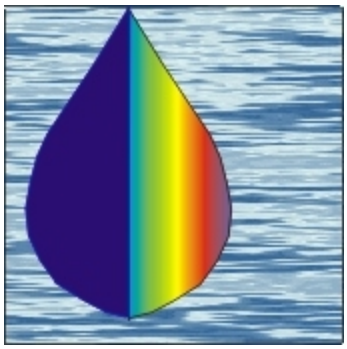
The Water Colour Simulator WASI

User manual for version 3

Peter Gege



WASI

This document can be cited as follows:

> Gege, P. (2005): The Water Colour Simulator WASI. User manual for version 3. *DLR Internal Report IB 564-01/05, 83 pp.*

The actual version of the program and of this manual can be downloaded from the following ftp site:

Server:	ftp.dfd.dlr.de
User:	anonymous
Directory:	/pub/WASI

Copyright

WASI version: 3
Date: 26 August 2005
Author: Peter Gege
Contact: peter.gege@dlr.de

Table of contents

1. Introduction

The Water Colour Simulator WASI is a software tool for analyzing and simulating the most common types of spectra that are measured by ship-borne optical instruments. It summarises the experiences from 15 years of experimental and theoretical work performed mainly at Lake Constance by DLR's Inland Water Group. Early versions were presented and distributed on CD-ROM on conferences (Gege 2001a, 2001b). The deep-water version is described in Gege (2004), the shallow-water version in Gege and Albert (2005).

The spectrum types and major calculation options are listed in Table 1.1. A more comprehensive summary including the fit parameters is given in Appendix 6. WASI can be used to generate the spectra of Table 1.1 ("Forward mode"), or to analyze such spectra ("Inverse mode"). Both modes can be combined effectively for performing sensitivity studies ("Reconstruction mode"). The three modes of operation are described in chapter 3 (forward mode), chapter 4 (inverse mode) and chapter 5 (reconstruction mode). Model options are depicted in chapter 6, program options in chapter 7. The installation of WASI is described in Appendix 1.

Spectrum type	Model options
Absorption	Of water constituents Of natural water bodies
Attenuation	For downwelling irradiance
Specular reflectance	Wavelength dependent Constant
Irradiance reflectance	For deep water For shallow water
Remote sensing reflectance	Below surface for deep water Below surface for shallow water Above surface for deep water Above surface for shallow water
Bottom reflectance	For irradiance sensors For radiance sensors
Downwelling irradiance	Above surface Below surface
Upwelling radiance	Below surface Above surface

Table 1.1: Spectrum types and major model options.

Basis of all calculations are analytical models with experimentally easily accessible parameters. Most of them are well established among "ocean colour" modelers and experimentally and theoretically validated. They are described in detail in chapter 2, the corresponding references are cited in chapter 8.

The program consists of an executable file, WASI.EXE, an initialisation file, WASI.INI, and 28 input spectra. WASI.INI is an ASCII file that comprises all paths and file names of the data files, parameter values, constants and user settings. An example listening is given in Appendix 2. Much effort was spent to make the user interface as clear as possible. Since most

settings in the different pop-up windows are self-explanatory, not every detail is described in this manual.

Alternatively to the usual interactive mode of operation, WASI can also be started from another program through the command `WASI INI_File`. In this case the file `INI_File` is read instead of WASI.INI, then calculation is started automatically without user interaction, and finally WASI is terminated automatically after the calculations are finished. This mode of operation is useful for combining WASI with another program. For example, WASI has been combined with a radiative transfer simulation program for the atmosphere (6S) to estimate the influence of errors in atmospheric correction on the retrieval of phytoplankton, Gelbstoff and suspended matter from MERIS and MODIS data (Pyhälahti and Gege, 2001).

2. Models

2.1 Absorption

2.1.1 Water constituents

Absorption of a mixture of water constituents is the sum of the components' absorption coefficients:

$$a_{WC}(\lambda) = \sum_{i=0}^{5} C_i \cdot a_i^*(\lambda) + X \cdot a_X^*(\lambda) + Y \cdot a_Y^*(\lambda). \quad (2.1)$$

λ denotes wavelength. Three groups of absorbing water constituents are considered: phytoplankton, non-chlorophyllous particles, and Gelbstoff.

Phytoplankton. The high number of species that occur in natural waters causes some variability in phytoplankton absorption properties. This is accounted for by the inclusion of 6 specific absorption spectra $a_i^*(\lambda)$. If no phytoplankton classification is performed, the spectrum $a_0^*(\lambda)$ is selected to represent the specific absorption of phytoplankton. C_i indicates pigment concentration, where "pigment" is the sum of chlorophyll-a and phaeophytin-a.

The default spectra provided with WASI are shown in Fig. 2.1. They are based on measurements at Lake Constance. The five spectra $a_1^*(\lambda)$ … $a_5^*(\lambda)$ represent the lake's major optical classes "cryptophyta type L", "cryptophyta type H", "diatoms", "dinoflagellates", and "green algae" (Gege 1994, 1995, 1998b). The spectrum $a_0^*(\lambda)$, labeled "phytoplankton" in Fig. 2.1, is a weighted sum of these five spectra and represents a mixture which can be considered as typical for Lake Constance. It was calculated by Heege (2000) using phytoplankton absorption spectra[1] and pigment data[2] from 32 days in 1990 and 1991, and he validated it using 139 irradiance reflectance and 278 attenuation measurements[3] from 1990 to 1996.

Non-chlorophyllous particles. Absorption is calculated as the product of concentration X and specific absorption $a_X^*(\lambda)$. The spectrum $a_X^*(\lambda)$ provided with WASI is shown in Fig. 2.2 (left). It is taken from Prieur and Sathyendranath (1981) and normalized to 1 at the reference wavelength $\lambda_0 = 440$ nm.

Gelbstoff (dissolved organic matter). Gelbstoff absorption is the product of concentration Y and specific absorption $a_Y^*(\lambda)$. The spectrum $a_Y^*(\lambda)$ can either be read from file or calculated using the usual exponential approximation (Nyquist 1979; Bricaud et al. 1981):

$$a_Y^*(\lambda) = \exp[-S \cdot (\lambda - \lambda_0)], \quad (2.2)$$

where S denotes the spectral slope, and λ_0 is a reference wavelength with a_Y^* normalized to 1. Default values are $\lambda_0 = 440$ nm and $S = 0.014$ nm^{-1}, which can be considered representative of a great variety of water types (Bricaud et al. 1981; Carder et al. 1989).

[1] Derived from above-water reflectance spectra by inverse modelling (Gege 1994, 1995).
[2] Measured at the University of Constance by Beese, Richter, and Kenter.
[3] Measured by Tilzer, Hartig, and Heege (Tilzer et al. 1995, Heege 2000).

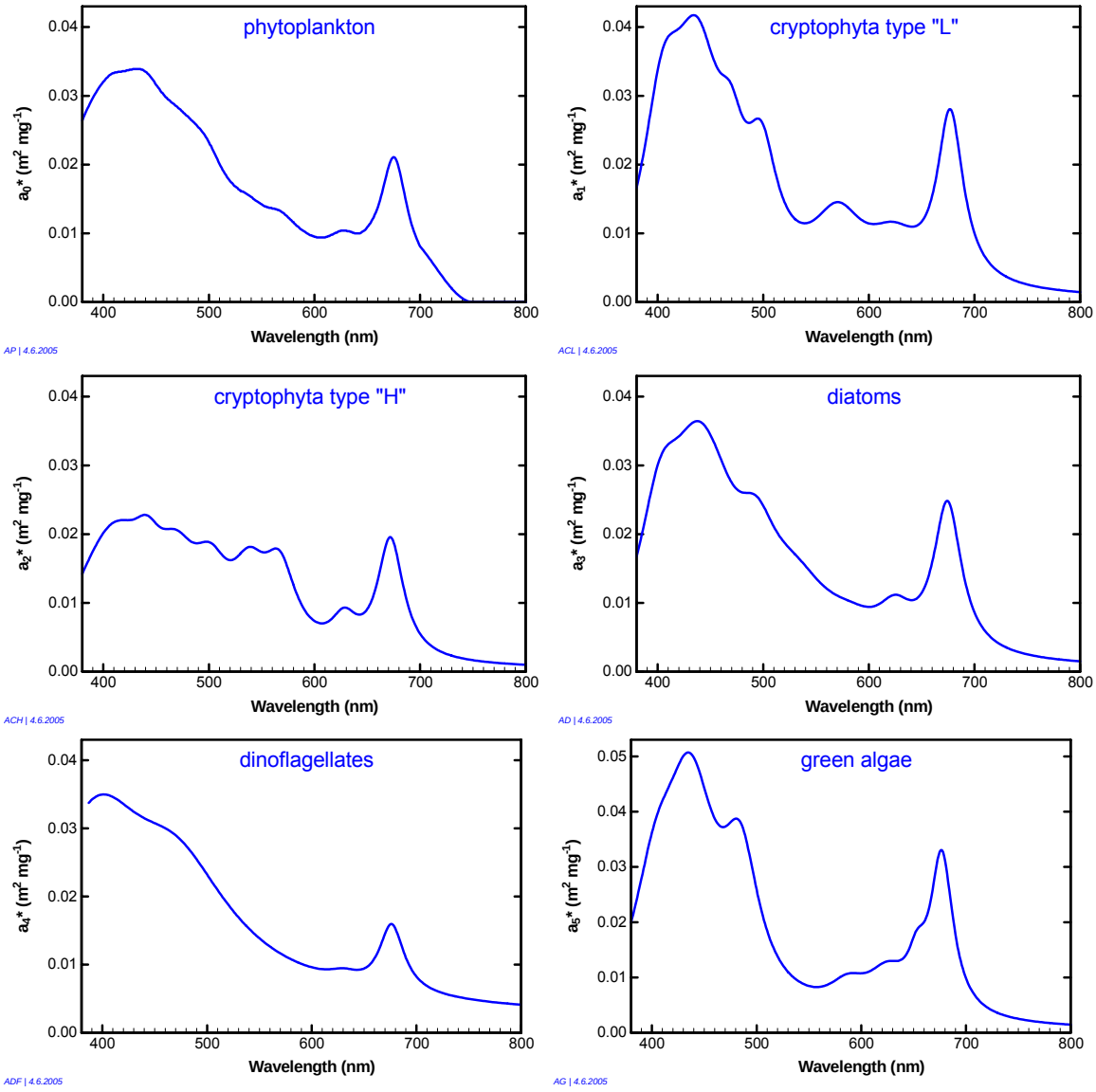


Fig. 2.1: Specific absorption spectra of 6 phytoplankton classes.

Gelbstoff absorption is calculated in WASI by default using the exponential approximation of eq. (2.2). However, Gege (2000) showed that this approximation provides model errors below 10 % only for the wavelength interval of $[\lambda_0 - 60\ \text{nm}, \lambda_0 + 60\ \text{nm}]$, and a better approximation is a sum of 3 Gaussian distributions (the x-axis must be transformed from the wavelength scale (nm) to the engergy scale (cm^{-1})). The Gaussian model is physically more reasonable than the exponential model and offers a deeper understanding of the chemical interactions affecting CDOM molecular structure (Schwarz et al. 2002). Thus, a spectrum (Y.A) is provided with WASI which was calculated using the Gaussian model (eq. (3) in Gege 2000) and the average model parameters determined for Lake Constance (Table 1 in Gege 2000). It is shown in Fig. 2.2 (right) on a logarithmic scale.

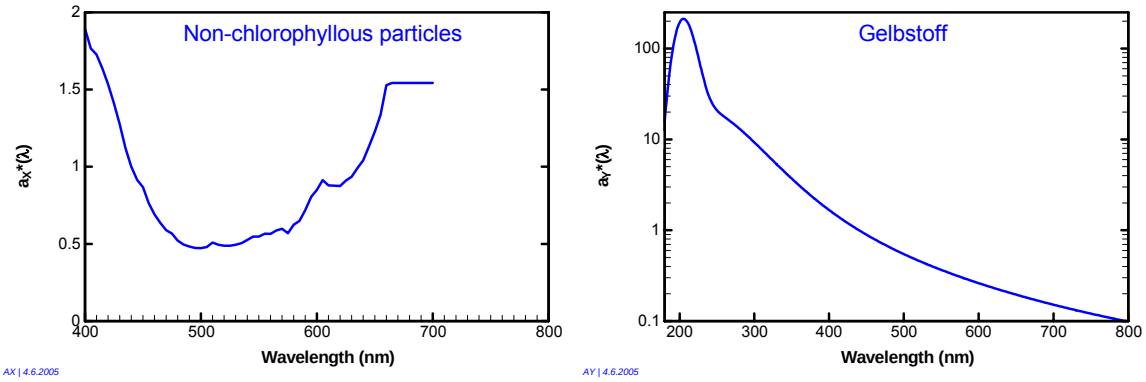


Fig. 2.2: Normalised absorption spectra of non-chlorophyllous particles, $a_X^*(\lambda)$, and Gelbstoff, $a_Y^*(\lambda)$.

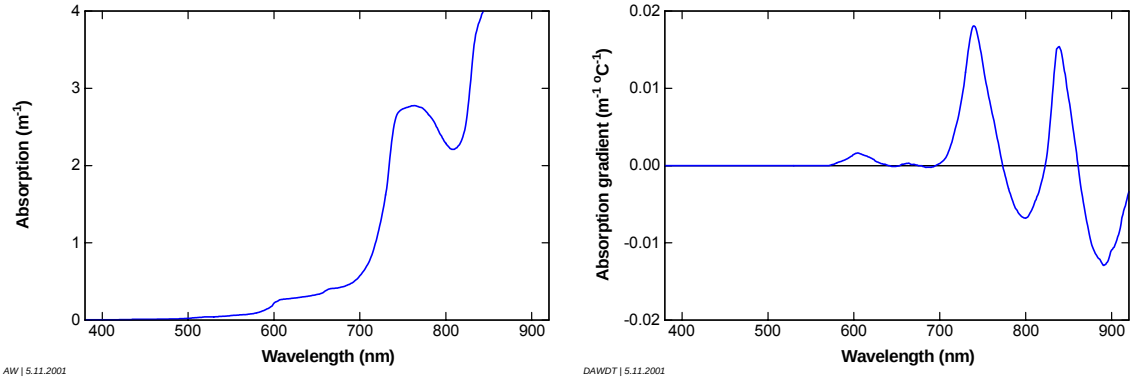


Fig. 2.3: Pure water absorption, $a_W(\lambda)$, and temperature gradient of water absorption, $da_W(\lambda)/dT$.

2.1.2 Natural water

The bulk absorption of a natural water body is the sum of absorption of pure water and of the water constituents:

$$a(\lambda) = a_W(\lambda) + (T - T_0) \cdot \frac{da_W(\lambda)}{dT} + a_{WC}(\lambda). \qquad (2.3)$$

Absorption of pure water is split up into a temperature-independent term a_W, which is valid at a reference temperature T_0, and a temperature gradient da_W/dT with T being the actual water temperature. The spectra $a_W(\lambda)$ and $da_W(\lambda)/dT$ are shown in Fig. 2.3.

The spectrum $a_W(\lambda)$ provided with WASI is a combination from different sources for a temperature of T_0 = 20 °C. 196-227 nm: Quickenden & Irvin (1980); 228-390 nm: Interpolation between Quickenden & Irvin (1980) and Buiteveld et al. (1994); 391-787 nm: Buiteveld et al. (1994); 788-874 nm: own unpublished measurements on UV-treated pure water of 20°C; 875-2000 nm: Palmer & Williams (1974), 27°C. For $da_W(\lambda)/dT$ a spectrum is provided which was measured by Gege (unpublished data).

2.2 Backscattering

Backscattering b_b of a water body is the sum of backscattering by pure water (index "W") and suspended matter. For the latter, a distinction between large ($\gtrsim$5 µm, index "L") and small ($\lesssim$5 µm, index "S") particles is made. Thus, the following parameterization is chosen:

$$b_b(\lambda) = b_{b,W}(\lambda) + C_L \cdot b_{b,L}^* \cdot b_L(\lambda) + C_S \cdot b_{b,S}^* \cdot (\lambda/\lambda_S)^n. \quad (2.4)$$

2.2.1 Pure water

For pure water, the empirical relation of Morel (1974) is used: $b_{b,W}(\lambda) = b_1 \cdot (\lambda/\lambda_1)^{-4.32}$. The specific backscattering coefficient, b_1, depends on salinity. It is $b_1 = 0.00111$ m^{-1} for fresh water and $b_1 = 0.00144$ m^{-1} for oceanic water with a salinity of 35–38 ‰, when $\lambda_1 = 500$ nm is chosen as reference wavelength.

2.2.2 Large particles

Backscattering by large particles is calculated as the product of concentration C_L, specific backscattering coefficient $b_{b,L}^*$, and normalized scattering function $b_L(\lambda)$. The user has several options for calculation:

- C_L can be treated either as an independent parameter, or $C_L = C_0$ can be set, where C_0 is the concentration of phytoplankton class no. 0 (see eq. 1). The latter is useful for Case 1 water types where the concentrations of particles and phytoplankton are highly correlated.

- $b_{b,L}^*$ can be treated either as constant with a default value of 0.0086 m^2 g^{-1} (Heege 2000), or as $b_{b,L}^* = A \cdot C_L^B$. Such a non-linear dependency of scattering on concentration was observed for phytoplankton (Morel 1980). It may be used for Case 1 water types, while $b_{b,L}^*$ = constant is appropriate for Case 2 waters with significant sources of non-phytoplankton suspended matter. Typical values of the empirical constants are $A = 0.0006$ m^2 g^{-1} and $B = -0.37$ (Sathyendranath et al. 1989), which are set as defaults in WASI.

- $b_L(\lambda)$ can either be read from file, or it can be calculated as $b_L(\lambda) = a_0^*(\lambda_L) / a_0^*(\lambda)$, where $a_0^*(\lambda)$ is the specific absorption spectrum of phytoplankton class no. 0 (see eq. 1), and λ_L denotes a reference wavelength ($\lambda_L = 550$ nm by default). This method assumes that backscattering by large particles originates mainly from phytoplankton cells, and couples absorption and scattering according to the Case 1 waters model of Sathyendranath et al. (1989). However, such coupling may be used in exceptional cases only, since living algae have a negligible influence on the backscattering process by oceanic waters (Ahn et al. 1992), and in Case 2 waters particle scattering is weakly related to phytoplankton absorption in general. In WASI, $b_L(\lambda) = 1$ is set as default.

2.2.3 Small particles

Backscattering by small particles is calculated as the product of concentration C_S, specific backscattering coefficient $b_{b,S}$*, and a normalized scattering function $(\lambda/\lambda_S)^n$. The exponent n, which determines the spectral shape, depends on particle size distribution. n is typically in the order of −1 (Sathyendranath et al. 1989) and $b_{b,S}$* in the order of 0.005 $m^2\ g^{-1}$ for λ_S = 500 nm.[4] Default values in WASI are n = −1 and $b_{b,S}$* = 0.0042 $m^2\ g^{-1}$.

[4] The empirical data given in Sathyendranath et al. (1989) correspond to $b_{b,S}$* = 0.015 $m^2\ g^{-1}$; however, the calculations in that paper were done using $b_{b,S}$* = 0.0042 $m^2\ g^{-1}$ (personal communication Sathyendranath).

2.3 Attenuation

The diffuse attenuation coefficient of irradiance E is defined as K = –(1/E) dE/dz, where z is the depth. Similarly, the attenuation coefficient of radiance L is defined as k = –(1/L) dL/dz. Attenuation is an apparent optical property (AOP) and depends not only on the properties of the medium, but additionally on the geometric distribution of the illuminating light field.

2.3.1 Diffuse attenuation for downwelling irradiance

The most important attenuation coefficient is K_d, which describes attenuation for downwelling vector irradiance. Gordon (1989) has shown for Case 1 waters that the geometric structure of the light field can be corrected, and the corrected attenuation coefficient, $\overline{\mu}_d K_d$, is, to a high degree of accuracy, an inherent optical property which can be related to absorption $a(\lambda)$ and backscattering $b_b(\lambda)$. The correction factor is the ratio of downwelling vector irradiance to downwelling scalar irradiance: $\overline{\mu}_d = E_d / E_{0d}$. $\overline{\mu}_d$ is also called the average cosine of the downwelling light field, since it were $\overline{\mu}_d = \cos\theta'_{sun}$ if there were no atmosphere, with θ'_{sun} the sun zenith angle in water. Gordon showed by Monte Carlo simulations that, for sun zenith angles below 60°, the difference between $\overline{\mu}_d$ and $\cos\theta'_{sun}$ is usually below 3 % near the water surface. Thus, the following parameterization of K_d is adapted from Gordon (1989):

$$K_d(\lambda) = \kappa_0 \cdot \frac{a(\lambda) + b_b(\lambda)}{\cos\theta'_{sun}}. \qquad (2.5)$$

$a(\lambda)$ is calculated according to eq. (2.3), $b_b(\lambda)$ using eq. (2.4). The coefficient κ_0 depends on the scattering phase function. Gordon (1989) determined a value of κ_0 = 1.0395 from Monte Carlo simulations in Case 1 waters, Albert and Mobley (2003) found a value of κ_0 = 1.0546 from simulations in Case 2 waters using the radiative transfer program Hydrolight (Mobley et al. 1993). Some authors use eq. (2.5) with κ_0 = 1 (Sathyendranath and Platt 1988, 1997; Gordon et al. 1975). In WASI, κ_0 is read from the WASI.INI file; the default value is 1.0546.

2.3.2 Diffuse attenuation for upwelling irradiance

For upwelling irradiance two attenuation coefficients are used: K_{uW} for the radiation backscattered in the water, and K_{uB} for the radiation reflected from the bottom. The following parameterization is adopted from Albert and Mobley (2003):

$$K_{uW}(\lambda) = \left[a(\lambda) + b_b(\lambda)\right] \cdot \left[1 + \omega_b(\lambda)\right]^{1.9991} \cdot \left[1 + \frac{0.2995}{\cos\theta'_{sun}}\right]. \qquad (2.6)$$

$$K_{uB}(\lambda) = \left[a(\lambda) + b_b(\lambda)\right] \cdot \left[1 + \omega_b(\lambda)\right]^{1.2441} \cdot \left[1 + \frac{0.5182}{\cos\theta'_{sun}}\right]. \qquad (2.7)$$

The function $\omega_b(\lambda)$ depends on absorption $a(\lambda)$ and backscattering $b_b(\lambda)$ of the water body:

$$\omega_b(\lambda) = \frac{b_b(\lambda)}{a(\lambda) + b_b(\lambda)}. \qquad (2.8)$$

Eqs. (2.6) and (2.7) are used implicitely in the model of irradiance reflectance in shallow waters, see eq. (2.16). The spectra $K_{uW}(\lambda)$ and $K_{uB}(\lambda)$ cannot be calculated explicitely using WASI.

2.3.3 Attenuation for upwelling radiance

For upwelling radiance two attenuation coefficients are used: k_{uW} for the radiation backscattered in the water, and k_{uB} for the radiation reflected from the bottom. The following parameterization is adopted from Albert and Mobley (2003):

$$k_{uW}(\lambda) = \frac{a(\lambda)+b_b(\lambda)}{\cos\theta'_v} \cdot \left[1+\omega_b(\lambda)\right]^{3.5421} \cdot \left[1-\frac{0.2786}{\cos\theta'_{sun}}\right]. \quad (2.9)$$

$$k_{uB}(\lambda) = \frac{a(\lambda)+b_b(\lambda)}{\cos\theta'_v} \cdot \left[1+\omega_b(\lambda)\right]^{2.2658} \cdot \left[1+\frac{0.0577}{\cos\theta'_{sun}}\right]. \quad (2.10)$$

These equations are used implicitely in the model of remote sensing reflectance in shallow waters, see eq. (2.19). The spectra $k_{uW}(\lambda)$ and $k_{uB}(\lambda)$ cannot be calculated explicitely using WASI.

2.4 Specular reflectance

An above-water radiance sensor looking down to the water surface measures the sum of two radiance components: one from the water body, one from the surface. The first comprises the desired information about the water constituents, the second is an unwanted add-on which has to be corrected. However, correction is difficult. For example, the method from the SeaWiFS protocols (Mueller and Austin 1995), which is widely used in optical oceanography, leads to rms errors of the corrected water leaving radiance as large as 90 % under typical field conditions (Toole et al. 2000). Thus, WASI offers different methods.

The radiance reflected from the surface, $L_r(\lambda)$, is a fraction σ_L of sky radiance $L_s(\lambda)$:

$$L_r(\lambda) = \sigma_L \cdot L_s(\lambda). \tag{2.11}$$

$L_s(\lambda)$ is the average radiance of that area of the sky that is specularly reflected into the sensor. It can be imported from file or calculated using eq. (2.26). σ_L is the Fresnel reflectance and depends on the angle of reflection. The value can either be specified by the user or it can be calculated from the viewing angle θ_v using the Fresnel equation for unpolarized light (Jerlov 1976):

$$\sigma_L = \frac{1}{2}\left|\frac{\sin^2(\theta_v - \theta'_v)}{\sin^2(\theta_v + \theta'_v)} + \frac{\tan^2(\theta_v - \theta'_v)}{\tan^2(\theta_v + \theta'_v)}\right|. \tag{2.12}$$

θ'_v is the angle of refraction, which is related to θ_v by Snell's law $n_W \, sin\theta'_v = sin\theta_v$, where $n_W \approx 1.33$ is the refractive index of water. For viewing angles near nadir, $\sigma_L \approx 0.02$.

