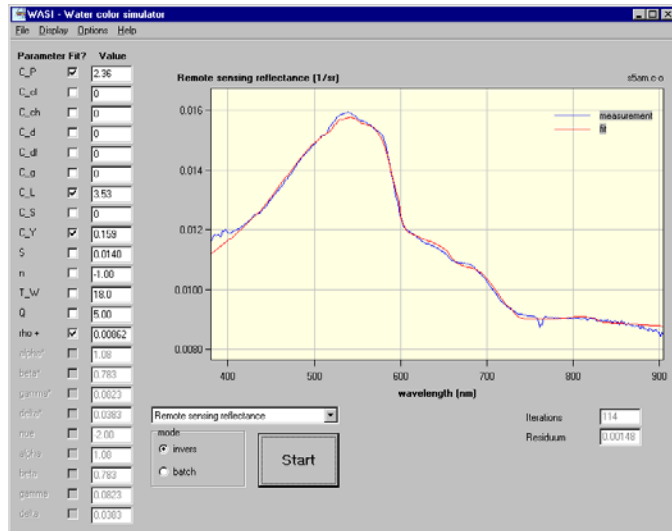


Fig. 3. Inverse modeling using WASI.

spectrum with a modeled curve. The latter was calculated iteratively in a least-squares fit (Simplex algorithm) according to eq. (6).

The parameters of the model curve are initialised using the values from the initialisation file. The user may change them by editing the list at the left side of the main window or by editing a more detailed popup window which allows to alter additional parameters, for example the allowed range of variation for each parameter, and which displays also the physical units of all parameters. The "Fit" box of each parameter determines if that parameter is treated as a fit variable or kept constant during fitting.

After the initial values are defined, the fit procedure is started by pressing the "Start" button. The resulting fit curve is displayed together with the measurement, and the list of parameters is updated. In the example of Fig. 2, a phytoplankton concentration of $C_P = 2.36 \mu\text{g/l}$, a Gelbstoff absorption at 440 nm of $C_Y = 0.159 \text{ m}^{-1}$ and a suspended matter concentration (large particles) of $C_L = 3.53 \text{ mg/l}$ were obtained by the program; all other parameters of the water body were pre-defined by the user and not optimised during fitting. Surface reflections were treated as wavelength-independent, i.e. the parameters of the radiance reflected at the surface (α^* , β^* , γ^* , δ^*) were set equal to those of $E_d(\lambda)$; only the Fresnel reflection factor was calculated as $\rho^+ = 0.00862$. After 114 iterations the fit had converged (CPU time below 1 sec). The relative difference between measurement and fit (residuum) is 0.00148, averaged from 400 to 900 nm.

VI. APPLICATIONS

Applications of WASI are visualisation of spectral changes upon altered parameters, data analysis of optical in-situ spectra from different instruments, and data generation for remote sensing simulations and sensitivity studies in different types of waters. For example, WASI and 6S, a radiative transfer simulation program for the atmosphere, were used together to estimate the influence of errors in atmospheric correction on the retrieval of phytoplankton, Gelbstoff and suspended matter from MERIS and MODIS data [10].

VII. SUMMARY AND OUTLOOK

The water colour simulator WASI is a tool for visualisation, simulation and data analysis of bulk optical properties of different types of natural waters. The calculations are easily adaptable to regional specifics, because all input data are taken from files in ASCII format.

Further developments will focus on replacing the empirical parameterisation of $E_d(\lambda)$ by a model-based one and on the parameterisation of Q in terms of sun zenith angle and optical properties of the water body. Algorithms for other types of spectra will be developed, validated and included in WASI, for example diffuse attenuation, vector and scalar irradiances in the water and reflection at the bottom [11] [12]. Online help will be included.

A general problem of inverse modeling is that the result may depend on the initial values of the fit parameters. This problem is caused by local minima of the residuum and increases with the number of fit parameters. WASI has already been tuned to handle this problem, but further improvements are necessary and planned.

The software is available free of charge. Please contact the author (peter.gege@dlr.de).

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