The ratio of the radiance reflected from the water surface to the downwelling irradiance,

$$R_{rs}^{surf}(\lambda) = \frac{L_r(\lambda)}{E_d(\lambda)} = \sigma_L \cdot \frac{L_s(\lambda)}{E_d(\lambda)}, \tag{2.13a}$$

is called specular reflectance. $E_d(\lambda)$ and $L_s(\lambda)$ can either be imported from file, or one or both can be calculated using eq. (2.23) or (2.26). If the wavelength-independent model of surface reflection is chosen, it is

$$R_{rs}^{surf} = \frac{\sigma_L}{\pi}. \tag{2.13b}$$

Toole et al. (2000) showed that $R_{rs}^{surf}(\lambda)$ is nearly spectrally flat at overcast sky, but clearly not for clear-sky conditions. Thus, eq. (2.13a) should be used in general, and eq. (2.13b) at most for days with overcast sky.

2.5 Irradiance reflectance

The ratio of upwelling irradiance to downwelling irradiance in water, $R(\lambda) = E_u^-(\lambda) / E_d^-(\lambda)$, is called irradiance reflectance (Mobley 1994). It is an apparent optical property (AOP) and depends not only on the properties of the medium, but also on the geometric distribution of the incoming light.

2.5.1 Deep water

A suitable parameterization which separates to a large extent the parameters of water and of the illumination was found by Gordon et al. (1975):

$$R(\lambda) = f \cdot \omega_b(\lambda). \tag{2.14}$$

The function $\omega_b(\lambda)$, which is given by eq. (2.8), depends only on inherent optical properties of the water body, absorption and backscattering. The factor f comprises the illumination dependencies. It can be treated either as an independent parameter with a default value of 0.33 according to Gordon et al. (1975), or the relationship of Albert and Mobley (2003) can be used:

$$f = 0.1034 \cdot \left(1 + 3.3586 \cdot \omega_b - 6.5358 \cdot \omega_b^2 + 4.6638 \cdot \omega_b^3\right) \cdot \left(1 + \frac{2.4121}{\cos \theta'_{sun}}\right). \tag{2.15}$$

θ'_{sun} is the sun zenith angle in water. Eq. (2.15) takes into consideration the fact that f depends not only on the geometric structure of the light field, expressed by the parameter θ'_{sun}, but also on the absorption and scattering properties of the water. Some alternate models of f are also included in WASI and can be used if desired, namely those of Kirk (1984), Morel and Gentili (1991), and Sathyendranath and Platt (1997). The equations are given in chapter 6.2.

Independently from Gordon, Prieur (1976) found the relation $R(\lambda) = f' \cdot b_b(\lambda) / a(\lambda)$. It is also included in WASI. However, the Gordon algorithm (2.14) is favoured and set as default, because it restricts the ω_b values to the physically reasonable range from 0 to 1, which is not the case for the Prieur equation.

2.5.2 Shallow water

For shallow water, the parameterization found by Albert and Mobley (2003) is used:

$$\begin{aligned} R^{sh}(\lambda) = R(\lambda) \cdot \left[1 - A_1 \cdot \exp\left\{-\left(K_d(\lambda) + K_{uW}(\lambda)\right) \cdot z_B\right\}\right] \\ + A_2 \cdot R^b(\lambda) \cdot \exp\left\{-\left(K_d(\lambda) + K_{uB}(\lambda)\right) \cdot z_B\right\} \end{aligned} \tag{2.16}$$

The first term on the right-hand side is the reflectance of a water layer of thickness z_B, the second term the contribution of the bottom. Bottom reflectance $R^b(\lambda)$ is calculated using eq. (2.21). The K's account for attenuation within the water layer and are calculated using eqs. (2.5), (2.6), and (2.7). The empirical constants are set to $A_1 = 1.0546$ and $A_2 = 0.9755$ according to Albert and Mobley (2003) and cannot be changed by the user.

2.6 Remote sensing reflectance

The ratio of upwelling radiance to downwelling irradiance, $R_{rs}(\lambda) = L_u(\lambda) / E_d(\lambda)$, is called remote sensing reflectance (Mobley 1994). It is an apparent optical property (AOP), i.e. it depends on the geometric distribution of the incoming light.

2.6.1 Deep water

The remote sensing reflectance below the water surface is, for deep water, proportional to $R(\lambda)$:

$$R_{rs}^{-}(\lambda) = \frac{R(\lambda)}{Q}. \tag{2.17a}$$

This follows from the definitions $R_{rs}^{-} \equiv L_u^{-} / E_d^{-}$, $Q \equiv E_u^{-} / L_u^{-}$, and $R \equiv E_u^{-} / E_d^{-}$. $R(\lambda)$ is either calculated using eq. (2.14), or imported from file. The factor Q, which is a measure of the anisotropy of the light field in water, is treated in WASI as a wavelength-independent parameter with a default value of 5 sr. It depends on the geometric distribution of the upwelling and downwelling light, and thus on the scattering and absorption properties of the water body. Consequently, Q depends on wavelength. However, this is not accounted for in WASI, since no convenient parameterization of Q is known. Yet, an alternative to eq. (2.17a) with a convenient parameterization of the factor f_{rs} was found by Albert and Mobley (2003):

$$R_{rs}^{-}(\lambda) = f_{rs} \cdot \omega_b(\lambda). \tag{2.17b}$$

The following parameterization of the factor f_{rs} is valid for both deep and shallow waters (Albert and Mobley 2003):

$$f_{rs} = 0.0512 \cdot \left(1 + 4.6659 \cdot \omega_b - 7.8387 \cdot \omega_b^{\,2} + 5.4571 \cdot \omega_b^{\,3}\right) \cdot \left(1 + \frac{0.1098}{\cos\theta'_{sun}}\right) \cdot \left(1 + \frac{0.4021}{\cos\theta'_{v}}\right). \tag{2.18}$$

Parameters of f_{rs} are ω_b of eq. (2.8), the sun zenith angle in water, θ'_{sun}, and the viewing angle in water, θ'_v. Alternately, f_{rs} can be calculated in WASI as $f_{rs} = f / Q$ using the ill-favoured parameter Q.

2.6.2 Shallow water

For shallow water, the following parameterization is chosen (Albert and Mobley 2003):

$$R_{rs}^{sh-}(\lambda) = R_{rs}^{-}(\lambda) \cdot \left[1 - A_{rs,1} \cdot \exp\left\{-\left(K_d(\lambda) + k_{uW}(\lambda)\right) \cdot z_B\right\}\right] + A_{rs,2} \cdot R_{rs}^{b}(\lambda) \cdot \exp\left\{-\left(K_d(\lambda) + k_{uB}(\lambda)\right) \cdot z_B\right\} \tag{2.19}$$

The first term on the right-hand side is the reflectance of a water layer of thickness z_B, the second term the contribution of the bottom. Bottom reflectance $R^b_{rs}(\lambda)$ is calculated using eq. (2.22). K_d, k_{uW} and k_{uB} account for attenuation within the water layer and are calculated using

eqs. (2.5), (2.9), and (2.10), respectively. The empirical constants are set to $A_{rs,1} = 1.1576$ and $A_{rs,2} = 1.0389$ according to Albert and Mobley (2003) and cannot be changed by the user.

2.6.3 Above the surface

The remote sensing reflectance above the water surface is related to radiance and irradiance spectra in water as follows:

$$R_{rs}(\lambda) = \frac{L_u(\lambda)}{E_d(\lambda)} = \frac{\frac{1-\sigma_L^-}{n_W^2}\cdot L_u^-(\lambda)}{E_d(\lambda)} + \frac{\sigma_L \cdot L_s(\lambda)}{E_d(\lambda)} = \frac{\frac{(1-\sigma_L^-)(1-\sigma)}{n_W^2}\cdot L_u^-(\lambda)}{E_d^-(\lambda) - \sigma^- \cdot E_u^-(\lambda)} + \sigma_L \cdot \frac{L_s(\lambda)}{E_d(\lambda)}.$$

Eq. (2.29) was used to replace $L_u(\lambda)$, and eq. (2.24) to express $E_d(\lambda)$ in terms of $E_d^-(\lambda)$ and $E_u^-(\lambda)$. The first term on the right-hand side describes reflection in the water, the second at the surface. By using $L_u^-(\lambda) = E_u^-(\lambda) / Q$, multiplying numerator and denominator of the first term with $R(\lambda) / E_u^-(\lambda)$ (where $R(\lambda) = E_u^-(\lambda) / E_d^-(\lambda)$), and expressing the second term as $R_{rs}^{surf}(\lambda)$ according to eq. (2.13a), the following equation is obtained:

$$R_{rs}(\lambda) = \frac{(1-\sigma)(1-\sigma_L^-)}{n_w^2 \cdot Q} \cdot \frac{R(\lambda)}{1-\sigma^- \cdot R(\lambda)} + R_{rs}^{surf}(\lambda). \qquad (2.20a)$$

Replacing $R(\lambda)$ by $R_{rs}(\lambda)$ according to eq. (2.17a) yields the following relationship:

$$R_{rs}(\lambda) = \frac{(1-\sigma)(1-\sigma_L^-)}{n_w^2} \cdot \frac{R_{rs}^-(\lambda)}{1-\sigma^- \cdot Q \cdot R_{rs}^-(\lambda)} + R_{rs}^{surf}(\lambda). \qquad (2.20b)$$

This eq. was used, for example, by Lee et al. (1998) for comparing simulated remote sensing reflectance spectra above and below the surface and calculating the conversion factors, for which they found as typical values $(1-\sigma)(1-\sigma_L^-)/n_W^2 = 0.518$ and $\sigma^- \cdot Q = 1.562$. The factor Q, which is difficult to assess in practice, can be avoided by replacing in the denominator $Q \cdot R_{rs}^-$ by R:

$$R_{rs}(\lambda) = \frac{(1-\sigma)(1-\sigma_L^-)}{n_w^2} \cdot \frac{R_{rs}^-(\lambda)}{1-\sigma^- \cdot R(\lambda)} + R_{rs}^{surf}(\lambda). \qquad (2.20c)$$

The three equations (2.20a), (2.20b), and (2.20c) are formally identical. The first term on the right-hand side of each equation describes reflection in the water, the second at the surface. Frequently, the first term alone is called remote sensing reflectance (e.g. Mobley 1994). In WASI, the reflection at the surface is also included in the R_{rs} definition. It is calculated using eq. (2.13a) or (2.13b) and can easily be excluded by setting the reflection factor σ_L equal to zero.

The factors σ, σ_L^-, and σ^- are the reflection factors for E_d, L_u^-, and E_u^-, respectively. σ depends on the radiance distribution and on surface waves. Typical values are 0.02 to 0.03 for clear sky conditions and solar zenith angles below 45°, and 0.05 to 0.07 for overcast skies (Jerlov 1976; Preisendorfer and Mobley 1985, 1986). It is set to $\sigma = 0.03$ by default. σ_L^- can either be calculated as a function of θ_v using eq. (2.12), or a constant value can be taken. σ^- is

in the range of 0.50 to 0.57 with a value of 0.54 being typical (Jerome et al. 1990; Mobley 1999). The defaults of the other constants are set to Q = 5 sr and n_W = 1.33.

Which of the equations is used, depends on the application:

- Eq. (20a) is useful when $R_{rs}(\lambda)$ shall be connected to $R(\lambda)$, for example if in-situ measurements of $R(\lambda)$ were performed as "ground truth" for a remote sensing instrument.
- Eq. (20b) links remote sensing reflectance in water to that in air. Since the same spectrum type is used above and below the water surface, it is the most convenient parameterisation. This equation is used by default.
- Eq. (20c) avoids the use of the factor Q, which is difficult to assess. The equation is useful, for example, for optical closure experiments which investigate the consistency of measurements above and below the water surface by measuring simultaneously the spectra $R_{rs}(\lambda)$, $R(\lambda)$, and $R_{rs}^{-}(\lambda)$.

Eq. (2.20a), (2.20b) or (2.20c) is also used to calculate the corresponding spectrum $R^{sh}_{rs}(\lambda)$ for shallow water. $R(\lambda)$ is replaced by $R^{sh}(\lambda)$, and $R_{rs}^{-}(\lambda)$ by $R_{rs}^{sh-}(\lambda)$ in the case of shallow water.

2.7 Bottom reflectance

The models of bottom reflectance are used to calculate reflectance and radiance spectra in shallow waters. However, they can be applied as well to land surfaces, if the input spectra are replaced by suitable albedo spectra from terrestrial bottom types.

2.7.1 For irradiance sensors

The irradiance reflectance of a surface is called albedo. When N different surfaces of albedo $a_n(\lambda)$ are viewed simultaneously, the measured albedo is the following sum:

$$R^b(\lambda) = \sum_{n=0}^{N-1} f_n \cdot a_n(\lambda) \,. \qquad (2.21)$$

f_n is the areal fraction of surface number n within the sensor's field of view; it is $\Sigma\, f_n = 1$. This equation is implemented in WASI for N = 6 bottom types. The spectra $a_n(\lambda)$ provided with WASI are shown in Fig. 2.4. They were measured by Pinnel (2005) using a submersible RAMSES spectroradiometer. Three of them represent bare bottom, the other green makrophytes:

0. constant: an artificial spectrum with constant albedo of 10 %;
1. sand: sandy bottom in a coastal shallow area in Bolivar (South Australia);
2. silt: fine-grained sediment in 50 cm water depth close to the shoreline of Starnberger See (Germany);
3. Chara *aspera*: green makrophyte from Bodensee (Lake Constance, Germany);
4. Potamogeton *perfoliatus*: green makrophyte from Starnberger See (Germany);
5. Potamogeton *pectinatus*: green makrophyte from Starnberger See (Germany).

2.7.2 For radiance sensors

When the upwelling radiation is measured by a radiance sensor, the corresponding remote sensing reflectance can be expressed as follows:

$$R_{rs}^b(\lambda) = \sum_{n=0}^{N-1} f_n \cdot B_n \cdot a_n(\lambda) \,. \qquad (2.22)$$

B_n is the proportion of radiation which is reflected towards the sensor. In WASI, the B_n's of all surfaces are assumed to be angle-independent. The default values are set to $B_n = 1/\pi = 0.318\ sr^{-1}$, which represents isotropic reflection (Lambertian surfaces).

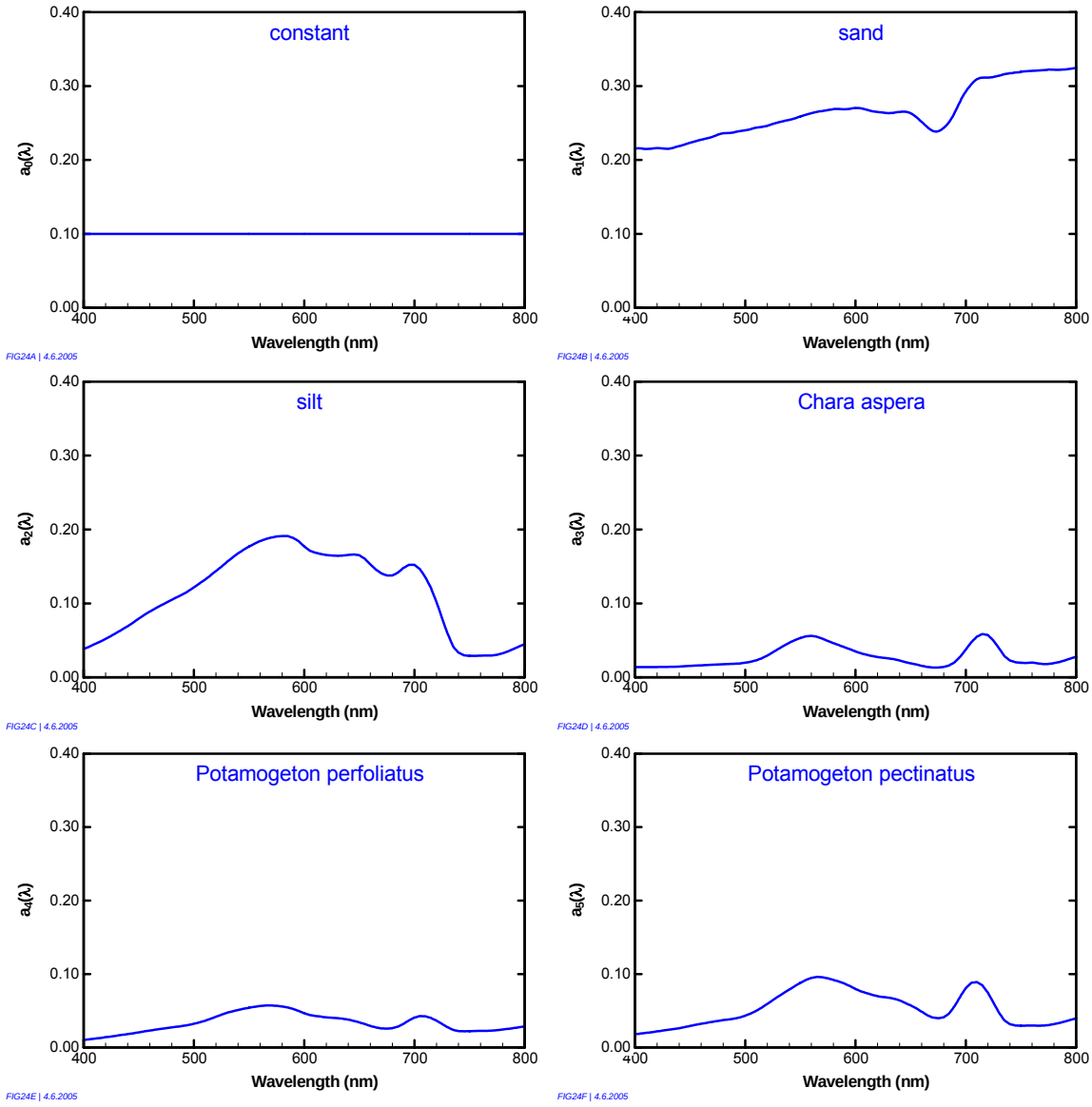


Fig. 2.4: Albedo spectra of 6 bottom types.

2.8 Downwelling irradiance

2.8.1 Above water surface

An analytic model of the downwelling irradiance spectrum $E_d(\lambda)$ with only few parameters was developed by Gege (1994, 1995). It fits to measured spectra with a high degree of accuracy (average rms error of 0.1 %). The radiation illuminating the water surface is parameterized as the sum of four spectrally different components: (1) the direct solar radiation, (2) the blue sky (Rayleigh scattering), (3) radiation scattered by aerosols (Mie scattering), and (4) clouds. Each component is expressed in terms of a wavelength-dependent fraction of the extraterrestrial solar irradiance $E_0(\lambda)$:

$$E_d(\lambda) = [\ \alpha \cdot t_A(\lambda) + \beta \cdot (\lambda/\lambda_R)^{-4.09} + \gamma \cdot (\lambda/\lambda_M)^{\nu} + \delta \cdot t_C(\lambda)\ ] \cdot E_0(\lambda). \qquad (2.23)$$

The four functions $t_i(\lambda) = \{t_A(\lambda), (\lambda/\lambda_R)^{-4.09}, (\lambda/\lambda_M)^{\nu}, t_C(\lambda)\}$ are transmission spectra which spectrally characterize the four light sources. Their weights $\alpha, \beta, \gamma, \delta$ may change from one measurement to the next, but the $t_i(\lambda)$ themselves are assumed to be constant.

In order to make the weights $\alpha, \beta, \gamma, \delta$ the relative intensities of the four light sources, each $t_i(\lambda)$ is normalized as $\int t_i(\lambda)\ E_0(\lambda)\ d\lambda = \int E_0(\lambda)\ d\lambda$; the integration interval is set to 400 to 800 nm by default. The functions $(\lambda/\lambda_R)^{-4.09}$ and $(\lambda/\lambda_M)^{\nu}$ are calculated during run-time. Normalization yields their scaling factors: λ_R = 533 nm, and λ_M is typically between 563 nm (ν=–1) and 583 nm (ν=1). The exponent ν parameterizes the wavelength dependency of aerosol scattering. The two other functions $t_A(\lambda)$ and $t_C(\lambda)$ are read from file. After import they are nor-

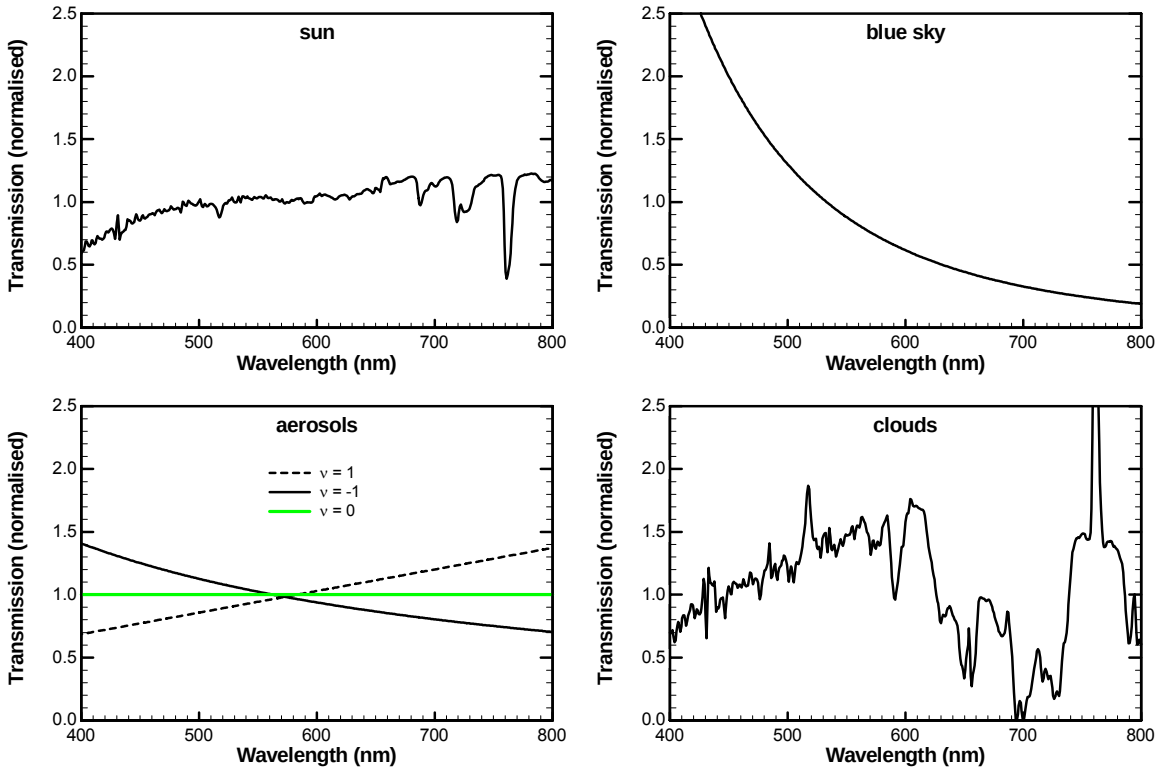


Fig. 2.4: The four base spectra of the model of the downwelling irradiance.

malized. The two spectra provided with WASI were determined from measurements at Lake Constance. The four functions $t_i(\lambda)$ are shown in Fig. 2.4.

2.8.2 Below water surface

The downwelling irradiance in water, E_d^-, is related to the downwelling irradiance in air, E_d, through

$$E_d^-(\lambda) = (1-\sigma) \cdot E_d(\lambda) + \sigma^- \cdot E_u^-(\lambda). \quad (2.24)$$

σ is the reflection factor for downwelling irradiance in air, σ^- for upwelling irradiance in water, and E_u^- is the upwelling irradiance in water. Using the irradiance reflectance $R = E_u^- / E_d^-$ yields the following expression:

$$E_d^-(\lambda) = \frac{1-\sigma}{1-\sigma^- \cdot R(\lambda)} \cdot E_d(\lambda) . \quad (2.25)$$

This equation is used in WASI for calculating $E_d^-(\lambda)$. $R(\lambda)$ is calculated using eq. (2.14). $E_d(\lambda)$ can either be calculated according to eq. (2.23), or a measured spectrum can be taken. Making use of measurements is useful for reducing the number of fit parameters when upwelling radiance spectra are inverted. Default values of the reflection factors are $\sigma = 0.03$ and $\sigma^- = 0.54$.

Downwelling irradiance below the surface in shallow water, $E_d^{sh-}(\lambda)$, is also calculated using eq. (2.25), but using $R^{sh}(\lambda)$ instead of $R(\lambda)$.

2.9 Sky radiance

The same parameterization as for $E_d(\lambda)$ is also implemented for $L_s(\lambda)$:

$$L_s(\lambda) = [\ \alpha^* \cdot t_A(\lambda) + \beta^* \cdot (\lambda/\lambda_R)^{-4.09} + \gamma^* \cdot (\lambda/\lambda_M)^{\nu} + \delta^* \cdot t_C(\lambda)\ ] \cdot E_0(\lambda). \qquad (2.26)$$

The functions $E_0(\lambda)$, $t_A(\lambda)$, $(\lambda/\lambda_R)^{-4.09}$, $(\lambda/\lambda_M)^{\nu}$, and $t_C(\lambda)$ are those of eq. (2.23). Parameters of $L_s(\lambda)$ are the weights α^*, β^*, γ^*, δ^*, which represent the relative intensities of the four above-mentioned light sources for a radiance sensor, and the exponent ν.

This model of $L_s(\lambda)$ has been included for modeling specular reflection at the water surface. Its usefulness has been demonstrated (Gege 1998b). Capillary waves at the water surface, and moreover gravity waves, spread greatly the sky area that is reflected into the sensor, and change the angle of reflection. Consequently, measurements of $L_s(\lambda)$ are frequently not reliable. For these cases, and if no $L_s(\lambda)$ measurement is available, eq. (2.26) can be applied. If the user selects the wavelength-independent model of surface reflections, $L_s(\lambda) = E_d(\lambda)/\pi$ is set.

2.10 Upwelling radiance

The upwelling radiance is that part of the downwelling irradiance which is reflected back from the water into a down-looking radiance sensor. Calculation is based on a model of R_{rs} and a model or a measurement of E_d.

2.10.1 Below the water surface

In water, eq. (2.25) is used for calculating $E_d^-(\lambda)$, and eq. (2.17a), (2.17b) or (2.19) for $R_{rs}^-(\lambda)$. The upwelling radiance is then calculated as follows:

$$L_u^-(\lambda) = R_{rs}^-(\lambda) \cdot E_d^-(\lambda) \; . \tag{2.27}$$

In shallow waters, $R_{rs}^{sh-}(\lambda)$ is used instead of $R_{rs}^-(\lambda)$, and $E_d^{sh-}(\lambda)$ instead of $E_d^-(\lambda)$.

2.10.2 Above the water surface

The upwelling radiance after crossing the water-air boundary is related to the upwelling radiance in water, L_u^-, as follows:

$$L_u(\lambda,\theta_v) = \frac{1-\sigma_L^-(\theta'_v)}{n_W^2} \cdot L_u^-(\lambda,\theta'_v) + \sigma(\theta_v) \cdot L_d(\lambda,-\theta_v) \; . \tag{2.28}$$

θ_v is the zenith angle of the observer in air, θ'_v in water. These two angles are related to each others according to Snell's law via $n_W \, sin\theta'_v = sin\theta_v$ with n_W = refractive index of water. The first term on the right-hand side of eq. (2.28) is the radiance upwelling in the water, weakened at the interface by Fresnel reflection (factor $1-\sigma_L^-(\theta'_v)$) and refraction (flux dilution by widening of the solid angle, factor $1/n_w^2$). The second term are specular reflections of downwelling radiance at the surface. Eq. (2.28) is valid for a flat surface, i.e. without waves. Integration of eq. (2.28) over the upper hemisphere yields eq. (2.24).

Omitting for simplicity the symbol θ_v and using the more general model (2.11) for the radiance reflected from the surface, the following equation is obtained:

$$L_u(\lambda) = \frac{1-\sigma_L^-}{n_W^2} \cdot L_u^-(\lambda) + \sigma_L \cdot L_s(\lambda) \; . \tag{2.29}$$

This equation is used in WASI for calculating $L_u(\lambda)$. $L_u^-(\lambda)$ is calculated using eq. (2.27). The sky radiance $L_s(\lambda)$ can either be calculated using eq. (2.26), or a measured spectrum can be imported from file. The reflection factor for upwelling radiance is set to $\sigma_L^- = 0.02$ by default. This value, which is valid for a nadir-looking sensor, can be changed in the WASI.INI file. The reflection factor for downwelling radiance, σ_L, can either be calculated using the Fresnel equation (2.12), or it can be set constant. The default $\sigma_L = 0.02$ is valid for a nadir-looking sensor. By setting $\sigma_L = 0$ the water leaving radiance can be calculated. Furtheron, $n_W = 1.33$ is set as default.

3. Forward mode

The forward mode allows to calculate a single spectrum or a series of spectra according to user-specified parameter settings. The supported spectrum types are listed in Table 1.1.

3.1 Graphical user interface

The appearance of WASI's graphical user interface (GUI) depends slightly on the spectrum type. Fig. 3.1 shows the GUI at the example of the spectrum type "Remote sensing reflectance". The GUI consists of 8 elements:

(1) Drop-down list for selecting the spectrum type. The user selects one of the spectrum types from Table 1.1. If the spectrum type is changed, the parameter list (3) is updated in the way that only the parameters relevant for the selected type are displayed, and accordingly the model options (5) are updated.

(2) Check box for switching between forward and inverse mode. In the forward mode, this box is not checked.

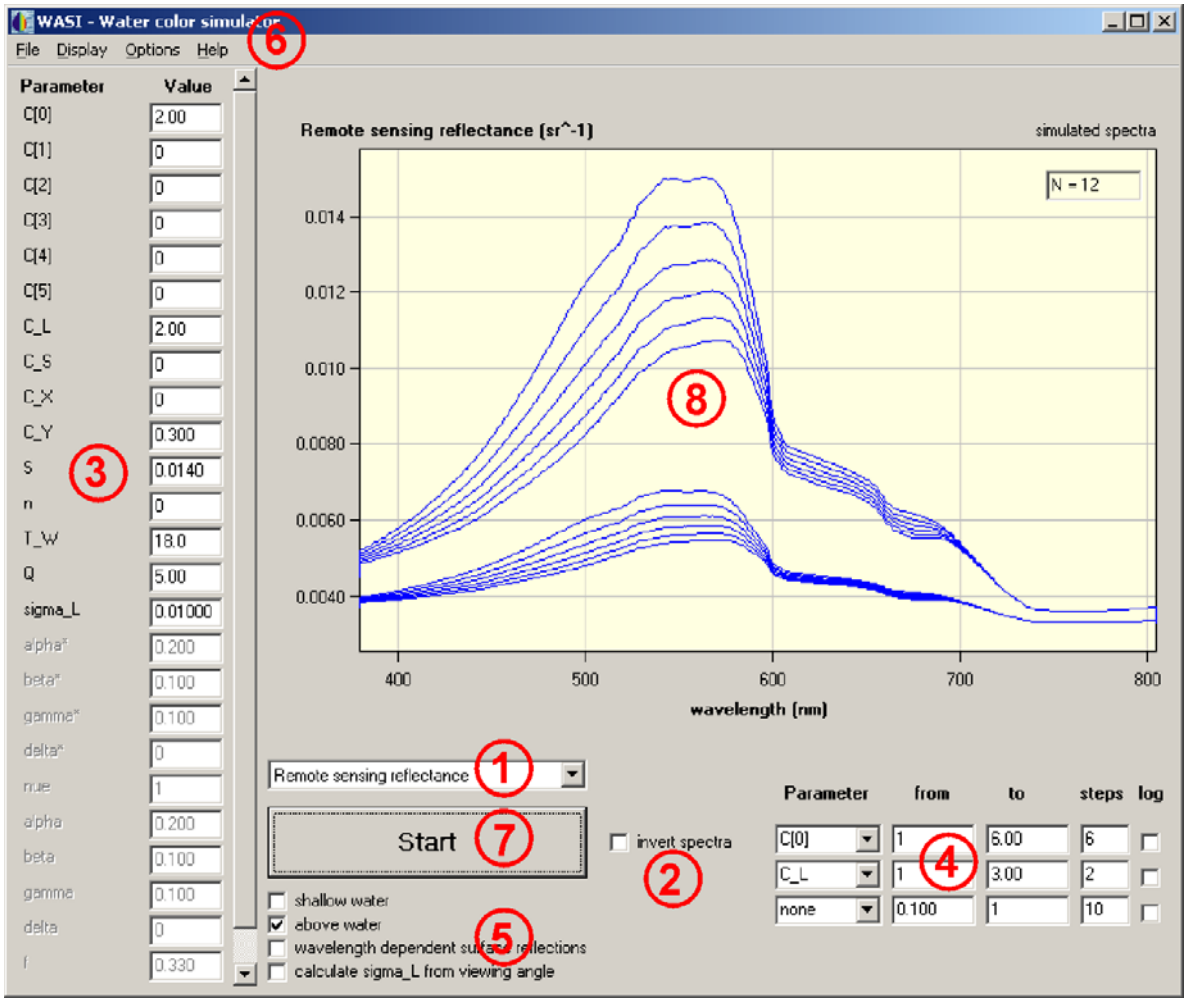


Fig. 3.1: Graphical user interface of the forward mode. 1 = Drop-down list for selecting the spectrum type, 2 = Check box for switching between forward and inverse mode, 3 = Parameter list (model specific), 4 = Selection panel for specifying the parameter iterations, 5 = Check boxes for selecting model options (model specific), 6 = Menu bar, 7 = Start button, 8 = Plot window.

(3) Parameter list. This list tabulates the parameters which are relevant for the selected spectrum type. It displays the parameters' symbols (in WASI notation, see Appendix 3) and their actual values. Default values are read from the WASI.INI file, actual values are set by the user by editing the corresponding "Value" fields. Depending on the model options, not all parameters may be relevant. Irrelevant parameters are disabled, i.e. the corresponding symbol and value is displayed in gray colour, and the value cannot be edited.

(4) Selection panel for specifying the iterations. Up to 3 parameters can be iterated simultaneously during one run, thus the panel has 3 rows, one for each parameter. The iterated parameters are selected in the "Parameter" drop-down lists, their minimum and maximum values in the "from" and "to" fields, and their numbers of values in the "steps" fields. The "log" check boxes specify whether the intervals are equidistant on a linear scale (no hook) or on a logarithmic scale (hook).

(5) Check boxes for selecting model options. Several spectrum types support options which further specify the model, cf. Table 1.1. Each option is either switched on or off.

(6) Menu bar. Further details concerning the model, data storage and visualisation can be specified in various pop-up windows, which are accessed via the menu bar.

(7) Start button. Calculation is started by pressing this button.

(8) Plot window. Each spectrum is plotted in this window after calculation. All curves are plotted together in order to visualize the spectral changes for the chosen iterations. A counter in the upper right corner is updated after each plot.

3.2 Calculation of a single spectrum

3.2.1 Mode selection

For calculating a single spectrum in the forward mode, the following settings must be made:

- Set forward mode: the "invert spectra" box (② in Fig. 3.1) is unchecked;
- No parameter iteration: select "none" in each "parameter" drop-down list (④ in Fig. 3.1).

3.2.2 Spectrum type selection

WASI allows to calculate 8 different types of spectra, see Table 1.1. The desired type is selected in the main window from the drop-down list① of Fig. 3.1.

Several types of spectra support further options, see Table 1.1. If that is the case for the selected type, the options are displayed at the bottom of the main window (⑤ in Fig. 3.1). Each option is either switched on or off. The selection is done by marking the corresponding check box with a hook. In the example of Fig. 3.1 three options are available:

(1) Above water. Since the check box is marked, the remote sensing reflectance will be calculated for a sensor above the water surface; when the hook is removed, calculation is performed for below the surface.

(2) Wavelength dependent surface reflections. Since the check box is unmarked, the surface reflections will be treated as constant ($R_{rs}^{surf}(\lambda) = \sigma_L/\pi$ according to chapter 2.5).

(3) Calculate sigma_L from viewing angle. Since the check box is unmarked, the reflectance factor for sky radiance, σ_L, is treated as a parameter that can be defined by the user. Otherwise, σ_L would be calculated from the viewing angle using eq. (2.18).

3.2.3 Parameter selection

All model parameters are read during program start from the WASI.INI file. The parameters which are relevant for the actual spectrum type are listed at the left side of the main window (③ in Fig. 3.1). This list can be edited.

3.2.4 Calculation options

Several calculation settings are made in the pop-up window "Forward calculation settings". This pop-up window is accessed from the menu bar via "Options - Forward calculation" (see Fig. 7.1) and displayed in Fig. 3.2.

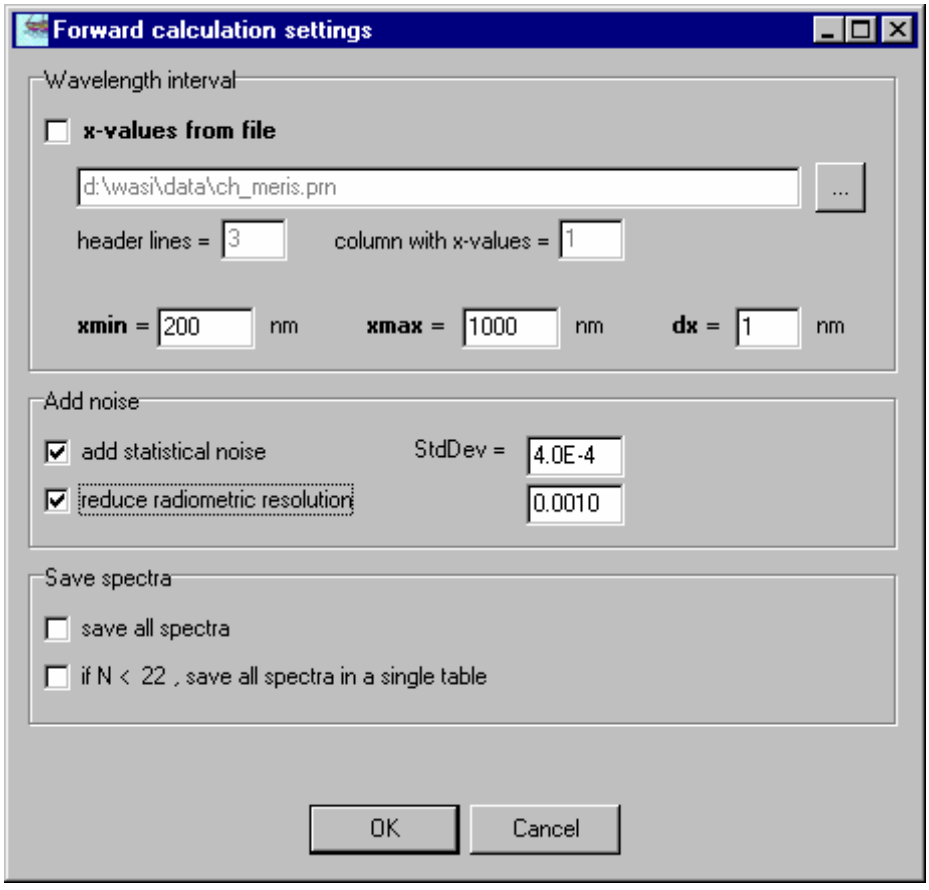


Fig. 3.2: The pop-up window "Forward calculation settings".

Wavelength interval. The wavelength range and the data interval of the calculated spectra can be selected in two ways:

- For non-equidistant intervals, e.g. if calculations should be performed for channels of a specific sensor, the wavelengths are read from an ASCII table.[5] In this case the box "x-values from file" must be marked with a hook, and the corresponding file must be selected. The pre-selected file can be changed by pressing the button ... , which causes the opening of a file-selection window. The number of lines in the ASCII file that are skipped are specified in the "header lines" input field; the column with the wavelengths is specified in the "column with x-values" field.

- If the spectra shall be calculated at equidistant wavelengths, the check box "x-values from file" has to be deselected. The first wavelength is specified in the "xmin" field, the last wavelength in the "xmax" field, and the intervals in the "dx" field.

Add noise. Two types of sensor characterics deterioriating data quality can be simulated: noise and dynamics.

- If the check box "add statistical noise" is marked with a hook, Gaussian distributed noise is added to each calculated value. Its standard deviation is specified in the input field "StdDev". If no noise is added, the "StdDev" input field is not displayed.

- If the check box "reduce radiometric resolution" is marked with a hook, the numerical accuracy is limited to the value shown in the corresponding input field. For example, 0.001 rounds original real numbers such that values of 0.000, 0.001, 0.002, 0.003, etc. result. If "reduce radiometric resolution" is not selected, the corresponding input field is not displayed.

Save spectra. Automatic saving of calculated spectra is activated by a hook in the check box "save all spectra". The directory is selected in the "Directories" window, see section 7.1 (Fig. 7.2). The calculated spectrum is stored in ASCII format as file B1.FWD. Note: If a file with the name B1.FWD already exists, it will be overwritten without warning. Two additional files are created automatically in the same directory as the spectrum. First, a copy of the initialisation file WASI.INI containing the actual parameter settings. It documents the data and parameters used for calculation. Second, a file CHANGES.TXT, which can be ignored; it is relevant only if a series of spectra is calculated.

The check box "if N < 22, save all spectra in a single table" is not relevant for calculating a single spectrum.

3.2.5 Start calculation

Calculation is started by pressing the "Start" button (⑦ in Fig. 3.1).

After calculation, the resulting curve is plotted in the main window (⑧ in Fig. 3.1) and stored automatically, if spectra saving is activated in the pop-up window "Forward calculation settings", see section 7.1 (Fig. 7.2).

[5] Spectral weighting using sensor-specific response functions is not supported.

3.2.6 Example

An example of a spectrum calculated in the forward mode is given in Fig. 3.3. The spectrum type is irradiance reflectance in deep water. The values of the model parameters are listed in the parameter list at the left-hand side: phytoplankton concentration C[0] = 3 µg/l, concentration of large suspended particles C_L = 1 mg/l, Gelbstoff absorption C_Y = 0.3 m^{-1} at 440 nm, Gelbstoff exponent S = 0.014 nm^{-1}, n is irrelevant since C_S = 0, water temperature T_W = 18 °C, sun zenith angle sun = 47.0°; the concentrations of all other substances are zero. The factor Q is irrelevant for the chosen model, which is indicated by gray text color. The fact that the displayed spectrum is a model curve (and not a measurement) is indicated by "simulated spectra" at top right.

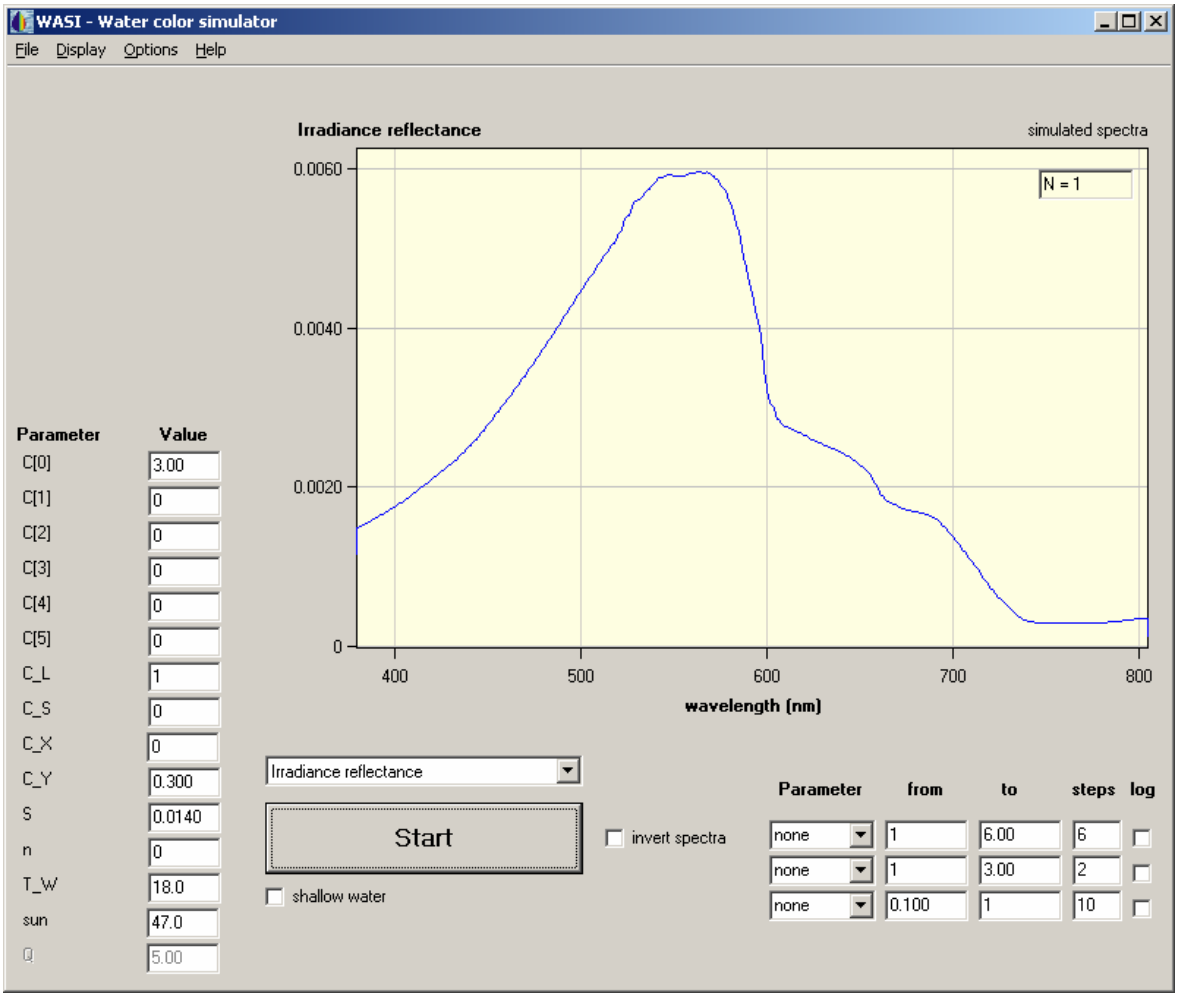


Fig. 3.3: A single irradiance reflectance spectrum calculated in the forward mode.

A listening of the first lines of the calculated spectrum is shown in Fig. 3.4. The header of the spectrum file contains the information that the spectrum has been created by the program WASI, gives the software version ("latest update"), lists the files which contain additional information (WASI.INI, CHANGES.TXT) and indicates the spectrum type ("y = "). It follows the calculated spectrum.

```
This file was generated by the program WASI
Version 3 - Latest update: 29 May 2005
Parameter values in files: WASI.INI, CHANGES.TXT

y = Irradiance reflectance



380.00  0.001482
381.00  0.001495
382.00  0.001507
383.00  0.001519
384.00  0.001532
385.00  0.001544
386.00  0.001557
387.00  0.001570
388.00  0.001583
389.00  0.001596
390.00  0.001610
```

Fig. 3.4: Listening of the first lines of the spectrum from Fig. 3.3.

3.3 Calculation of a series of spectra

3.3.1 General

Calculating a series of spectra in the forward mode is very similar to calculating a single spectrum. The only difference is that the parameter iterations have to be specified. Hence the settings are as follows:

- Define the spectrum type: select the type from the drop-down list (① in Fig. 3.1);
- Set forward mode: the "invert spectra" box (② in Fig. 3.1) is unchecked;
- Specify the parameter values: set the values of all model parameters in the parameter list (③ in Fig. 3.1).

Up to three model parameters can be iterated simultaneously as described below. For these, the parameter list entries are irrelevant since the values are set during iteration.

3.3.2 Specification of the iteration

3.3.2.1 Iteration over 1 parameter

For studying the dependence of a spectrum on a certain parameter, the values of that parameter can be iterated over its typical range of variation. WASI allows to iterate the parameters of Appendix 3. As shown in Fig. 3.5, the parameter to be iterated has to be selected from one of the three "Parameter" drop-down lists of the selection panel ④ of Fig. 3.1 (it is irrelevant, which of the 3 lists); the selection in the two other drop-down lists must be "none". The range of variation of the iterated parameter is specified by a minimum and a maximum value ("from", "to"), and the number of calculated spectra by the number of steps ("steps"). If the check box "log" is marked with a hook, the parameter intervals are equidistant on a logarithmic scale, otherwise they are equidistant on a linear scale.

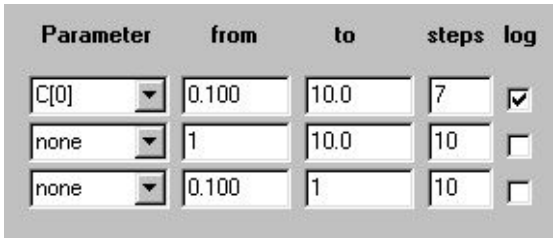


Fig. 3.5: Iteration over 1 parameter.

In the example of Fig. 3.5, the phytoplankton concentration C[0] is iterated from 0.100 to 10 µg/l in 7 steps which are equidistant on a logarithmic scale, i.e. 7 spectra with concentrations of 0.100, 0.215, 0.464, 1.0, 2.15, 4.64 and 10 µg/l are calculated.

3.3.2.2 Iteration over 2 parameters

When 2 parameters should be iterated, these parameters, their range of variation and the number of steps must be specified analogously to iterating 1 parameter. This is illustrated in Fig. 3.6.

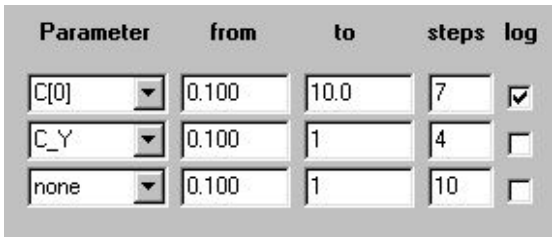


Fig. 3.6: Iteration over 2 parameters.

In the example of Fig. 3.6, the phytoplankton concentration C[0] is iterated as in Fig. 3.5 from 0.100 to 10 µg/l in 7 steps which are equidistant on a logarithmic scale, and Gelbstoff absorption at 440 nm, C_Y, is iterated from 0.100 to 1 m^{-1} in 4 steps which are equidistant on a linear scale, i.e. absorption values of 0.1, 0.4, 0.7 and 1.0 m^{-1} are taken. Spectra are calculated for each combination, hence the number of generated spectra is $7 \cdot 4 = 28$.

3.3.2.3 Iteration over 3 parameters

When 3 parameters should be iterated, these parameters, their range of variation and the number of steps must be specified analogously to iterating 1 or 2 parameters. This is illustrated in Fig. 3.7.

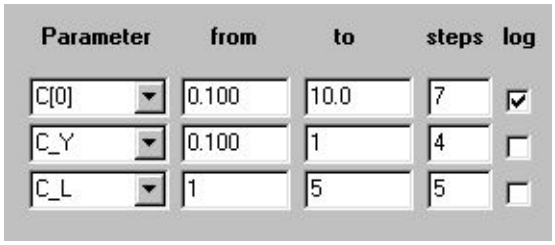


Fig. 3.7: Iteration over 3 parameters.

In the example of Fig. 3.7, phytoplankton concentration C_P and Gelbstoff absorption C_Y are iterated as in Fig. 3.6, but additionally the concentration of large suspended particles, C_L, is iterated from 1 to 5 mg/l in 5 steps which are equidistant on a linear scale, i.e. concen-

trations of 1, 2, 3, 4 and 5 mg/l are taken. Spectra are calculated for each combination, hence the number of generated spectra is 7 · 4 · 5 = 140.

3.3.3 Data storage

Calculated spectra are stored automatically if saving is activated in the "Forward calculation settings" pop-up window shown in Fig. 3.2. Each spectrum is stored in a separate file; the file names are `Bnr.fwd` with `nr` = file number. The extension `fwd` indicates that the spectra are the result of forward calculations. The parameters which change from one spectrum to the next are listed in the file `changes.txt`. A copy of the `WASI.INI` file is created for documenting completely all parameters and input files. The directory where all the files are stored is selected as described in section 7.1.

If the number of calculated spectra is below 22, the spectra can alternately be stored in a single file, `spec.fwd`. This option is selected by marking the check box "if N < 22, save all spectra in a single table" in the "Forward calculation settings" pop-up window (see Fig. 3.2).

3.3.4 Example

An example of a series of spectra calculated in the forward mode is given in Fig. 3.8.

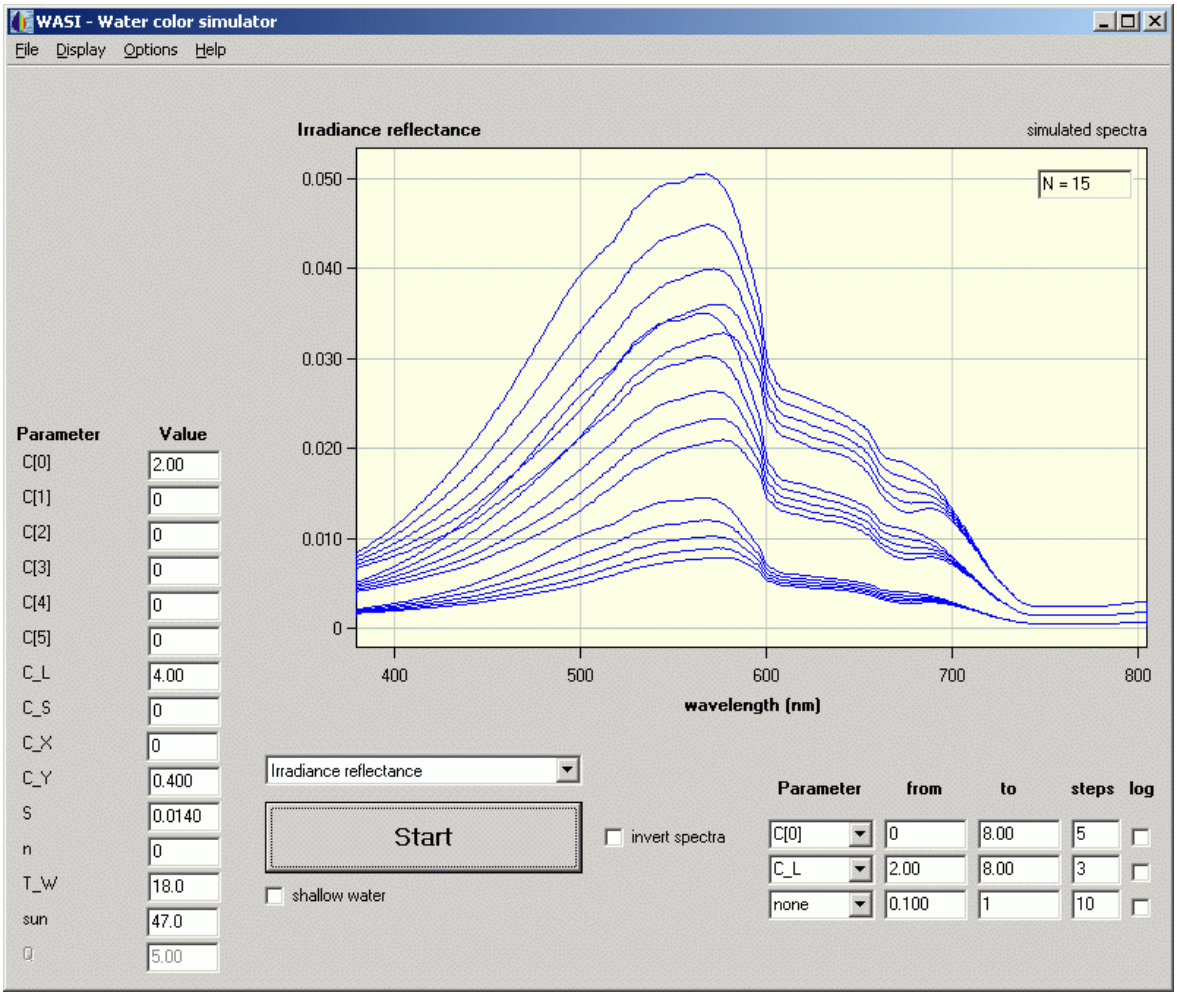


Fig. 3.8: A series of irradiance spectra calculated in the forward mode.

The spectrum type of Fig. 3.8 is irradiance reflectance. N = 15 spectra have been calculated by iterating two parameters: phytoplankton concentration, C[0], was changed from 0 to 8 µg/l in 5 steps, i.e. concentrations of 0, 2, 4, 6, 8 µg/l were taken, and the concentration of large suspended particles, C_L, was changed from 2 to 8 mg/l in 3 steps, i.e. concentrations of 2, 5 and 8 mg/l were taken. The values of the other parameters are shown in the parameter list at the left side. The list values of the iterated parameters, C[0] and C_L, are invalid.

When "save all spectra" is activated in the "Forward calculation settings" popup-window (see Fig. 3.2), all 15 spectra are saved in ASCII format as separate files in the specified directory; an example listening of such a file was given above in Fig. 3.4. The file names are `B01.fwd, B02.fwd, ... B15.fwd`.

If the number of calculated spectra is less than 22, and if the check box "if N<22, save all spectra in a single table" of the "Batch mode options" menu is marked with a hook, a single table with the file name `SPEC.FWD` is created instead of separate files. An example of that table is shown in Fig. 3.9.

```
This file was generated by the program WASI
Version 3 - Latest update: 29 May 2005
Parameter values in files: WASI.INI, CHANGES.TXT

y = Irradiance reflectance

               1         2         3         4         5         6

380.00  0.002158  0.005170  0.008426  0.002035  0.004880  0.007951
381.00  0.002186  0.005244  0.008552  0.002057  0.004942  0.008057
382.00  0.002214  0.005320  0.008679  0.002081  0.005006  0.008164
383.00  0.002243  0.005397  0.008808  0.002104  0.005070  0.008272
384.00  0.002272  0.005476  0.008939  0.002128  0.005135  0.008382
385.00  0.002301  0.005555  0.009072  0.002152  0.005201  0.008493
386.00  0.002331  0.005636  0.009208  0.002176  0.005268  0.008605
387.00  0.002362  0.005718  0.009345  0.002201  0.005336  0.008719
388.00  0.002393  0.005801  0.009484  0.002226  0.005404  0.008834
389.00  0.002424  0.005886  0.009625  0.002251  0.005474  0.008951
390.00  0.002456  0.005972  0.009768  0.002277  0.005544  0.009069
```

Fig. 3.9: The first lines and the first 6 columns of the file SPEC.FWD of the spectra series of Fig. 3.8.

The parameter values and input files used for calculating the spectra are documented by a copy of the WASI.INI file, which is stored automatically in the directory of the spectra. The values of the iterated parameters are tabulated in the file `CHANGES.TXT`. An example of that file is given in Fig. 3.10.

```
This file was generated by the program WASI
Version 3 - Latest update: 29 May 2005

List of parameter values which differ from one spectrum to the next
Common parameter set of all spectra in file: WASI.INI
All spectra are the results of forward calculations
Spectra = Irradiance reflectance

  Spectrum      C[0]       C_L

   B01.fwd         0     2.000
   B02.fwd         0     5.000
   B03.fwd         0     8.000
   B04.fwd     2.000     2.000
   B05.fwd     2.000     5.000
   B06.fwd     2.000     8.000
   B07.fwd     4.000     2.000
   B08.fwd     4.000     5.000
   B09.fwd     4.000     8.000
   B10.fwd     6.000     2.000
   B11.fwd     6.000     5.000
   B12.fwd     6.000     8.000
   B13.fwd     8.000     2.000
   B14.fwd     8.000     5.000
   B15.fwd     8.000     8.000
```

Fig. 3.10: The file CHANGES.TXT of the spectra series of Fig. 3.8.

4. Inverse mode

Inverse modeling is the determination of model parameters for a given spectrum. More precisely, those values of the model parameters must be determined for which the correspondence between fit curve and given spectrum is maximal.

Three modes of operation are implemented for inverse modeling of spectra:

- **Single spectrum mode.** Inversion is performed for a single spectrum which the user loads from file. After calculation, an overlay of imported spectrum and fit curve is automatically shown on screen and resulting fit values, number of iterations, and residuum are displayed. This mode allows to inspect the results for individual measurements. It is useful for optimizing the choice of initial values and the fit strategy before starting a batch job.

- **Batch mode.** A series of spectra from file is inverted. After each fit, an overlay of imported spectrum and fit curve is automatically shown on screen. This mode is useful for processing large data sets.

- **Reconstruction mode.** Combines forward and inverse modes. Inversion is performed for a series of forward calculated spectra which are not necessarily read from file. The model parameters can be chosen differently for forward and inverse calculations. This mode is useful for performing sensitivity studies.

4.1 Graphical user interface

The appearance of WASI's graphical user interface (GUI) depends on the spectrum type and on the operation mode. Fig. 4.1 shows the GUI for the example of the spectrum type "Remote sensing reflectance" and the single spectrum mode. The GUI consists of 8 elements:

(1) Drop-down list for selecting the spectrum type. As in the forward mode.

(2) Check boxes for specifying the operation mode. In the inverse mode, the box "invert spectra" is checked. A hook in the "batch mode" check box indicates that a series of spectra is analyzed. Otherwise, a single spectrum is inverted (single spectrum mode). The check box "read from file" selects whether the spectra are read from files (hook), or if previously forward calculated spectra are used (reconstruction mode, no hook).

(3) Parameter list. The list tabulates the start values of the fit parameters. Defaults are read from the WASI.INI file, the user can change them by editing the "Value" fields. A hook in a "Fit?" check box makes the corresponding parameter to a fit parameter, otherwise the parameter is kept constant during inversion. In the single spectrum mode, the resulting fit values are displayed after inversion is finished.

(4) The appearance of this area depends on the mode of operation. In the single spectrum mode, the residuum and the number of iterations are shown here after calculation is finished. In the batch mode, this area is empty. In the reconstruction mode, the panel of the forward mode for specifying the parameter iterations is displayed.

(5) Check boxes for selecting model options. As in the forward mode.

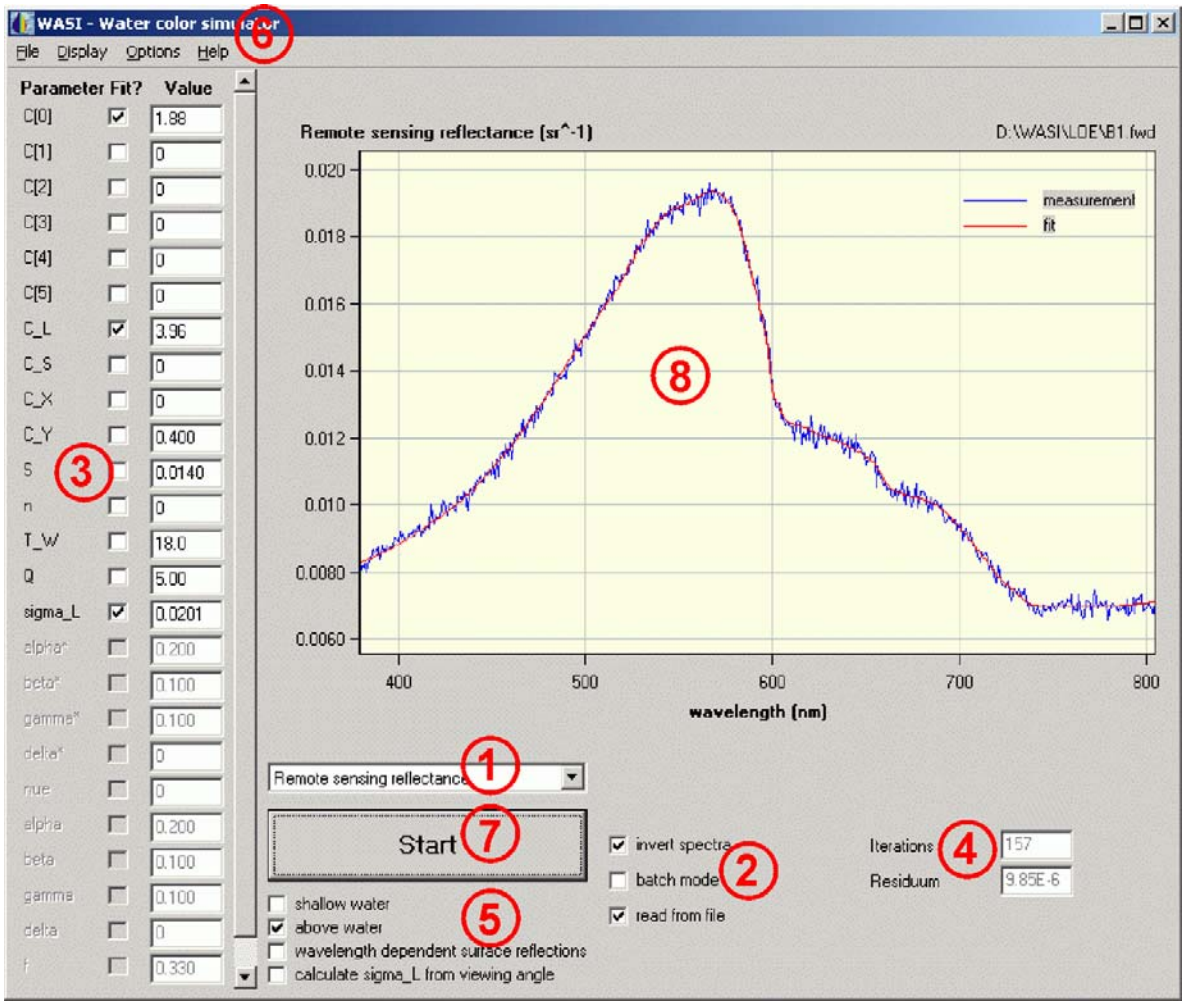


Fig. 4.1: Graphical user interface of the inverse mode. 1 = Drop-down list for selecting the spectrum type, 2 = Check boxes for specifying the operation mode, 3 = Parameter list (model specific), 4 = Display elements depending on mode of operation, 5 = Check boxes for selecting model options (model specific), 6 = Menu bar, 7 = Start button, 8 = Plot window.

(6) Menu bar. As in the forward mode.

(7) Start button. Inverse modeling is started by pressing this button.

(8) Plot window. The input spectrum is displayed in blue, the fit curve in red. The window is refreshed before a new pair of spectra is plotted, thus only the last pair remains on screen when a series of spectra is analyzed. The file name of the imported spectrum is shown on top right.

In the example of Fig. 4.1, a remote sensing reflectance spectrum above water, imported from the file B1.fwd, was inverted in the single spectrum mode. The spectrum had been previously generated in the forward mode, where noise with a standard deviation of $2 \cdot 10^{-4}$ sr^{-1} was added. During inversion three parameters were fitted (C[0], C_L, sigma_L), the other parameters were kept constant. Fit results are C[0] = 1.88 µg l^{-1}, C_L = 3.96 mg l^{-1}, and sigma_L = 0.201. The fit converged after 157 iterations at a residuum of $9.85 \cdot 10^{-6}$ sr^{-1}.

4.2 Inversion of a single spectrum

4.2.1 Spectrum selection

A single spectrum from file is selected as follows:

- Define the spectrum type: select the type from the drop-down list (① in Fig. 4.1);
- Load the spectrum.

Loading the spectrum is illustrated in Fig. 4.2. The pull-down menu "File" is opened from the menu bar, and "Load" is selected (top). Then a pop-up window for file selection opens, where the desired file is selected (bottom). Note: The layout of the file selection window depends on the operating system and the language; here the version of Windows 2000 in German is shown.

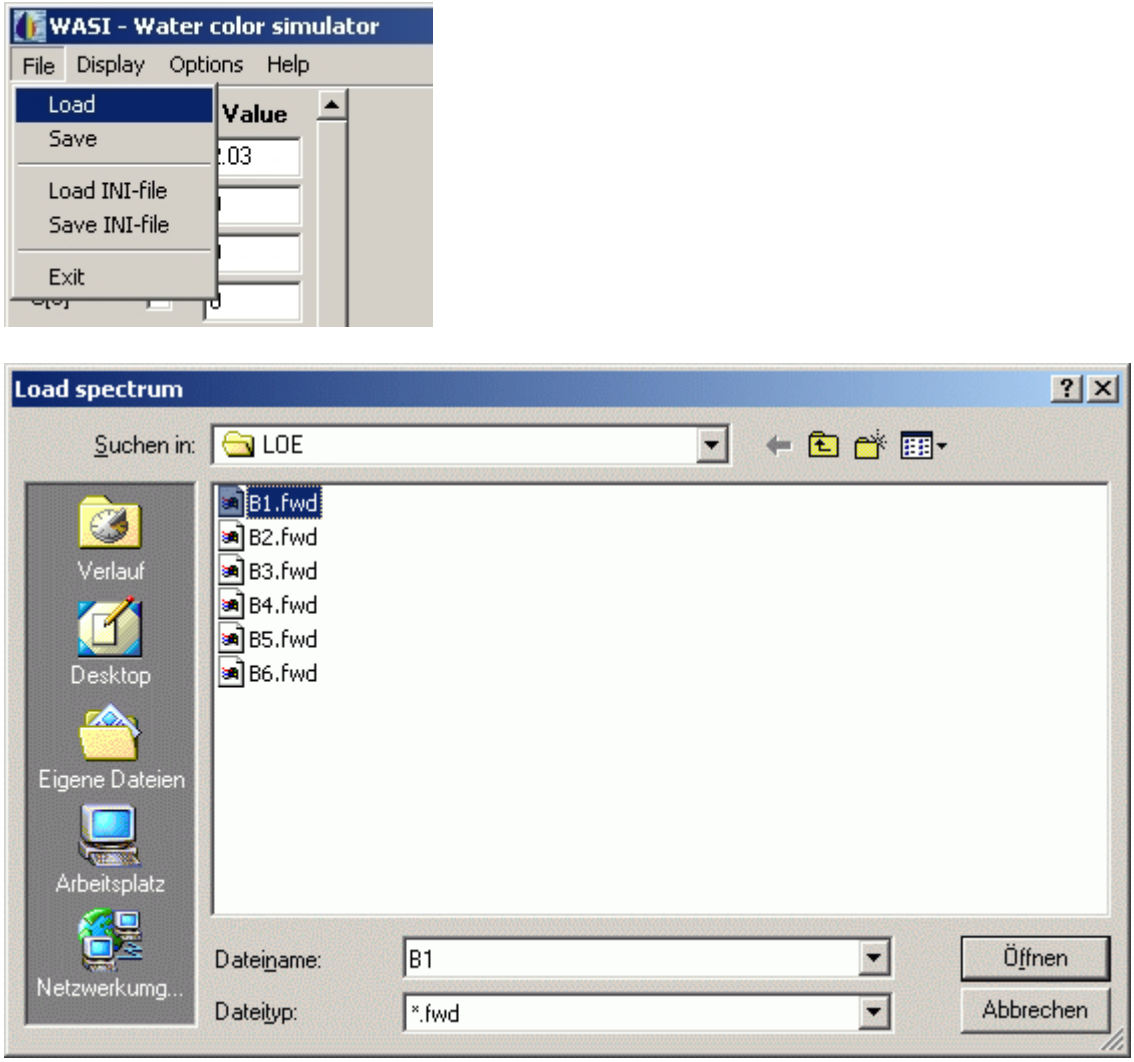


Fig. 4.2: Loading a single spectrum for inversion. Top: Menu bar and pull-down menu "File". Bottom: Pop-up window for selecting the file.

After the spectrum is loaded, it is automatically displayed in the plot window ⑧ of Fig. 4.1, and the program mode is automatically set to "single spectrum mode", i.e. the check boxes ② of Fig. 4.1 are set as shown in Fig. 4.3. No user action is required.

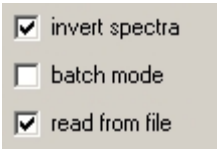


Fig. 4.3: Check box settings of the single spectrum mode.

4.2.2 Definition of initial values

Initial values of each fit parameter are read from the WASI.INI file. The user can change them either in the parameter list ③ of Fig. 4.1, or in the "Fit parameters" pop-up window, which is shown in Fig. 4.4.

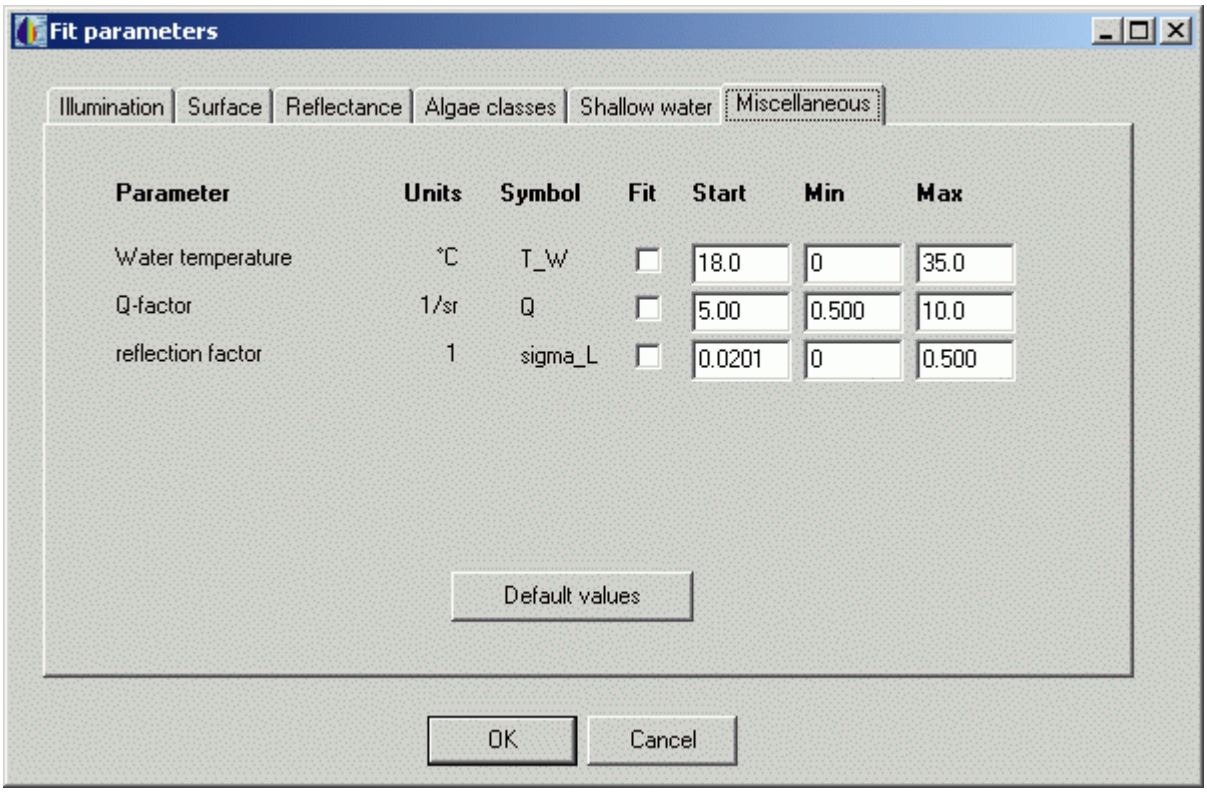


Fig. 4.4: The pop-up window "Fit parameters" with the register card "Miscellaneous".

Only the parameters relevant for the selected spectrum type are displayed in the main window (in the parameter list ③ of Fig. 4.1). For the example of Fig. 4.1, these are the parameters of the remote sensing reflectance model. The acronym, a check box, and a value is depicted for each parameter. The check box "Fit?" is used for selecting whether the parameter is treated as constant (no hook) or as fit parameter (hook) during inversion. In the example of Fig. 4.1 the parameters C[0], C_L, and sigma_L will be fitted, while all other parameters will be kept constant. The entry in the "Value" field has a different meaning before inversion is started and after it is finished: Before, the initial values are displayed; afterwards, the fit results are shown.

More details about the fit parameters contains the pop-up window "Fit parameters" (Fig. 4.4). It is accessed from the menu bar via "Options - Inverse calculation - Fit parameters" (see Fig. 7.1). It has six register cards which sort the parameters according to the categories Illumination, Surface, Reflectance, Algae classes, Shallow water, and Miscellaneous. Fig 4.4 shows as example the register card "Miscellaneous".

For each parameter the "Fit parameters" pop-up window displays a description, the physical units, and the acronym; furtheron it shows a check box for determining whether the parameter is fit variable or constant, and it specifies the start value and minimum and maxium values that are allowed for the fit routine. The user can change the settings of the "Fit" check box and of start, minimum and maximum value. The complete set of start values of a displayed register card can be overwritten by default values from the WASI.INI file by pressing the "Default values" button. These default values are stored separately from the start values in the WASI.INI file and can be changed only by editing the WASI.INI file.

4.2.3 Fit strategy

The values of the model parameters are determined iteratively. In the first iteration a fit curve is calculated using the initial values as parameters, and as a measure of correspondence between measured and fitted curve the residual is calculated. In all further iterations the fit parameters are altered and the new residual is compared with the previous one. If the new residual is smaller, the correspondence between measurement and fit is better, hence the new parameter set is the better one. The calculation is stopped when the difference between the residuals of two subsequent steps is smaller than some threshold, or if the number of iterations is above some threshold. The parameter values of the step with the smallest residuum are the fit results.

The residuum is a measure of the correspondence between the measured spectrum and a fit curve. WASI supports two calculation options:

- wavelength dependent weighting,
- 6 different minimisation methods.

The residuum is calculated by averaging the weighted differences between measured and fit curve over all wavelengths. The weighting function is specified in the "Weights" register card of the pop-up window "Fit tuning", which is shown in Fig. 4.5 and accessed from the menu bar via "Options - Invers calculation - Fit tuning" (see Fig. 7.1). Path and file name of that function are displayed in the "File" field; the file can be exchanged by opening a file selection window by pressing the "..." button. The number of header lines and the columns of the x- and y-values have to be specified also. If all wavelengths shall be weighted equally, the file must contain a constant function, at the best with 1 as y-values. Such a file, `EINS.PRN`, is set as default in WASI.

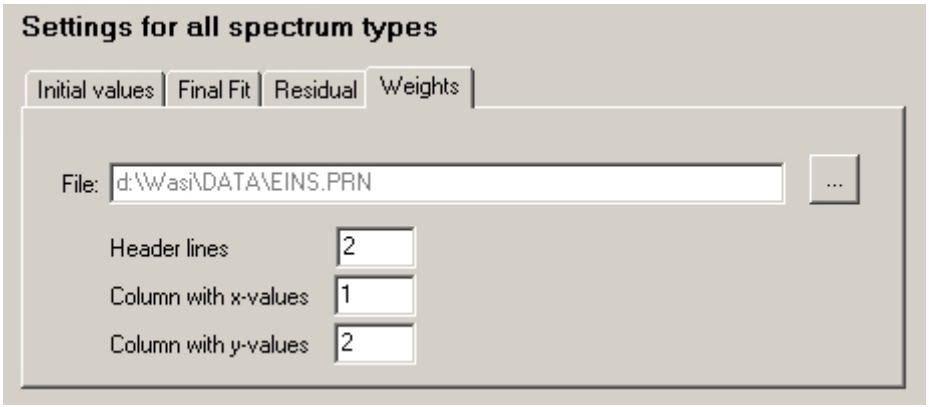


Fig. 4.5: The register card "Weights" of the popup window "Fit tuning".

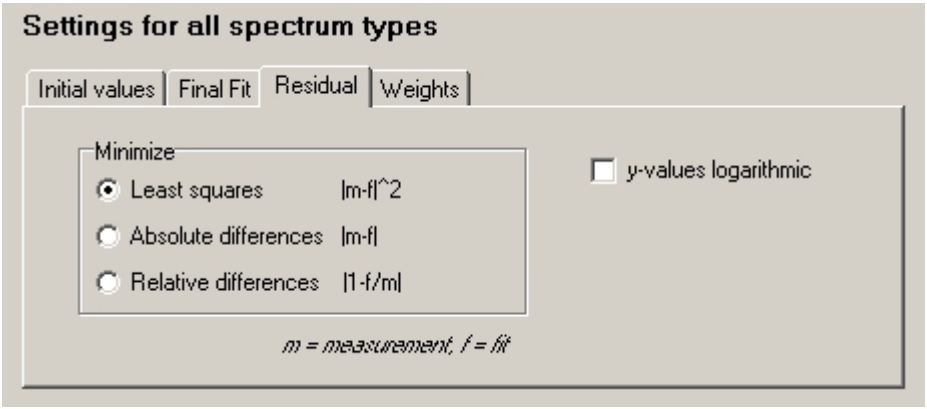


Fig. 4.6: The register card "Residual" of the popup window "Fit tuning".

The minimization method is selected in the "Residual" register card of the pop-up window "Fit tuning", which is shown in Fig. 4.6. The equations of calculation are summarized in Table 4.1.

no.	method	y-values	minimize
1	least squares	linear	$\Sigma\, g_i \cdot \lvert m_i - f_i \rvert^2$
2	absolute differences	linear	$\Sigma\, g_i \cdot \lvert m_i - f_i \rvert$
3	relative differences	linear	$\Sigma\, g_i \cdot \lvert 1 - f_i / m_i \rvert$
4	least squares	logarithmic	$\Sigma\, g_i \cdot \lvert \ln(m_i) - \ln(f_i) \rvert^2$
5	absolute differences	logarithmic	$\Sigma\, g_i \cdot \lvert \ln(m_i) - \ln(f_i) \rvert$
6	relative differences	logarithmic	$\Sigma\, g_i \cdot \lvert 1 - \ln(f_i) / \ln(m_i) \rvert$

Table 4.1: Methods for calculating residuals. g_i = weight of channel i, m_i = measurement of channel i, f_i = fit of channel i.

4.2.4 Definition of fit region and number of iterations

Which part of the spectrum is fitted and which data interval is taken for calculating the residuals is specified in the "Final fit" register card of the "Fit tuning" menu, as shown in Fig. 4.7. The pop-up window is accessed from the menu bar via "Options - Invers calculation - Fit tuning" (see Fig. 7.1). The maximum number of iterations forces the fit routine to stop; the number should be set high enough that a forced stop is exceptional.

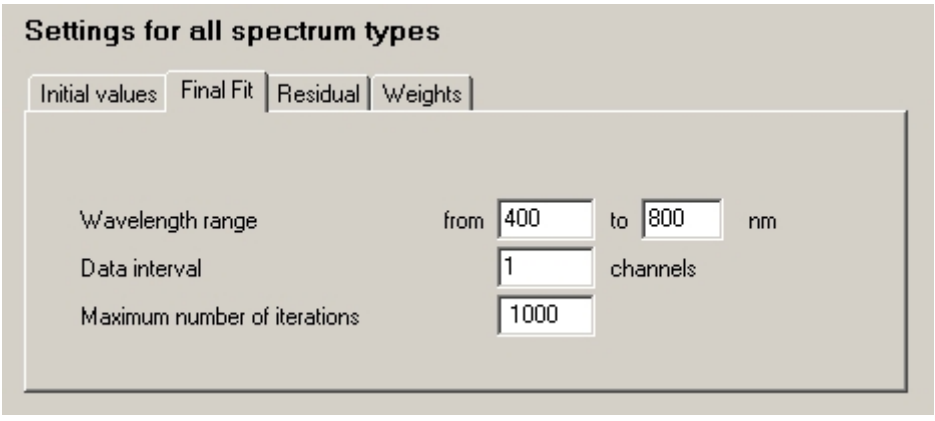


Fig. 4.7: The register card "Final fit" of the pop-up window "Fit tuning".

4.3 Inversion of a series of spectra

4.3.1 Selection of spectra

A series of spectra is selected for inversion as follows:

- the path of the input spectra is set in the menu "Options - directories", field "Read spectra";
- the path for storing the results is set in the menu "Options - directories", field "Save results", input line "Inversion";
- reading of spectra is activated in the menu "Options - Invers calculation - Data in/out", field "Input": mark the box "read spectra" with a hook;
- the file characteristics of the input spectra are set in the menu "Options - Invers calculation - Data in/out", field "Input": specify file extension, number of header lines in the files, column of x-values, column of y-values;
- saving of fit spectra is activated or deactivated in the menu "Options - Invers calculation - Data in/out", field "Output": select or deselect the box "save all spectra".

As a result of inversion, the fit results are stored in the table `FITPARS.TXT`. This table is generated at the specified path, irrespective whether saving of spectra is activated or deactivated. If saving of spectra is activated, for each input spectrum a file is generated which lists the spectral values of input and fit curve. The file names are identical to the input file names, but the file extensions are set to `INV`.

4.3.2 Definition of initial values

When a series of spectra shall be inverted, the initial values can either be chosen identically for every spectrum, or they are determined individually. The selection of the method is done in the "Initial values" register card of the pop-up window "Fit tuning" menu, as shown in Fig. 4.8. The pop-up window is accessed from the menu bar via "Options - Invers calculation - Fit tuning".

If the box "identical for all spectra" is marked with a hook, the initial values for every spectrum are taken from the parameter list, as described in section 4.1.3. Otherwise, there are two options: either the results from the previous fit are taken as start values for the subsequent fit, or some start values are determined from the spectrum itself. Which of these options is taken is specified individually for each spectrum type in the register card "Settings for individual spectra types". However, determination of start values from the spectrum itself is not possible for every spectrum type. If there is no register card for a specific spectrum type, or if the register card does not include a box labeled "automatic determination of initial values", the results from the previous fit are taken as start values.

Fig. 4.8 shows as an example the register card for the spectrum type `Irradiance reflectance`. "Automatic determination of initial values" is activated, i.e. the initial values are determined from the spectra themselves. The implemented algorithms for automatic determination and the relevant user interfaces are described in chapter 4.3 "Optimisation of inversion".

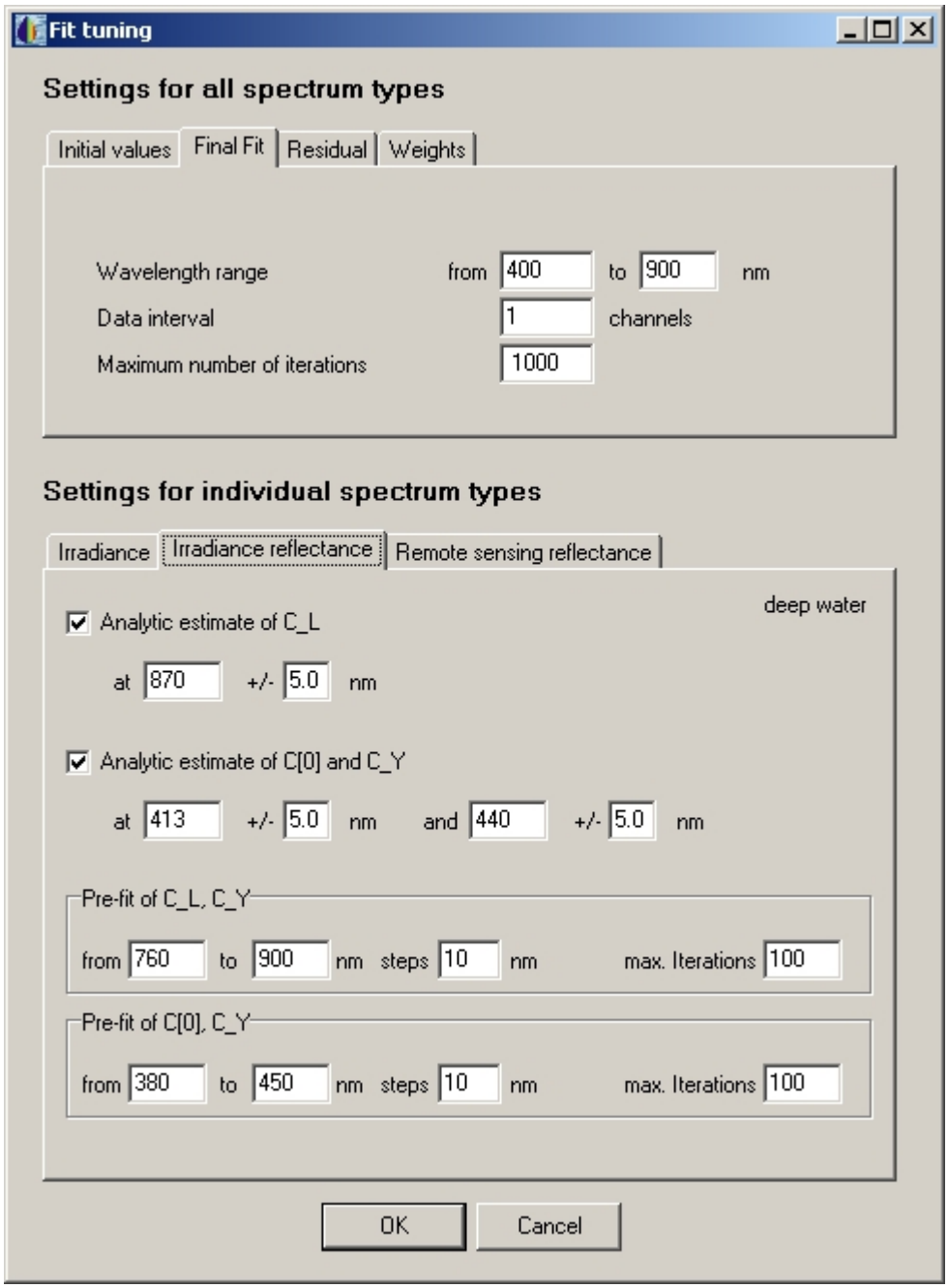


Fig. 4.8: The pop-up window "Fit tuning" with the opened register cards "Initial values" and "Irradiance reflectance" of deep water.

4.4 Optimisation of inversion

4.4.1 Irradiance reflectance of deep water

The most important parameters that can be determined from irradiance reflectance spectra of deep water are the concentrations of phytoplankton, Gelbstoff and suspended matter. A study has been performed which investigated their retrieval sensitivity to errors (Gege 2002). It resulted a very small sensitivity for suspended matter, some sensitivity for Gelbstoff, but very high sensitivity for phytoplankton. The study suggested a procedure for initial values determination, which has been optimised by further simulations. Finally the 5-steps-procedure summarised in Table 4.2 was implemented in WASI. The user can fine-tune the procedure in the "Fit tuning" pop-up window, which is shown in Fig. 4.8. It is accessed from the menu bar via "Options - Invers calculation - Fit tuning".

Step	determine	algorithm	Procedure
1	C_L, C_S	analytical	Determine a first estimate of C_L and C_S from an analytic equation at a wavelength in the Infrared.
2	Y, C_0	analytical	Determine a first estimate of Y and C_0 from analytic equations at two wavelengths; for C_L and C_S the values from step 1 are taken.
3	C_L, C_S, Y	fit	Determine initial values of C_L, C_s and Y by fit; C_0 is kept constant at the value from step 2, C_L, C_S and Y are initialized using the values from steps 1 and 2, respectively.
4	C_0, Y, S	fit	Determine initial values of C_0, Y and S by fit; C_L is kept constant at the value from step 3, Y is initialized using the value from step 3, S is initialized by the user-setting from the parameter list.
5	All parameters	fit	All parameters are fitted, starting with initial values for C_L, C_S, C_0, Y and S from steps 3 and 4.

Table 4.2: Procedure for inversion of irradiance reflectance spectra of deep water.

Fine-tuning of steps 1 to 4 is done in the "Irradiance reflectance" register card of the "Fit tuning" pop-up window. It is shown in Fig. 4.9. Steps 1 and 2 are performed if the check boxes "Analytic estimate of ..." are marked with a hook. Otherwise the initial values from the parameter list or from the previous fit are taken, as described in section 4.2.2. Steps 3 and 4 are tuned in the "Pre-fit" frames. The pre-fits are performed if "max. iterations" is set to a value larger than 1. At step 5 the user can define the wavelength range to be fitted, the intervals between data points, and the maximum number of iterations. The relevant user interface is shown in Fig. 4.7.

Step 1. Suspended matter backscattering B_0 can be calculated analytically from the reflectance at any wavelength, for which phytoplankton and Gelbstoff absorption are either known or can be neglected. The equation of determination is obtained from the irradiance reflectance model described in section 2.5.1. Two models are implemented:

$$R(\lambda) = f \cdot \frac{b_{b,W}(\lambda) + B_0}{a(\lambda) + b_{b,W}(\lambda) + B_0}, \tag{4.1a}$$

$$R(\lambda) = f \cdot \frac{b_{b,W}(\lambda) + B_0}{a(\lambda)}. \tag{4.1b}$$

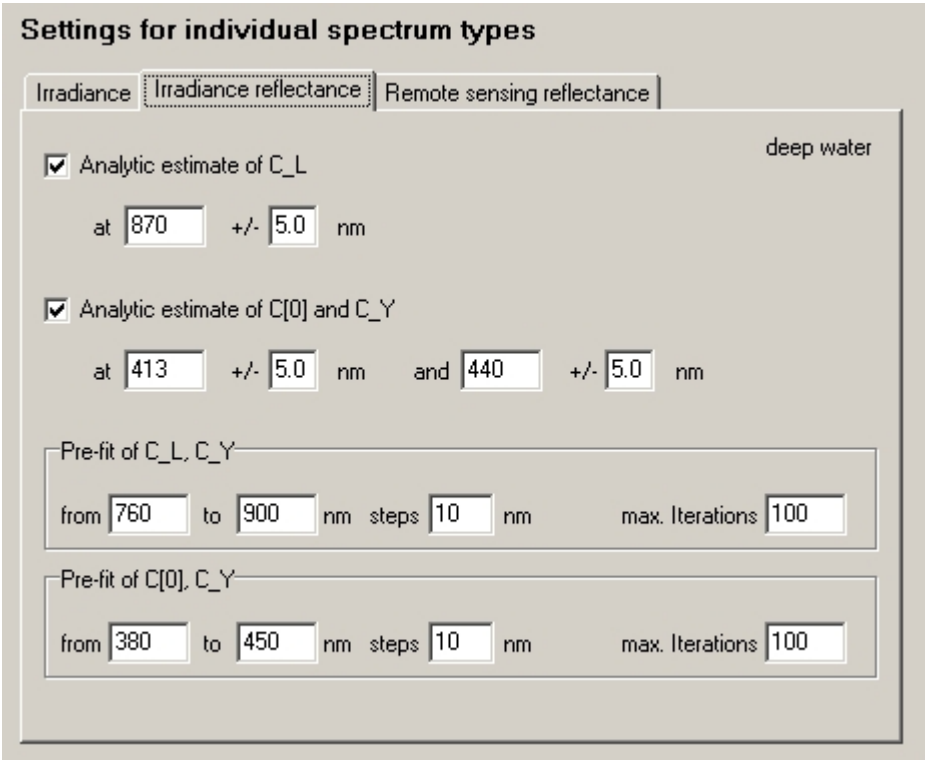


Fig. 4.9: The register card "Irradiance reflectance" for deep water of the pop-up window "Fit tuning".

Eq. (4.1a) is the Gordon et al. (1975) model, eq. (4.1b) the Prieur (1976) model, see section 2.5.1. If absorption of water and its constituents, a, is known at a certain wavelength λ_{IR}, B_0 is calculated as follows:

$$B_0 = \frac{a(\lambda_{IR}) \cdot R(\lambda_{IR})}{f - R(\lambda_{IR})} - b_{b,W}(\lambda_{IR}), \tag{4.2a}$$

$$B_0 = \frac{a(\lambda_{IR}) \cdot R(\lambda_{IR})}{f} - b_{b,W}(\lambda_{IR}). \tag{4.2b}$$

These equations are obtained by solving eqs. (4.1a) and (4.1b) for B_0, respectively. Which is used for calculating B_0 depends on the selected R model. $a(\lambda_{IR})$ is calculated according to eq. (2.3) using as inputs the values from the parameter list; typically $a(\lambda_{IR})$ is very close to pure water absorption, $a_W(\lambda_{IR})$, except for high Gelbstoff concentration.

The calculation of f depends on the selected f model, cf. chapter 6.2. If f is parameterised solely as a function of the sun zenith angle (eqs. 6.1, 6.3), the f value resulting from the given sun zenith angle is taken. If f is parameterised additionally as a function of backscattering (eqs. 6.2, 6.4), f is calculated in two steps. First, the values from the parameter list are taken to calculate backscattering at wavelength λ_{IR} using eq. (2.4); with that result a first estimate of f is calculated. In the second step, eq. (4.2a) or (4.2b) is applied to calculate B_0 using the f value from the first step. Then f is calculated again using eq. (6.2) or (6.4).

A special algorithm has been implemented for the f model f = constant. Obviously a constant f value needs no further consideration for applying eq. (4.2a) or (4.2b). However, if that f model is selected, f can be treated as a fit parameter. If fitting of f is activated, an initial value for f can be calculated in addition to B_0 as described in the following.

Special case: Initial values for f and B_0

Calculation is based on reflectance values at two wavelengths $\lambda_{IR,1}$ and $\lambda_{IR,2}$ ($\lambda_{IR,2} > \lambda_{IR,1}$). It requires that $R(\lambda_{IR,1}) \neq R(\lambda_{IR,2})$; if that is not the case, f is kept constant at the value from the parameter list, and B_0 is calculated as described above. Initial values determination makes use of eq. (4.1a); no corresponding algorithm for eq. (4.1b) is implemented.

First the factor f is eliminated by taking the ratio of eq. (4.1a) for two wavelengths $\lambda_{IR,1}$ and $\lambda_{IR,2}$:

$$\frac{R(\lambda_{IR,1})\cdot\left(a(\lambda_{IR,1})+b_{b,W}(\lambda_{IR,1})+B_0\right)}{R(\lambda_{IR,2})\cdot\left(a(\lambda_{IR,2})+b_{b,W}(\lambda_{IR,2})+B_0\right)}=\frac{b_{b,W}(\lambda_{IR,1})+B_0}{b_{b,W}(\lambda_{IR,2})+B_0}. \tag{4.3}$$

Eq. (4.3) assumes that B_0 is the same at $\lambda_{IR,1}$ and $\lambda_{IR,2}$. Multiplication of eq. (4.3) with the product of both denominators leads to a quadratic expression in B_0 of the form

$$\alpha\cdot B_0^2+\beta\cdot B_0+\gamma=0, \tag{4.4}$$

with

$$\alpha = R(\lambda_{IR,1})-R(\lambda_{IR,2}); \tag{4.5a}$$

$$\beta = R(\lambda_{IR,1})\cdot\left(a(\lambda_{IR,1})+b_{b,W}(\lambda_{IR,1})+b_{b,W}(\lambda_{IR,2})\right)- R(\lambda_{IR,2})\cdot\left(a(\lambda_{IR,2})+b_{b,W}(\lambda_{IR,1})+b_{b,W}(\lambda_{IR,2})\right); \tag{4.5b}$$

$$\gamma = R(\lambda_{IR,1})\cdot\left(a(\lambda_{IR,1})+b_{b,W}(\lambda_{IR,1})\right)\cdot b_{b,W}(\lambda_{IR,2})- R(\lambda_{IR,2})\cdot\left(a(\lambda_{IR,2})+b_{b,W}(\lambda_{IR,2})\right)\cdot b_{b,W}(\lambda_{IR,1}). \tag{4.5c}$$

It has two solutions:

$$B_0=\frac{-\beta\pm\sqrt{\beta^2-4\alpha\gamma}}{2\alpha}. \tag{4.6}$$

The positive solution gives the correct value of B_0. This is the algorithm for calculating B_0. The algorithm for calculating f is obtained directly from eq. (4.1a):

$$f = R(\lambda_{IR,2})\cdot\frac{a(\lambda_{IR,2})+b_{b,W}(\lambda_{IR,2})+B_0}{b_{b,W}(\lambda_{IR,2})+B_0}. \tag{4.7}$$

It has been investigated how the accuracy of the retrieved C_L values depends on the choice of the wavelengths $\lambda_{IR,1}$ and $\lambda_{IR,2}$ and on the errors of the initial Y and C_L values. The more $\lambda_{IR,1}$ and $\lambda_{IR,2}$ are shifted towards longer wavelengths, the better are the results. For Gelbstoff concentrations below 1 m^{-1} the relative error of C_L is always below 20 % if both wavelengths are above 820 nm. For the MERIS channels $\lambda_{IR,1}$ = 870 nm and $\lambda_{IR,2}$ = 900 nm the relative errors are always below 5 % for Y ≤ 0.5 m^{-1} and below 12 % for Y ≤ 1 m^{-1}. Hence, for sensors equipped with two or more channels above 820 nm and for moderate Gelbstoff concentrations the analytical equations are well-suited to determine initial values of C_L and f.

The conversion from optical units B_0 to gravimetric concentrations C_L, C_S is based on eq. (2.4) assuming $b_L(\lambda) = 1$. Accordingly it is $B_0 \equiv b_b(\lambda) - b_{b,W}(\lambda) = C_L \cdot b_{b,L}^* + C_S \cdot b_{b,S}^* \cdot (\lambda/\lambda_S)^n$. If $C_S = 0$, C_L is calculated as

$$C_L=\frac{B_0}{b_{b,L}^*}. \tag{4.8a}$$

Otherwise, i.e. for $C_S \neq 0$, the user-defined ratio $r_{LS} = C_L/C_S$ is retained, hence the initial values of C_L and C_S are calculated as follows:

$$C_L = \frac{B_0}{b^*_{b,L} + \frac{b^*_{b,S}}{r_{LS}} \cdot \left(\frac{\lambda_{IR}}{\lambda_S} \right)^n}; \qquad C_S = \frac{C_L}{r_{LS}}. \tag{4.8b}$$

C_L can be determined in that way with an accuracy in the order of 1 % (Gege and Albert 2005).

Step 2. A non-iterative procedure based on two channels was found to be practicable for calculating the initial concentrations of phytoplankton and Gelbstoff at an accuracy in the order of 30 % (Gege and Albert 2005). If suspended matter concentration and the factor f are known with little error, e.g. from step 1, the concentrations C_0 and Y can be determined analytically from two wavelengths λ_1 and λ_2. The equations of determination are obtained from the irradiance reflectance model described in chapter 2.5.1:

$$R(\lambda) = f \cdot \frac{b_b(\lambda)}{a_W(\lambda) + Y \cdot a^*_Y(\lambda) + C_0 \cdot a^*_0(\lambda) + b_b(\lambda)}. \tag{4.9}$$

Resolving the equation for the sum $Y \cdot a_Y^*(\lambda) + C_0 \cdot a_0^*(\lambda)$, and ratioing that equation for two wavelengths yields the following ratio R_A:

$$R_A := \frac{Y \cdot a^*_Y(\lambda_1) + C_0 \cdot a^*_0(\lambda_1)}{Y \cdot a^*_Y(\lambda_2) + C_0 \cdot a^*_0(\lambda_2)} = \frac{f \cdot \frac{b_b(\lambda_1)}{R(\lambda_1)} - a_W(\lambda_1) - b_b(\lambda_1)}{f \cdot \frac{b_b(\lambda_2)}{R(\lambda_2)} - a_W(\lambda_2) - b_b(\lambda_2)}. \tag{4.10}$$

Since all functions on the right-hand side of this equation are known, R_A can be calculated. Division of nominator and denominator of the center expression by C_0 leads to an equation which has as single unknown parameter the ratio Y/C_0. Rewriting this equation yields the following expression:

$$\frac{Y}{C_0} = \frac{R_A \cdot a^*_P(\lambda_2) - a^*_P(\lambda_1)}{a^*_Y(\lambda_1) - R_A \cdot a^*_Y(\lambda_2)}. \tag{4.11}$$

The ratio of Gelbstoff to phytoplankton concentration is calculated using this equation. It is a matter of optimisation to determine the best-suited wavelengths λ_1 and λ_2. By inserting $Y = (Y/C_0) \cdot C_0$ into eq. (4.9) and solving eq. (4.9) for C_0 the following expression is obtained:

$$C_0 = \frac{f \cdot \frac{b_b(\lambda_3)}{R(\lambda_3)} - a_W(\lambda_3) - b_b(\lambda_3)}{a^*_0(\lambda_3) + \frac{Y}{C_0} \cdot a^*_Y(\lambda_3)}. \tag{4.12}$$

Eq. (4.12) is used to calculate the phytoplankton concentration. It is a matter of optimisation to determine the best-suited wavelength λ_3. Gelbstoff concentration is then calculated using eq. (4.13) with the results from eqs. (4.11) and (4.12):

$$Y = \frac{Y}{C_0} \cdot C_0 . \tag{4.13}$$

It has been investigated how the accuracy of the ratio Y/C_0 and of the C_0 and Y values depends on the choice of the wavelengths λ_1, λ_2 and λ_3, on the errors of C_L determination from step 1 and on suspended matter concentration. The results of these studies are as follows:

- λ_1 should be chosen below 470 nm;
- λ_2 should be chosen below 500 nm;
- λ_3 should be chosen below 550 nm.

In each case, preference should be given to shorter wavelengths. A good choice is $\lambda_2 = \lambda_0$ since S errors don't affect Gelbstoff absorption at λ_0. For λ_3 no separate wavelength must be chosen, it can be set $\lambda_3 = \lambda_2$. Consequently, selection of only two wavelengths is implemented in WASI. Their defaults are: $\lambda_1 = 413$ nm, $\lambda_2 = 440$ nm.

Steps 3 and 4. These steps were suggested by Gege (2002). The newly developed steps 1 and 2 make them now unnecessary in most cases, but they are useful under certain conditions, for instance if no suitable infrared channel is available for accurate determination of C_L or C_S, or if S is fit parameter. Steps 3 and 4 improve the estimates for C_0, C_L, C_S and Y by including additional spectral information, and a start value of S can be determined. Wavelength range, data interval and maximum number of iterations for the fits of steps 3 and 4 are specified in the "Pre-fit" frames of the register card "Irradiance reflectance" of Fig. 4.9. If `max. Iterations` is set to 0 or 1, the respective fit is not performed.

Step 5. Wavelength range, data interval and maximum number of iterations for the fit of step 5 are specified in the "Final fit" register card of the "Fit tuning" pop-up window, see Fig. 4.7. The maximum number of iterations forces the fit routine to stop; the number should be set high enough that a forced stop is exceptional.

4.4.2 Irradiance reflectance of shallow water

Inversion of a shallow water irradiance reflectance spectrum determines in addition to the parameters of deep water several parameters related to the bottom: bottom depth z_B and areal fractions f_n of up to 6 bottom albedo spectra. The analytic function $R^{sh}(\lambda)$ used for inversion is given by eq. (2.16). Since it consists of as much as 21 parameters, it is very important to initialise the fit parameters with realistic values. Otherwise the probability is large that the Simplex gets lost in the high dimensional search space (up to 22 dimensions) and hence the fit provides completely wrong results. Albert (2004) developed the well-working methodology of Table 4.3 to increase step by step the number of estimated parameters, and he implemented it in WASI.

Step	determine	algorithm	Procedure
1	z_B	analytical	Determine a first estimate of z_B from an analytic equation at a wavelength interval in the red.
2	C_L, C_S	analytical	Determine a first estimate of C_L and C_S from an analytic equation at a wavelength in the Infrared using the z_B value from step 1.
3	$a_{WC}(\lambda)$	nested intervals	Estimate the total absorption spectrum of all water constituents for a wavelength interval in the visible using nested intervals. The required values of z_B, C_L and C_S are taken from steps 1 and 2.
4	C_0, Y	fit	Determine a first estimate of C_0 and Y by fitting the spectrum $a_{WC}(\lambda)$ of step 3.
5	f_n	f_n = 1/N	The areal fractions of all bottom types are set equal; N = number of considered bottom types.
6	C_L, C_S, Y, z_B	fit	Determine a second estimate of C_L, C_S, Y and z_B by fitting a wavelength interval in the infrared.
7	C_0, Y, S, z_B	fit	Determine a first estimate of S, a second of C_0, and a third of Y and z_B by fitting a wavelength interval in the blue.
8	All parameters	fit	All fit parameters are fitted.

Table 4.3: Procedure for inversion of irradiance reflectance spectra of shallow water.

Fine-tuning of steps 1, 2, 4, 6, and 7 is done in the "Irradiance reflectance" register card of the "Fit tuning" pop-up window. It is shown in Fig. 4.10. Steps 1 and 2 are performed if the check boxes "Analytic estimate of ..." are marked with a hook. Otherwise the initial values from the parameter list or from the previous fit are taken, as described in section 4.2.2. Steps 4, 6 and 7 are tuned in the "Pre-fit" frames. The pre-fits are performed if "max. iterations" is set to a value larger than 1. At step 8 the user can define the wavelength range to be fitted, the intervals between data points, and the maximum number of iterations. The relevant user interface is shown in Fig. 4.7.

Step 1. The equation (2.16), which parameterises irradiance reflectance of shallow water, is simplified by setting $K_{uW}(\lambda) = K_{uB}(\lambda) = K_d(\lambda)$. The resulting equation,

$$R^{sh}(\lambda) = R(\lambda) - A_1 \cdot R(\lambda) \cdot \exp\{-2K_d(\lambda) \cdot z_B\} + A_2 \cdot R^b(\lambda) \cdot \exp\{-2K_d(\lambda) \cdot z_B\}, \quad (4.14)$$

is solved for z_B:

$$z_B = \frac{1}{2K_d(\lambda)} \ln \frac{A_1 \cdot R(\lambda) - A_2 \cdot R^b(\lambda)}{R(\lambda) - R^{sh}(\lambda)}. \quad (4.15)$$

Various simulations were performed to study the accuracy of this equation depending on wavelength and on errors of concentration and bottom type (Albert 2004). The wavelength interval 600–650 nm was found to be best-suited, thus it is used by default in WASI. By averaging the z_B values of that interval, an accuracy of z_B of typically 20–40 % can be expected at moderate suspended matter concentration (< 10 mg/l) and z_B < 10 m. Such accuracy is sufficient to initialise z_B.

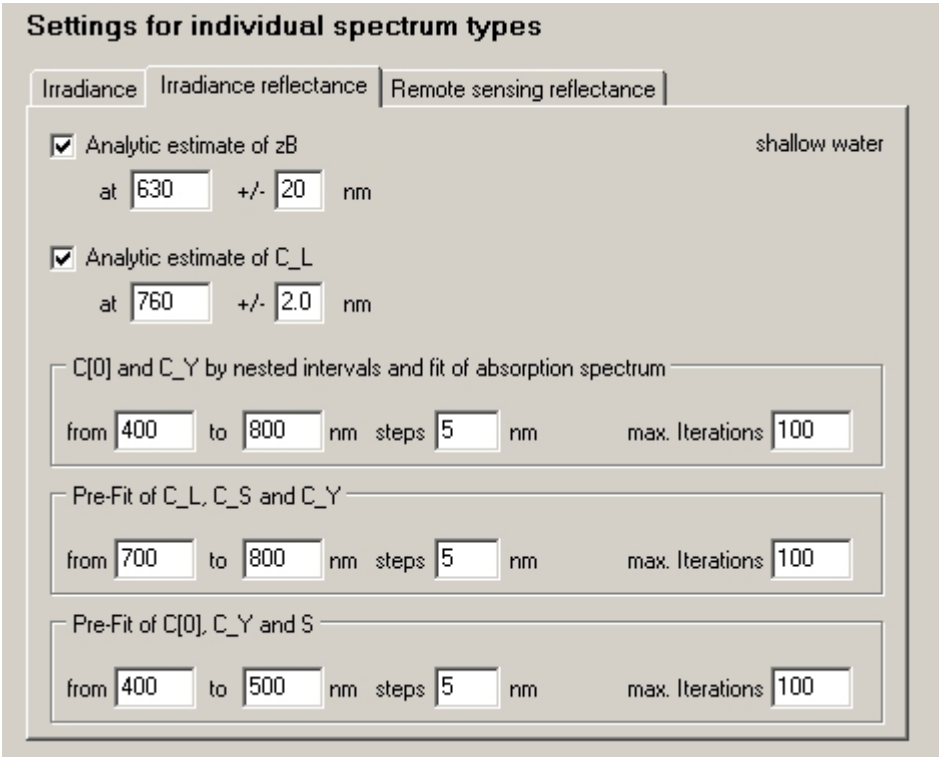


Fig. 4.10: The register card "Irradiance reflectance" for shallow water of the pop-up window "Fit tuning".

Step 2. Like in the deep water case, an analytic approximation of the reflectance spectrum is solved for suspended matter backscattering $B_0 \equiv b_b(\lambda) - b_{b,W}(\lambda)$ to obtain an analytic equation for B_0. The analytic approximation of the reflectance spectrum is given by eq. (4.14) in which $R(\lambda)$ is replaced by eq. (4.1a). Solving this equation for B_0 yields:

$$B_0 = \frac{\Re^0(\lambda)\cdot\left[a(\lambda)+b_{b,W}(\lambda)\right]-b_{b,W}(\lambda)}{1-\Re^0(\lambda)}, \tag{4.16}$$

where

$$\Re^0(\lambda) = \frac{1}{f}\cdot\frac{R^{sh}(\lambda)-A_2\cdot R^{b}(\lambda)\cdot\exp\{-2K_d(\lambda)\cdot z_B\}}{1-A_1\cdot\exp\{-2K_d(\lambda)\cdot z_B\}}. \tag{4.17}$$

The conversion from optical units B_0 to gravimetric units C_L, C_S uses eq. (4.8a) or (4.8b), as for deep water.

Simulations of Albert (2004) showed that for $z_B > 2$ m the accuracy is typically better than 20 % for $C_L + C_S < 5$ mg/l and better than 40 % for $C_L + C_S < 25$ mg/l if 760 nm is taken as reference wavelength, which is used as default in WASI. Such accuracy is sufficient for initialising C_L and C_S.

Step 3. Because eq. (4.14) cannot be solved analytically for C_0 and Y, an intermediate step is required to estimate the total absorption of all water constituents, a_{WC}. This is done iteratively by the method of nested intervals, which is described in the following.

At wavelengths of non-negligible absorption of water constituents the values of R and K_d depend on a_{WC}. When R is calculated using eq. (4.1a) and K_d using eq. (2.5), values for b_b and a

have to be assigned first. b_b is calculated using eq. (2.4); for its critical parameters C_L and C_S the values from step 2 are taken. a is calculated using eq. (2.3); the value of a_{WC} in that equation is treated as unknown and determined iteratively as follows. In the first step R and K_d are calculated using a start value A_0 for a_{WC} in eq. (2.3), and with these R and K_d values $R^{sh}{}_0$ is calculated using eq. (4.14). In the next steps A_0 is replaced in a systematic way with different A_i values until one of the following stop criteria is reached: (1) the ratio $\delta = R^{sh}{}_i / R^{sh} - 1$, which is a measure of the deviation between calculated value $R^{sh}{}_i$ and measurement R^{sh}, is below a threshold δ_{min}; (2) the number of iterations exceeds a threshold i_{max}. The rule for calculating A_{i+1} from A_i is as follows:

$$A_{i+1} = \begin{cases} A_i + \dfrac{\Delta}{i} & \text{if } \delta < 0 \\ A_i - \dfrac{\Delta}{i} & \text{if } \delta > 0 \end{cases} \tag{4.18}$$

The value of the last iteration, A_{i+1}, is assigned to a_{WC}. These iterations are performed wavelength for wavelength. The wavelength range 400–800 nm and a wavelength interval of 5 nm were found suitable, thus these are used by default in WASI. As a result an estimate of the spectrum $a_{WC}(\lambda)$ is obtained. $A_0 = 5\ m^{-1}$, $\Delta = 1\ m^{-1}$, $\delta_{min} = 0.01$ and $i_{max} = 100$ are set as defaults in WASI. Wavelength range, wavelength interval, and i_{max} can be changed in the frame labeled "C[0] and C_Y by nested intervals and fit of absorption spectrum" of Fig. 4.10. A_0, Δ, and δ_{min} can be changed by editing the WASI.INI file.

Step 4. A first estimate of the two parameters C_0 and Y is determined by fitting the spectrum $a_{WC}(\lambda)$ from step 3 with the Simplex algorithm using eq. (2.1). The parameters $C_1 \ldots C_5$ and X of eq. (2.1) are set to zero in this step. For wavelength range, wavelength interval, and i_{max} the same values are taken as in step 3.

Step 5. The areal fractions f_n of all those bottom types are set equal which are marked as fit parameters.

Steps 6 and 7. These steps can be tuned by the parameters in the two "Pre fit …" frames of Fig. 4.10.

Step 8. Wavelength range, data interval and maximum number of iterations are specified in the "Final fit" register card of the "Fit tuning" pop-up window, see Fig. 4.7. The maximum number of iterations forces the fit routine to stop; the number should be set high enough that a forced stop is exceptional.

4.4.3 Remote sensing reflectance of deep water

The remote sensing reflectance of deep water above the surface, $R_{rs}(\lambda)$, is calculated using eq. (2.20a), (2.20b) or (2.20c); that below the surface, $R_{rs}^-(\lambda)$, according to eq. (2.17a) or (2.17b). $R_{rs}(\lambda)$ has 25 parameters which may be fitted, $R_{rs}^-(\lambda)$ has 15. This high number of fit parameters makes fit tuning necessary. In particular it is important to find suitable start values of the parameters, i.e. to start with initial values which are not too different from the final results. The user interface for controlling fit tuning is shown in Fig. 4.11. It is accessed from the menu bar via "Options - Invers calculation - Fit tuning".

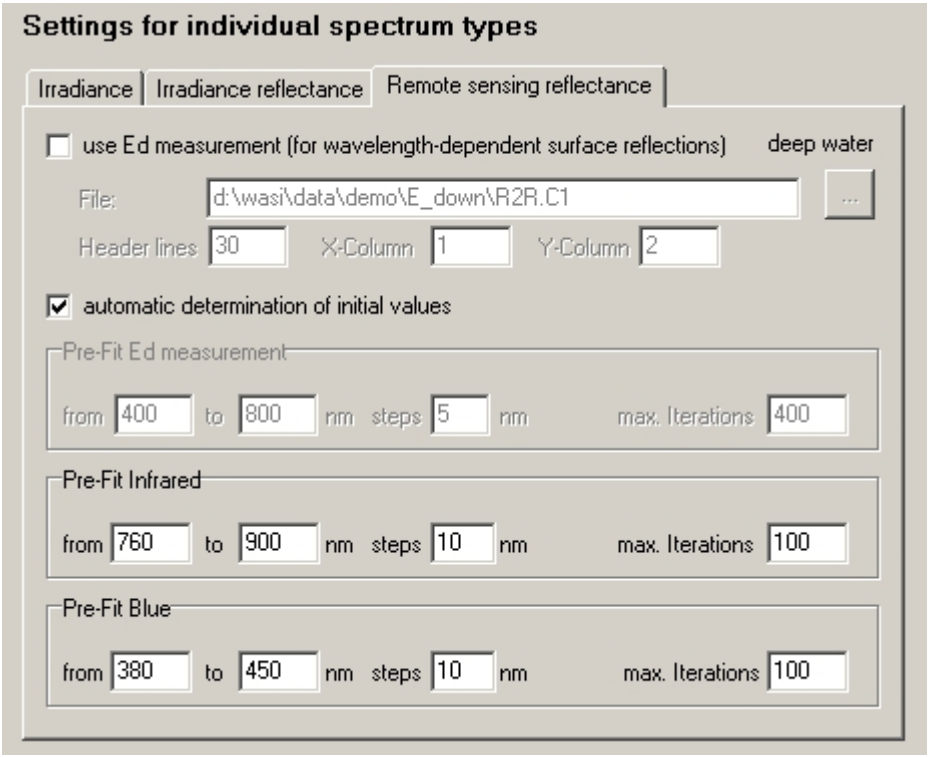


Fig. 4.11: The register card "Remote sensing reflectance" for deep water of the pop-up window "Fit tuning".

If a downwelling irradiance measurement is available, the number of fit parameters for $R_{rs}(\lambda)$ can be reduced by 4 (α, β, γ, δ). In this case the box "use Ed measurement" should be marked with a hook, and the measured spectrum has to be specified.

Most of the initial values are taken from the parameter list in the main window. However, for some parameters an automatic determination is possible: for α, β, γ, δ if an Ed measurement is available, for C_L and σ_L from a pre-fit in the Infrared, and for C_0, Y, S and Q from a pre-fit in the Blue. For doing so, the box "automatic determination of initial values" has to be marked with a hook. Subsequently, the wavelength intervals, steps and maximum number of iterations have to be specified for each pre-fit. If "max. Iterations" is set to 0 or 1, the corresponding pre-fit is not performed.

4.4.4 Remote sensing reflectance of shallow water

For inversion of remote sensing reflectance spectra also the 8 steps of Table 4.3 are performed. The only difference to the case of irradiance reflectance is that all R spectra are replaced by the corresponding R_{rs} spectra.

4.4.5 Downwelling irradiance

The downwelling irradiance above the water surface, $E_d(\lambda)$, is calculated according to eq. (2.1) as a weighted sum of 4 spectra. Since the curve forms of these spectra are quite different, it is not possible to obtain similar sum curves by using rather different sets of weights. In other words, the solution of the inversion is unequivocal. Consequently, no fine-tunig of the inversion scheme is necessary.

The downwelling irradiance below the water surface, $E_d^-(\lambda)$, is calculated according to eq. (2.4) using the above-water spectrum $E_d(\lambda)$. For $E_d(\lambda)$ either the parameterization of eq. (2.1) can be chosen, or a measured spectrum can be taken. The selection is done in the register card "Irradiance" of the pop-up window "Fit tuning", which is shown in Fig. 4.12. It is accessed from the menu bar via "Options - Invers calculation - Fit tuning".

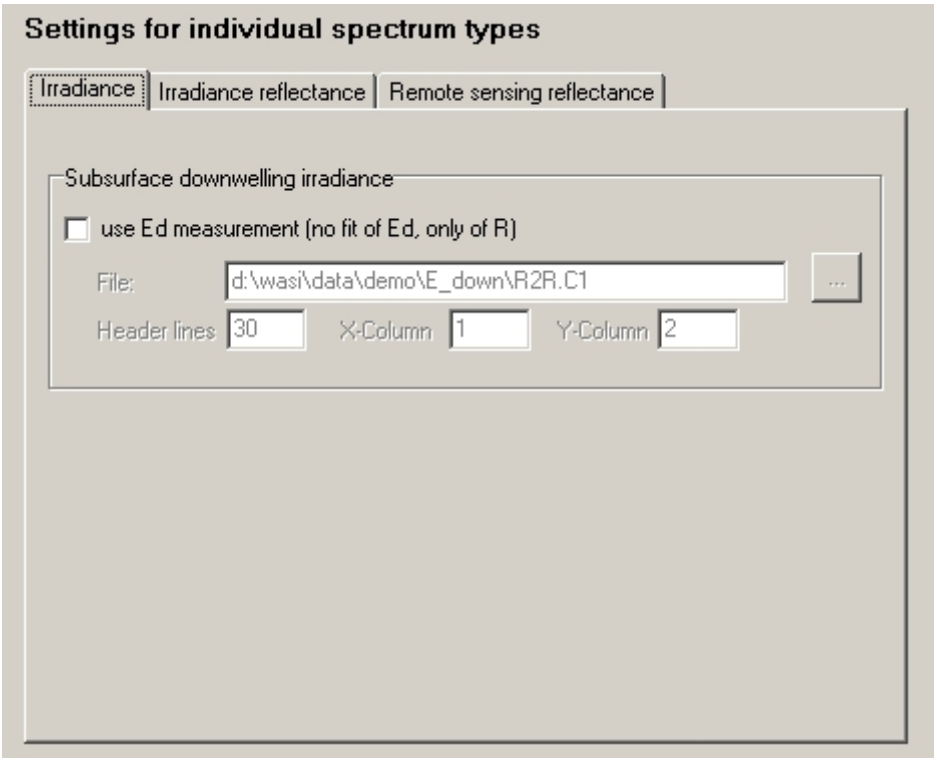


Fig. 4.12: The register card "Irradiance" of the pop-up window "Fit tuning".

Downwelling irradiance spectra below the water surface are not very different from those above the surface, i.e. the curve form of $E_d^-(\lambda)$ depends much more on the parameters of $E_d(\lambda)$ than on those of $R(\lambda)$. Hence small errors of $E_d(\lambda)$ cause large errors of the retrieved parameters of $R(\lambda)$. Thus the option of using $E_d(\lambda)$ measurements for fitting $E_d^-(\lambda)$ must be applied with care; in general it should not be used.[6]

[6] The option has been included for consistency reasons: $E_d(\lambda)$ measurements are useful for inversion of upwelling radiance and specular reflectance spectra.

5. Reconstruction mode

The reconstruction mode is a combination of forward and inverse mode: A spectrum is calculated in the forward mode, and subsequently this spectrum is fitted in the inverse mode. The model parameters of the forward calculation are stored together with the fit parameters of the inversion in one file; the spectrum may be saved or not. Analogously to the forward mode, up to three parameters can be iterated simultaneously. Parameters of the forward mode and of the inverse mode can be chosen differently. The mode is called reconstruction mode because inversion reconstructs model parameters of the forward mode at altered conditions. It is useful for sensitivity studies.

5.1 Definition of parameter values

Initial values of each fit parameter are read from the WASI.INI file. The user can change them most conveniently in the parameter list at the left side of the main window (or alternatively in the "Fit parameters" pop-up window, see Fig. 4.4). An example is shown in Fig. 5.1.

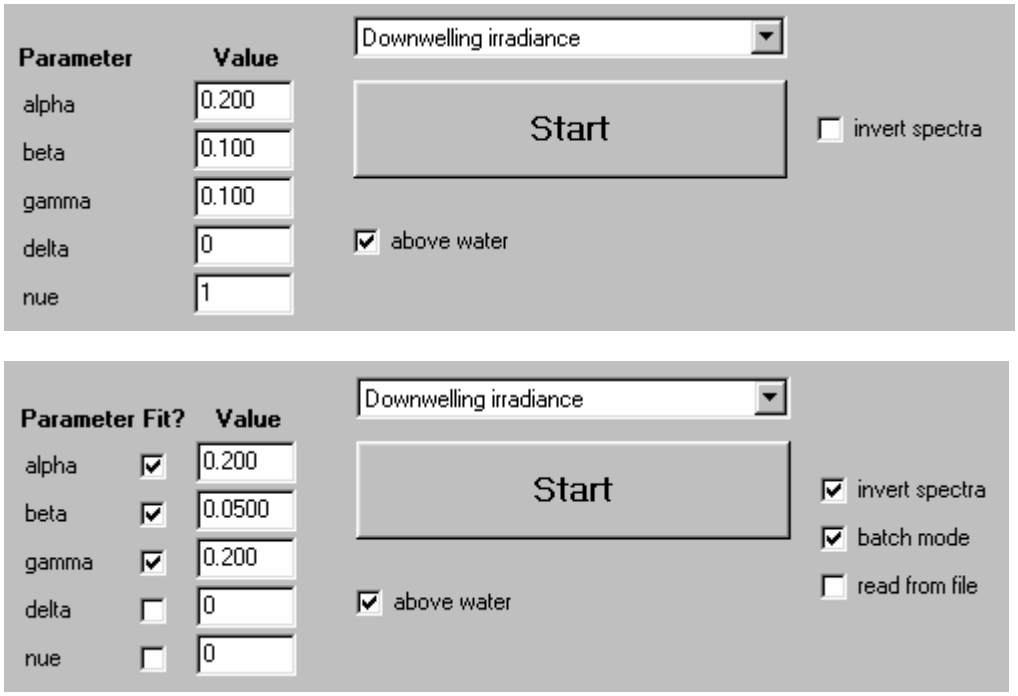


Fig. 5.1: Example of a parameter list. Top: values of forward modeling; bottom: start values of inversion.

By clicking the "invert spectra" check box, the user can quickly switch between the forward and inverse values. Fig. 5.1 shows as an example the parameter list of the downwelling irradiance model above the water surface. On top the forward values are shown, on bottom the start values of the inverse mode. The forward and inverse values are chosen identical for two parameters (alpha, delta), and differently for three other parameters (beta, gamma, nue).

Fig. 5.1 is an example how to study propagation of model errors. A different value of the parameter nue is chosen for forward and inverse calculation, and nue is not fitted. This is an efficient way to introduce a well-defined model error: the error of the inverse model is attributed to the parameter nue, and the error is given quantitatively as $nue^{wrong} - nue^{correct} = 0 - 1$.

Due to the wrong nue value, the fit cannot find the correct values of the fit parameters alpha, beta, gamma. The errors of these parameters depend only on the nue error. In this way, the sensitivity of alpha, beta, gamma on nue errors can be studied. Systematic investigations of such error propagation are the basis of sensitivity studies.

Error propagation can be investigated systematically by iterating the erroneous model parameter during forward calculation. The way to do this is explained in section 3.3.2. Fig. 5.2 shows as example how to study systematically the errors caused by wrong values of the parameter nue: nue is iterated from -1 to 1 in 11 steps. Thus, 11 spectra are calculated in the forward mode with nue values of -1, -0.8, ..., 1, and these spectra are subsequently fitted. If nue is fixed during inversion like in Fig. 5.1, a series of inversion results is obtained for a systematically changing error of the parameter nue.

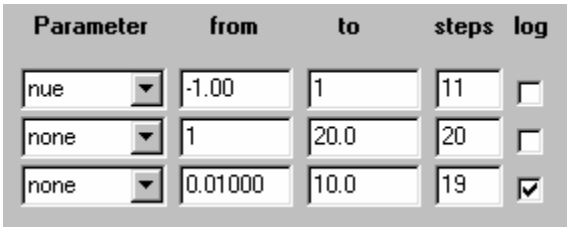


Fig. 5.2: Iteration of the parameter nue.

5.2 Definition of output information

The results of fitting a series of spectra are stored in a single file, `FITPARS.TXT`. Fig. 5.3 shows as an example a listening of this file for the settings of Figs. 5.1 and 5.2. The first lines explain the file content and summarize relevant information.

The first column of the data block of the file `FITPARS.TXT`, headed "File", lists the file names of the calculated spectra. Whether the spectra are saved or not, decides the user. As sensitivity

```
This file was generated by the program WASI
Version 2.4 - Latest update: 6 July 2004

List of fitted parameters which may differ from one spectrum to the next
Common parameter set of all spectra in file: WASI.INI
Errors are given in %: error = 100*(inv/fwd-1)

             fwd  Inversion                 inv      inv      inv    error    error    error
    File     nue Iterations   Residuum    alpha     beta    gamma    alpha     beta    gamma

     B01   -1.000        105      0.166    0.186   0.0741    0.146    -7.00    -25.9     46.0
     B02  -0.8000        111      0.129    0.189   0.0794    0.136    -5.50    -20.6     36.0
     B03  -0.6000        112     0.0957    0.192   0.0845    0.126    -4.00    -15.5     26.0
     B04  -0.4000        114     0.0654    0.195   0.0895    0.117    -2.50    -10.5     17.0
     B05  -0.2000        118     0.0383    0.197   0.0945    0.108    -1.50    -5.50     8.00
     B06 -5.551E-17      103     0.0147    0.199   0.0993   0.0998   -0.500   -0.700   -0.200
     B07   0.2000         99     0.0103    0.201    0.104   0.0919    0.500     4.00    -8.10
     B08   0.4000        110     0.0281    0.203    0.109   0.0844     1.50     9.00    -15.6
     B09   0.6000        111     0.0444    0.204    0.113   0.0773     2.00     13.0    -22.7
     B10   0.8000        142     0.0585    0.206    0.118   0.0705     3.00     18.0    -29.5
     B11        1         96     0.0703    0.207    0.123   0.0641     3.50     23.0    -35.9

   mean= -6.056E-17      111    0.06557   0.1981  0.09894   0.1019     2.86     13.2     22.3
    max=   -1.000        142     0.1663   0.2070   0.1230   0.1460    -7.00    -25.9     46.0
```

Fig. 5.3: Example of the output file FITPARS.TXT.

studies are generally based on a large number of spectra, usually not all spectra are saved, but only a few for illustration purposes. Thus, a study may be performed in two steps: in the first step, the parameters of interest are iterated over the interesting ranges with few steps, and the resulting spectra are saved; in the second step, the calculations of step 1 are repeated, but with much more steps, and without saving the spectra. How to save forward calculated spectra is described in sections 3.2.4 and 3.3.3, the corresponding pop-up window is shown in Fig. 3.2. How to save fit spectra is described in section 4.3.1. How the directories are selected is described in section 7.1, the corresponding pop-up window is shown in Fig. 7.2.

The second column of the data block lists the values of the parameter which is iterated during forward calculation. The abbreviation "fwd" in the heading of this column means "value of forward calculation", the heading's second line specifies the parameter name. If more than one parameter is iterated, similar columns are added. In the example of Fig. 5.3, 11 values of the parameter nue (-1.000, -0.800, ..., 1) were taken for forward calculation. Since the other model parameters were hold constant for the series of forward calculations, these are not included in this file; their values are documented in the WASI.INI file, as indicated in the header information.

All subsequent columns summarize the results which were obtained by fitting the forward calculated spectra. The column headed "Inversion Iterations" shows the required number of iterations of the fit routine (see 4.2.4). The next column, "Residuum", lists the residuals, which are a measure for the correspondence between the forward calculated spectrum and the fit curve (see 4.2.3.1). The next columns tabulate the resulting values of the fit parameters. The abbreviation "inv" in their heading means "value of inverse calculation", the heading's second line specifies the parameter name. Each parameter, for which in the parameter list the corresponding check box "Fit?" is marked with a hook, is represented by such a column. In the example of Fig. 5.3 these are the parameters alpha, beta, gamma.

The specific results of the reconstruction mode are tabulated in the last colums. These columns, labeled "error" and headed by parameter names, list the relative errors of user-selected parameters. The selection which parameters to tabulate, is done in the pop-up window "Reconstruction mode settings", which is shown in Fig. 5.4. This window is accessed from the menu bar via "Options – Reconstruction mode", see Fig. 7.1. The relative errors are calculated as 100 * (inv/fwd – 1), where "inv" is the fit result of inverse modeling and "fwd" is the parameter value used during forward calculation. Hence, the relative errors are the fit parameter's deviations from the "true" values in percent.

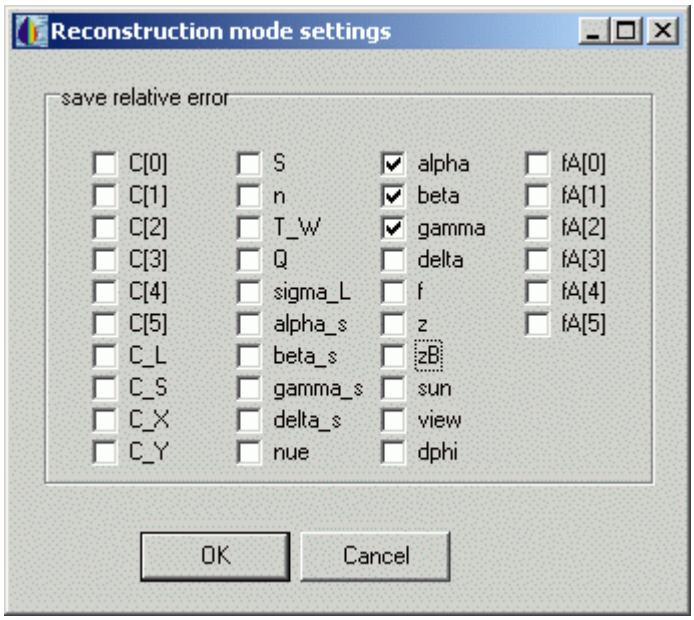


Fig. 5.4: The pop-up window "Reconstruction mode settings".

6. Model options

6.1 Downwelling irradiance

The spectrum type "Downwelling irradiance" is activated by selecting in the main window "Downwelling irradiance" from the drop-down list above the "Start" button, see Fig. 6.1 left. After the spectrum type is selected, the check box "above water" is displayed, and the according parameter list. If "above water" is selected, the parameter list shown in the center of Fig. 6.1 is displayed, otherwise the right one.

The above-water calculation is done using eq. (2.1), which requires the parameters α = alpha, β = beta, γ = gamma, δ = delta, ν = nue. The below-water calculation is done using eq. (2.4), which requires additionally the parameters of the irradiance model.

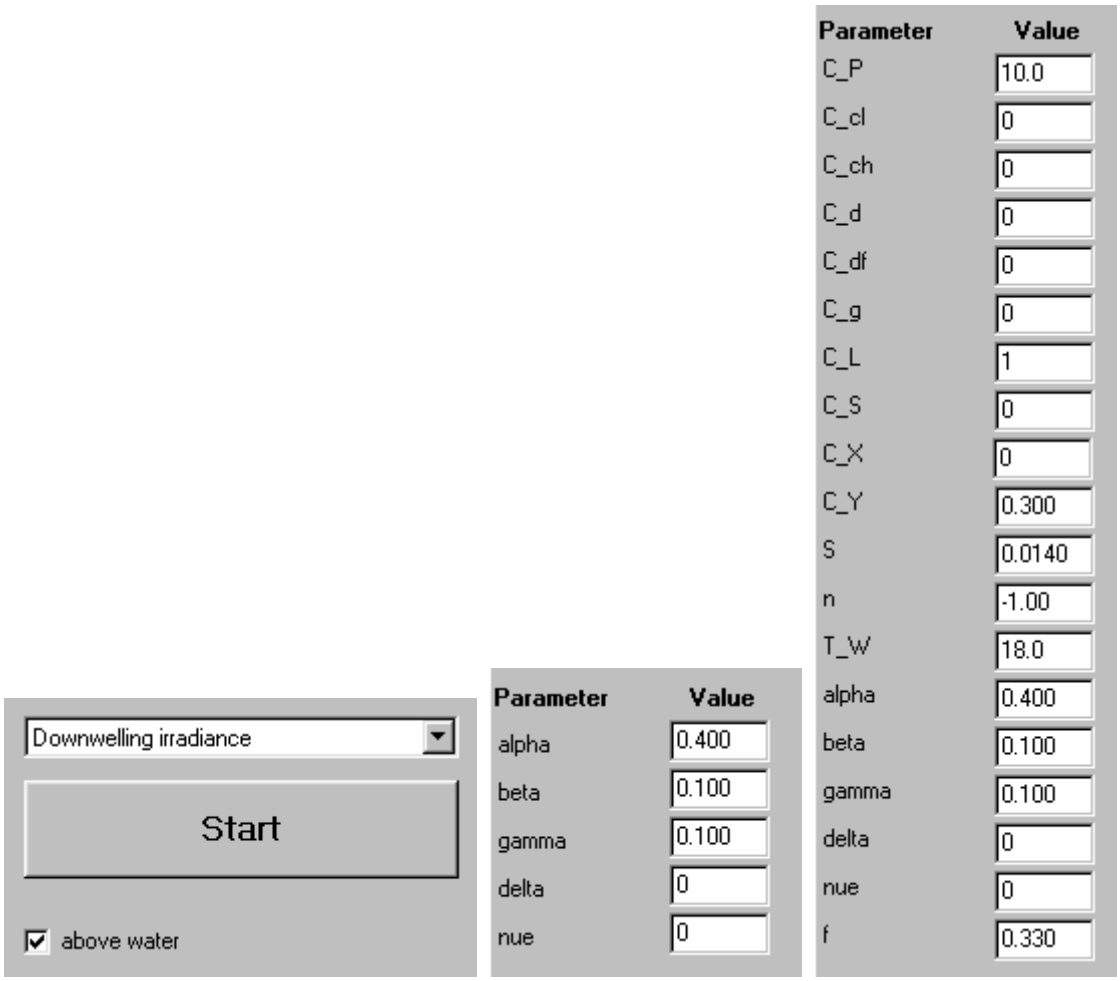


Fig. 6.1: Settings of the spectrum type "Downwelling irradiance" in the main window. Left: Drop-down list with "Downwelling irradiance" selected as spectrum type and "above water" check box. Center: Parameter list for above-water calculation. Right: Parameter list for in-water calculation.

6.2 Irradiance reflectance

The spectrum type "Irradiance reflectance" is activated by selecting this type in the main window from the drop-down list above the "Start" button, see Fig. 6.2 left. After the spectrum type is selected, one of the two parameter lists shown in Fig. 6.2 is displayed: if the check box "shallow water" below the "Start button" is not marked, the short list is displayed (Fig. 6.2 center), otherwise the long list is displayed (Fig. 6.2 right). Only 25 of the 36 parameters of the shallow water model can be displayed simultaneously; for displaying the hidden parameters, the scroll bar to the right of the "Value" fields has to be moved up- or downwards.

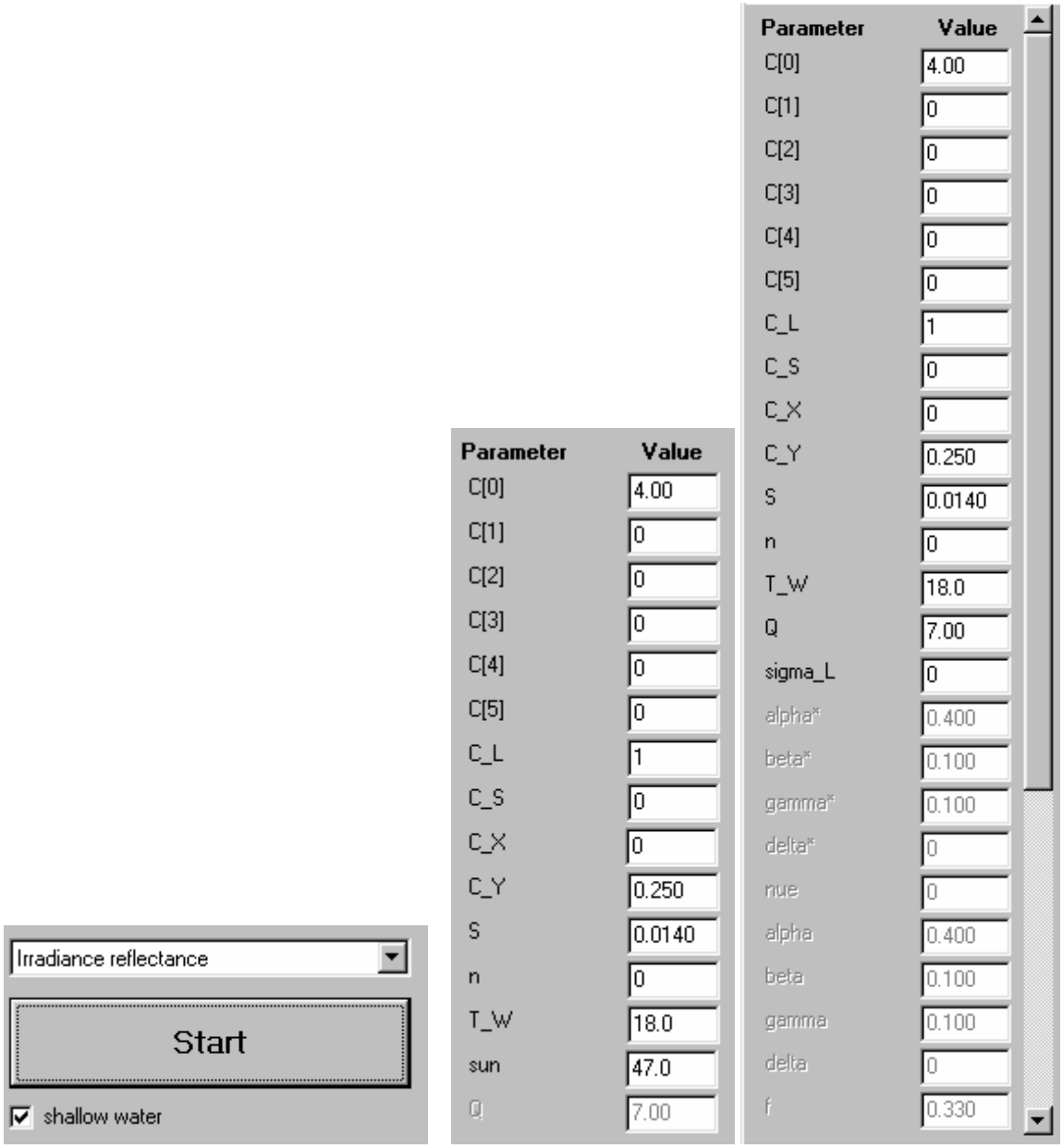


Fig. 6.2: Settings of the spectrum type "Irradiance reflectance" in the main window. Left: Drop-down list with "Irradiance reflectance" selected as spectrum type. Center: Parameter list of the deep-water model. Right: Parameter list of the shallow-water model.

Irradiance reflectance spectra R(λ) are calculated using the Gordon algorithm, see eq. (2.14a), or the Prieur algorithm, see eq. (2.14b). Both algorithms parameterize R(λ) as a function of absorption and backscattering and thus require as parameters the concentrations of the differ-

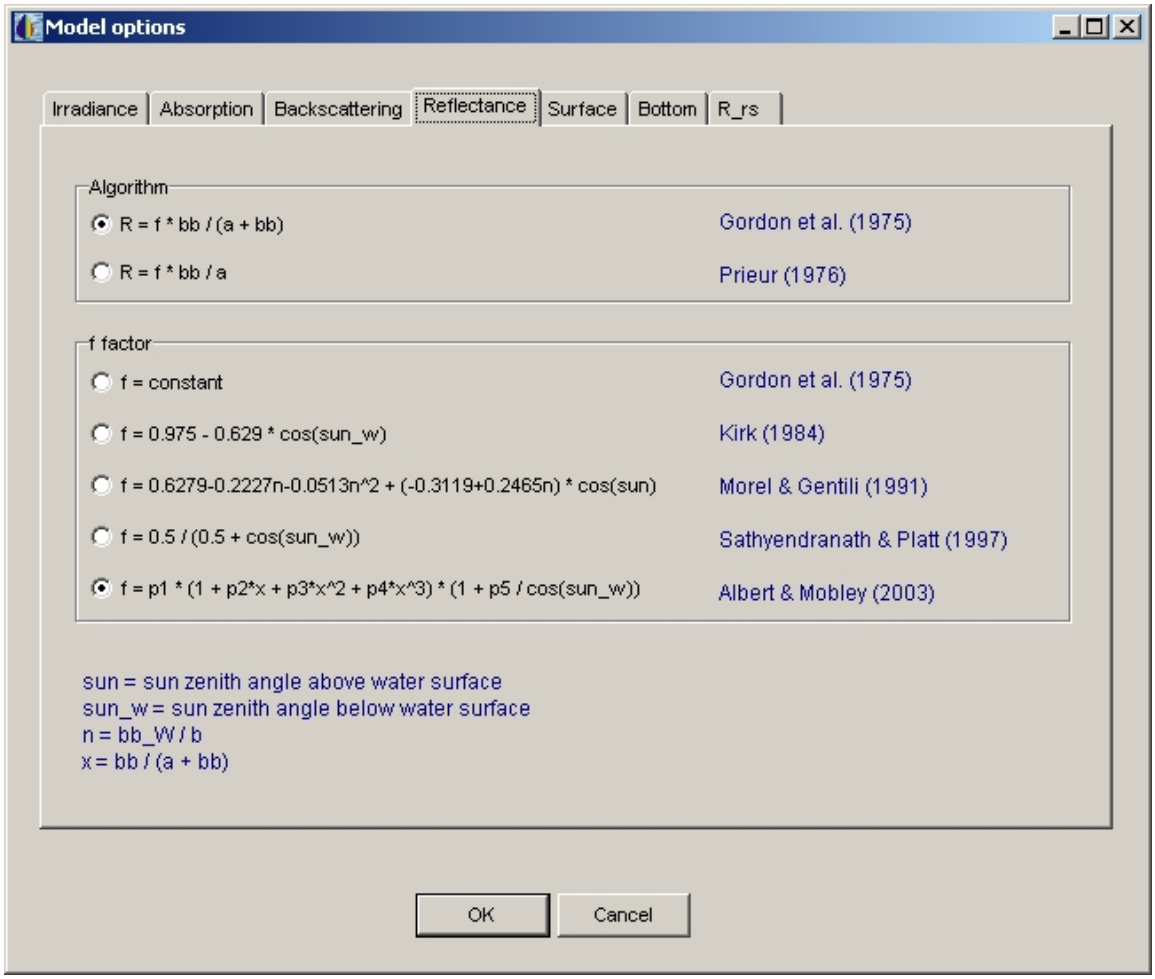


Fig. 6.3: The register card "Reflectance" of the pop-up window "Model options".

ent phytoplankton classes (C_i = C[i], i = 0, 1, ..., 5), of large (C_L = C_L) and small (C_S = C_S) suspended particles, of non-chlorophyllous particles (X = C_X) and of Gelbstoff (Y = C_Y), and the Angström exponent (n), water temperature (T = T_W), proportionality factor (f), and eventually Gelbstoff exponent (S). f can either be treated as a parameter, or it can be calculated as a function of absorption, backscattering and the sun zenith angle.

R algorithm and f calculation method are selected in the "Reflectance" register card of the "Model options" pop-up window, which is shown in Fig. 6.3. The pop-up window is accessed from the menu bar via "Options – Models".

The factor of proportionality, f, depends on the scattering properties of the water and on the illumination geometry. In WASI, f can either be treated as a parameter, or it can be calculated using one of the following algorithms:

$$f = 0.975 - 0.629 \cdot \cos \theta'_{sun} \tag{6.1}$$

$$f = 0.6279 - 0.2227 \cdot \eta_b - 0.0513 \cdot \eta_b^2 + (-0.3119 + 0.2465 \cdot \eta_b) \cdot \cos \theta_{sun} \tag{6.2}$$

$$f = \frac{0.5}{0.5 + \cos \theta_{sun}} \tag{6.3}$$

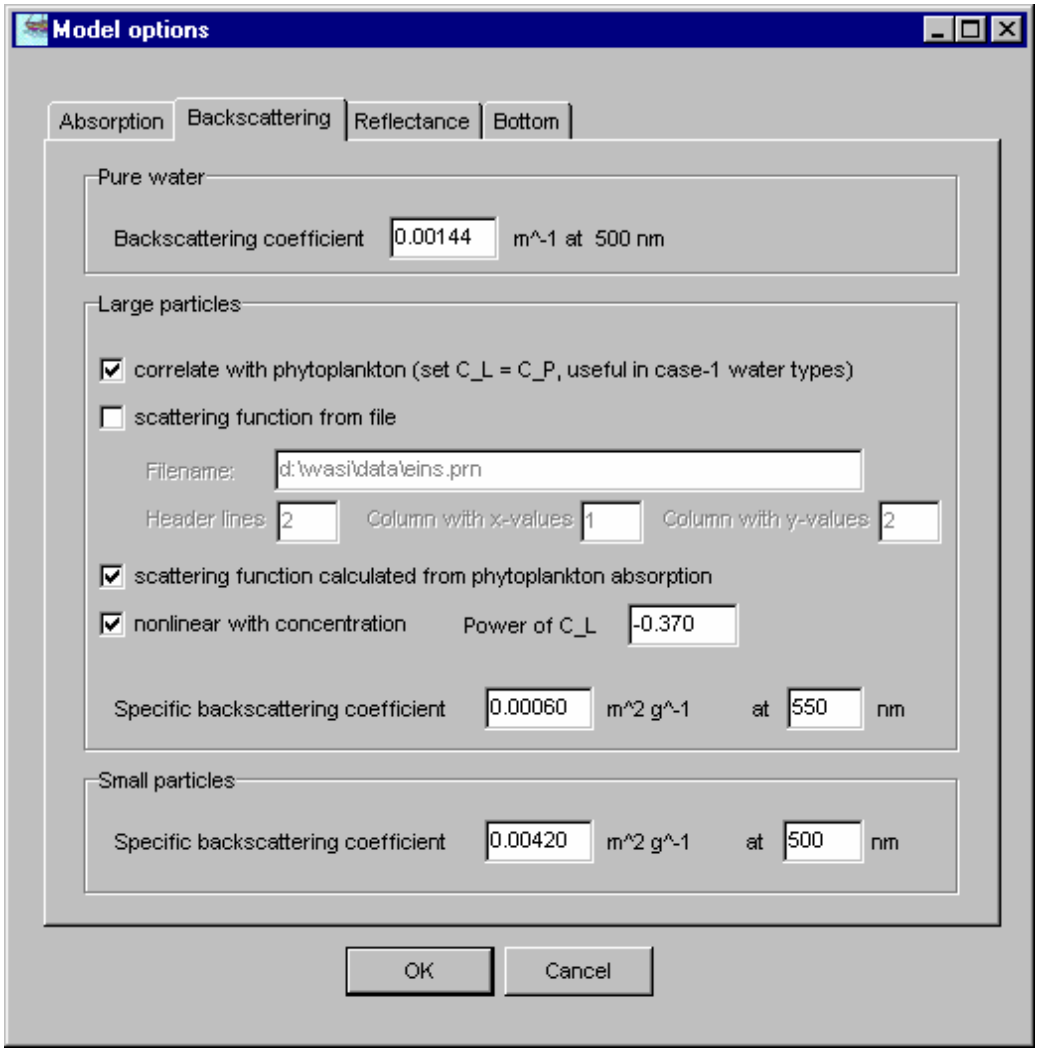


Fig. 6.4: The register card "Backscattering" of the pop-up window "Model options". The settings are not the default settings of WASI; they correspond to the model of Sathyendranath et al. (1989).

$$f = 0.1034 \cdot (1 + 3.3586 \cdot x - 6.5358 \cdot x^2 + 4.6638 \cdot x^3) \cdot (1 + \frac{2.4121}{\cos \theta'_{sun}}). \qquad (6.4)$$

Equation (6.1) is taken from Kirk (1984), (6.2) from Morel and Gentili (1991), (6.3) from Sathyendranath and Platt (1997), and (6.4) from Albert and Mobley (2003). θ_{sun} is the sun zenith angle above the water surface, θ'_{sun} below the surface. The factor η_b in eq. (6.2) is the ratio $b_{b,W}/b_b$. The factor x in eq. (6.4) is $b_b/(a+b_b)$ for the Gordon algorithm and b_b/a for the Prieur algorithm.

The options for calculating absorption are described in section 6.3. Those for calculating backscattering are set in the register card "Backscattering" of the pop-up window "Model options", see Fig. 6.4.

Backscattering by large particles

In Fig. 6.4 the box "correlate with phytoplankton" determines whether C_L of eq. (2.15) is treated as an independent parameter (no hook), or if $C_L = C_0$ is set, with $C_0 = C[0]$ denoting phytoplankton concentration (hook). In case-1 water types suspended matter is highly corre-

lated with phytoplankton, hence it is suggested to mark the box for case-1 waters, but not for case-2 waters.

The boxes "scattering function from file" and "scattering function calculated from phytoplankton absorption" are exclusive, i.e. exact one of both is marked with a hook. They determine how the function $b_L(\lambda)$ of eq. (2.15) is selected: it is either read from file ("scattering function from file" is marked) or it is calculated from the specific absorption spectrum of phytoplankton (the other box is marked). Calculation is useful when suspended matter and phytoplankton are highly correlated, i.e. for case-1 waters, otherwise a spectrum independent from phytoplankton should be taken. If no information about the spectral dependency of backscattering by large particles is available, it is a good idea to use a constant function $b_L(\lambda) = 1$. This provides good results for instance in Lake Constance (Heege 2000). By default, $b_L(\lambda) = 1$ is read from the file `eins.prn`. For reading another file, the WASI.INI file must be changed accordingly.

The box "nonlinear with concentration" determines whether the specific backscattering coefficient $b_{b,L}^*$ of eq. (2.15) is treated as constant (no hook), or if it is calculated as $A \cdot C_L^B$ (hook). B is the value in the input field "Power of C_L", which is visible only in the nonlinear case. The value in the input field "Specific backscattering coefficient" corresponds to $b_{b,L}^*$ in the linear case, and to A in the nonlinear case. The "at ... nm" input field of Fig. 6.4 specifies the wavelength where the specific backscattering coefficient is valid. After a scattering function is read from file or calculated from phytoplankton absorption, it is normalized at that wavelength.

Backscattering by small particles

The value in the input field "Specific backscattering coefficient" of the "Small particles" section of Fig. 6.4 corresponds to $b_{b,S}^*$ of eq. (2.15). The "at ... nm" input field specifies the wavelength λ_S of eq. (2.15).

6.3 Absorption

The spectrum type "Absorption" is activated by selecting in the main window "Absorption" from the drop-down list above the "Start" button, see Fig. 6.5 left. After the spectrum type is set to "Absorption", the check box "include pure water" (Fig. 6.5 left) and the parameter list shown in Fig. 6.5 right are displayed.

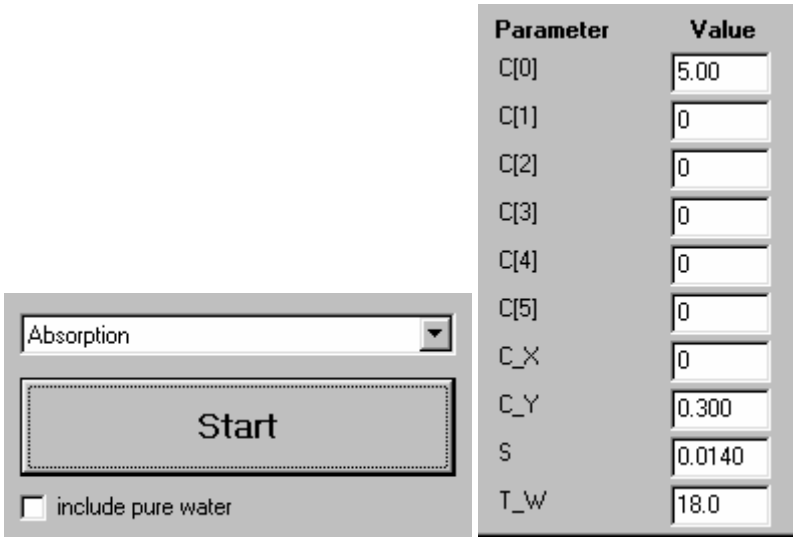


Fig. 6.5: Settings of the spectrum type "Absorption" in the main window. Left: Drop-down list with "Absorption" selected as spectrum type and "include pure water" check box. Right. Parameter list.

The spectrum type "Absorption" supports two options: include or exclude pure water absorption. If pure water absorption is included (check box is marked with a hook), the absorption spectrum of the water body is calculated using eq. (2.3). Otherwise (no hook) absorption of the water constituents alone is calculated using eq. (2.1).[7]

Parameters of the absorption model are the concentrations of the 6 phytoplankton classes (C_i = C[i], i = 0, 1, ..., 5), the concentration of non-chlorophyllous particles (X = C_X), Gelbstoff concentration (Y = C_Y), and eventually Gelbstoff exponent (S) and water temperature (T = T_W). T is model parameter if pure water absorption is included; it is not required for calculating absorption of the water constituents.

Whether S is model parameter or not depends on the choice of the specific Gelbstoff absorption spectrum $a_Y^*(\lambda)$. It can either be read from file, or it can be calculated during run-time using eq. (2.2). The selection is done in the "Absorption" register card of the pop-up window "Model options", which is shown in Fig. 6.6. The corresponding boxes "exponential function" and "specific absorption from file" are exclusive, i.e. exact one of both is marked with a hook. The input field "Normalize absorption spectrum at ... nm" specifies the wavelength λ_0 where $a_Y^*(\lambda)$ is normalised.

[7] Most spectrum types included in WASI depend on the absorption of the water body. For all types which use absorption implicitely, the absorption spectrum includes pure water, i.e. absorption is calculated according to eq. (2.3).

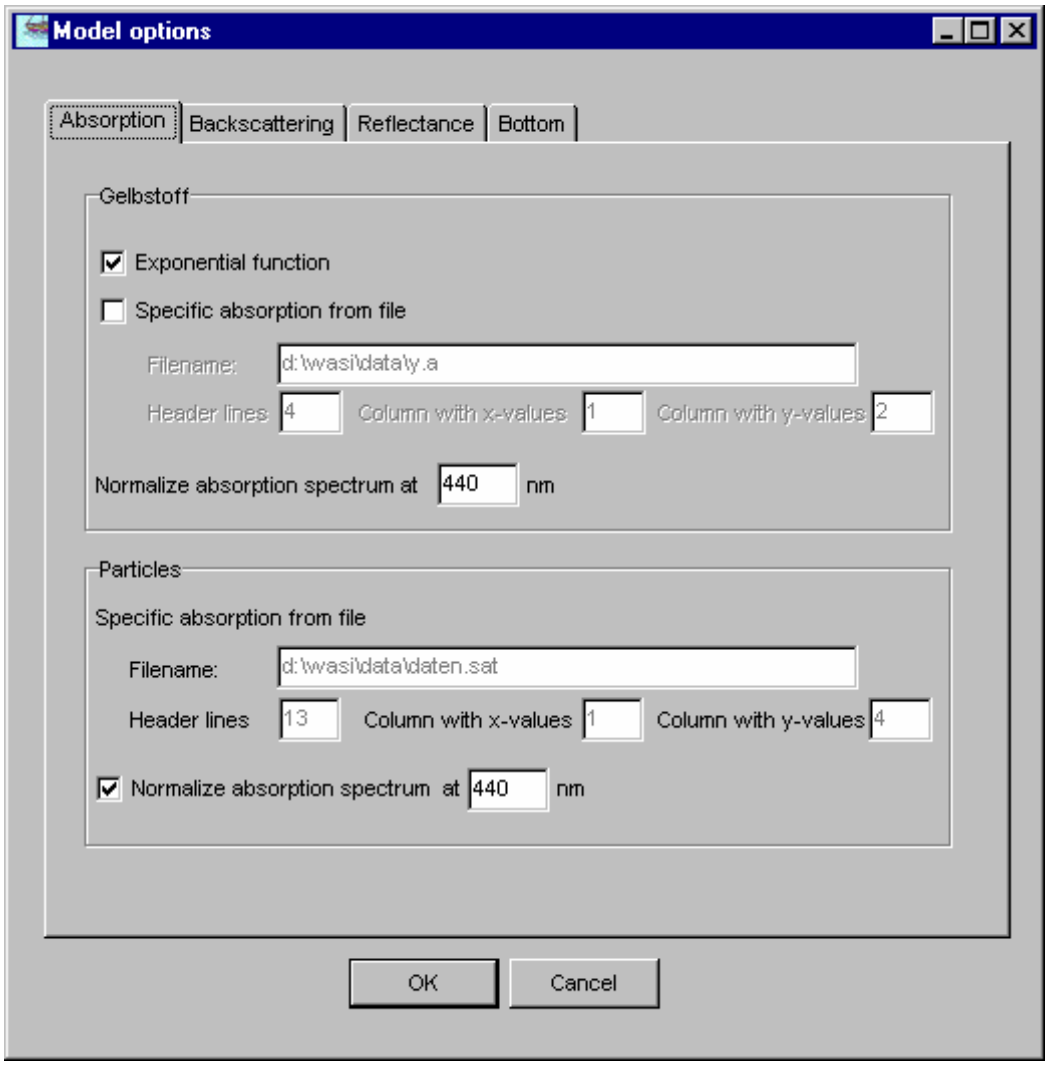


Fig. 6.6: The register card "Absorption" of the pop-up window "Model options".

The input spectrum $a_X^*(\lambda)$ may be normalized after it is read from file, or not. The selection is done in the check box "Normalize absorption spectrum" of the "Particles" section of Fig. 6.6. If normalization is selected, the corresponding wavelength λ_0 must be specified in the "at ... nm" input field. When $a_X^*(\lambda)$ is normalized, the concentration of large suspended particles is given in units of absorption at the reference wavelength λ_0, otherwise it is given in units related to the units of the input file. By default $a_X^*(\lambda)$ is normalized.

The 10 input spectra $a_W(\lambda)$, $da_W/dT(\lambda)$, $a_Y^*(\lambda)$, $a_X^*(\lambda)$, $a_i^*(\lambda)$ with i=0..5, are read from files which are specified in the initialisation file WASI.INI. If these spectra should be replaced by other spectra, the WASI.INI file must be changed accordingly.

6.4 Bottom reflectance

The spectrum type "Bottom reflectance" is activated by selecting this type in the main window from the drop-down list above the "Start" button, see Fig. 6.7 left. After the spectrum type is set to "Bottom reflectance", the check box "radiance sensor" (Fig. 6.7 left) and the parameter list shown in Fig. 6.7 right are displayed.

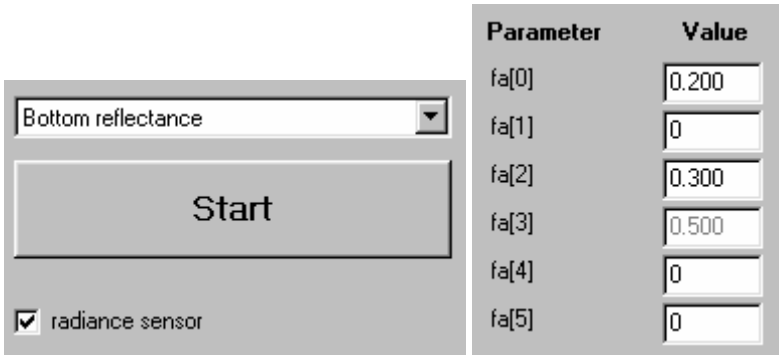


Fig. 6.7: Settings of the spectrum type "Bottom reflectance" in the main window. Left: Drop-down list with "Bottom reflectance" selected as spectrum type. Right: Parameter list of the forward mode.

If the check box "radiance sensor" is marked with a hook (like in Fig. 6.7 left), the bottom reflectance is calculated for a radiance sensor using eq. (2.22). Otherwise, it is calculated for an irradiance sensor using eq. (2.21).

Bottom albedo (irradiance reflectance) is calculated as a weighted sum of 6 albedo spectra. The weights f_n = fa[n], n = 0..5, are the relative areas of the 6 bottom types within the sensor's field of view. Consequently, it is $\Sigma f_n = 1$, thus only 5 of the f_n are independent parameters, while one is calculated using $\Sigma f_n = 1$. Which of the weights is adjusted in this manner is defined in the register card "Bottom" of the pop-up window "Model options", see Fig. 6.8. It is accessed from the menu bar via "Options – Models" (see Fig. 7.1). The selection is done in the box "Adjust bottom albedo". If "none" is selected, the weights are not automatically adjusted. In the example of Fig. 6.8 the weight for surface no. 3 is automatically adjusted. This is visible in the main window by an inactive input box for fa[3] in the parameter list, i.e. the calculated value is displayed in gray instead of black, see Fig. 6.7 right.

For a radiance sensor the bottom reflectance spectra are weighted additionally to f_n with reflection factors B_n, which are the ratio of radiance reflected in the direction of the sensor relative to the downwelling irradiance. For an isotropic (Lambertian) reflecting surface it is $B_n = 1/\pi = 0.318\ sr^{-1}$, thus $0.318\ sr^{-1}$ are the default values for all B_n's. The reflection factors can be set for each surface type individually in the register card "Bottom" of the pop-up window "Model options", see Fig. 6.8.

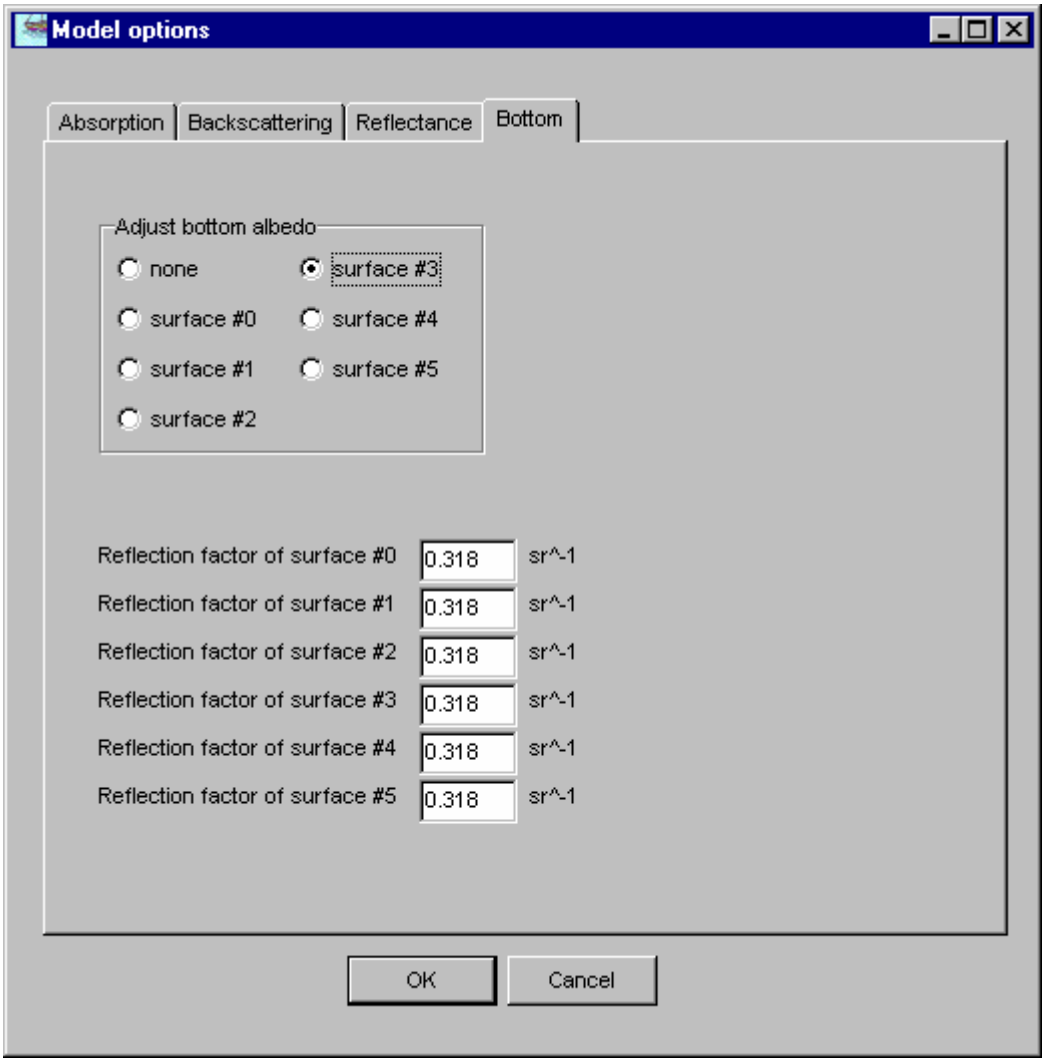


Fig. 6.8: The register card "Bottom" of the pop-up window "Model options".

7. Program options

The "Options" item of the menu bar on top of the WASI window is the entry point to all program settings. Fig. 7.1 shows the main menu bar of WASI and the structure of the "Options" item. The various program settings are grouped in 7 thematic areas; one of these ("Invers calculation) is further divided into 3 themes. When one of the themes is selected, a pop-up window shows up which allows to inspect and modify the settings.

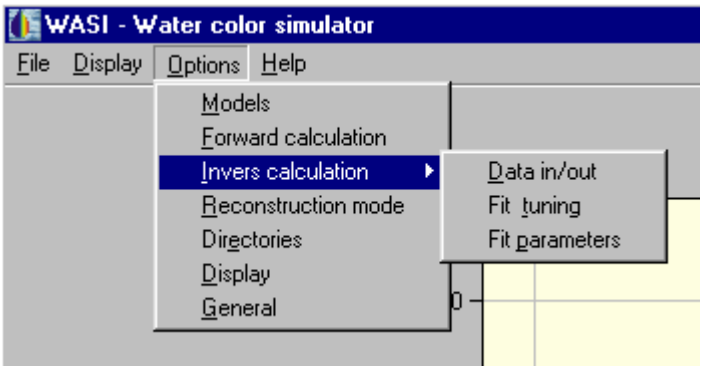


Fig. 7.1: The structure of the "Options" menu.

The pop-up menus of the first four thematic areas are described in the previous chapters: "Models" in chapter 6 (Figs. 6.3, 6.4, 6.6, 6.8), "Forward calculation" in chapter 3 (Fig. 3.2), "Invers calculation" in chapter 4 (Figs. 4.4 to 4.12), and "Reconstruction mode" in chapter 5 (Fig. 5.3). The pop-up menus of the three remaining themes are described in the following.

7.1 Directories

The directories for saving calculated spectra and for reading import spectra are selected in the "Directories" pop-up window. It is accessed from the menu bar via "Options – Directories" (see Fig. 7.1) and shown in Fig. 7.2. The pre-selected directories can be changed by entering a new directory name or by pressing the button ... and selecting a directory from the displayed directory tree (not shown).

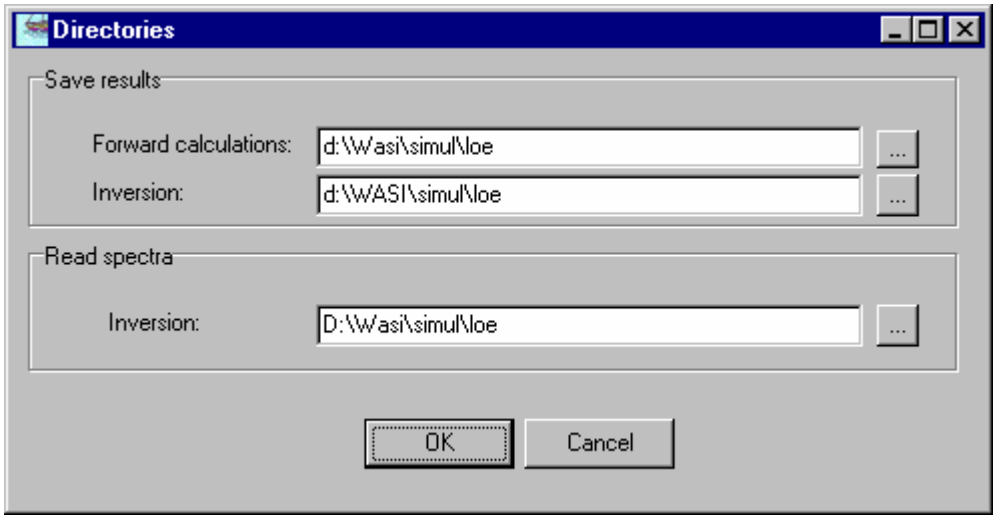


Fig. 7.2: The pop-up window "Directories".

7.2 Display options

The pop-up window for settings concerning visualisation is shown in Fig. 7.3. It appears when the thematic area "Display" is selected in the "Options" menu (see Fig. 7.1).

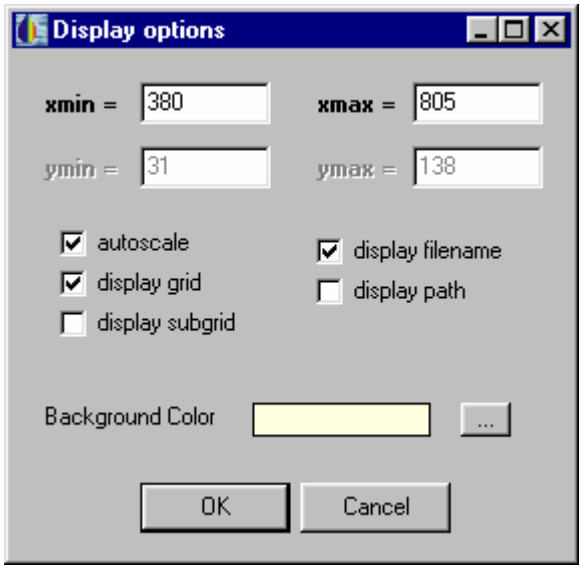


Fig. 7.3: The popup-window "Display options".

Range of x and y values. The range of the displayed x-values is defined by the values in the fields "xmin =" and "xmax =". The range of the displayed y-values is either defined by the values in the fields "ymin =" and "ymax =", or adjusted automatically to the actual spectrum if the check box "autoscale" is marked with a hook. In the latter case the input fields for ymin and ymax are deactivated. By default the autoscale option is activated.

Spectrum information. On top right of the plot window the file name of the actual spectrum can be displayed, either excluding or including the path. The selection is made using the check boxes "display filename" and "display path".

Layout. The spectra can be plotted either on a blank background, or on a coarse or fine grid. The selection is made using the check boxes "display grid" and "display subgrid". The background colour can be changed by pressing the ... button and selecting the desired colour in the upcoming popup-window (not shown).

7.3 General options

The pop-up window for some general settings is shown in Fig. 7.4. It appears when the thematic area "General" is selected in the "Options" menu (see Fig. 7.1).

Four yes-no-decisions can be made:

- The check box "save INI file automatically" selects whether or not the file WASI.INI is updated automatically at program termination.
- The check box "multiply spectrum Ed with factor" allows to multiply automatically each downwelling irradiance spectrum $E_d(\lambda)$, which is read from file, with a factor whose value

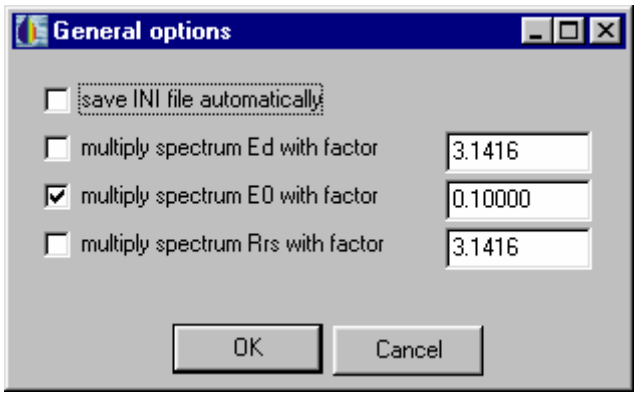


Fig. 7.4: The pop-up window "General options".

is set in the adjacent input field. This is useful if $E_d(\lambda)$ was measured as radiance upwelling from a horizontally oriented diffuse reflecting panel, $L_{up}(\lambda)$. In this case it is $E_d(\lambda) = \pi \cdot \rho \cdot L_{up}(\lambda)$, where ρ is the panel's reflectance. The conversion factor is set to $\pi = 3.1416$ by default, which corresponds to $\rho = 1$.

- The check box "multiply spectrum E0 with factor" allows to multiply automatically the spectrum of the extraterrestrial solar irradiance, $E_0(\lambda)$, with a conversion factor. This is useful if the spectrum $E_0(\lambda)$ is given in other units than the other irradiance spectra. For example, the spectrum $E_0(\lambda)$ provided with WASI is given in units of $\mu W\ cm^{-2}\ sr^{-1}$, while the common units in WASI are $mW\ m^{-2}\ sr^{-1}$. This leads to a conversion factor of 0.1.
- The check box "multiply spectrum Rrs with factor" allows to multiply automatically all remote sensing reflectance spectra $R_{rs}(\lambda)$ (those read from file as well as those forward calculated) with a factor whose value is set in the adjacent input field. This provides a fast way to convert $R_{rs}(\lambda)$ to irradiance reflectance $R(\lambda)$ using the model of Eq. (2.13a), $R_{rs}^{-}(\lambda) = R(\lambda)/Q$. The conversion factor is set to $Q = \pi = 3.1416$ by default, which represents the idealized case of isotropic reflection.

8. References

E. Aas (1987): Two-stream irradiance model for deep waters. *Applied Optics 26(11), 2095-2101.*

Y. H. Ahn, A. Bricaud, A. Morel (1992): Light backscattering efficiency and related properties of some phytoplankton. *Deep-Sea Res. 39, 1835-1855.*

A. Albert, C. D. Mobley (2003): An analytical model for subsurface irradiance and remote sensing reflectance in deep and shallow case-2 waters. *Optics Express 11, 2873-2890. http://www.opticsexpress.org/abstract.cfm?URI=OPEX-11-22-2873.*

A. Albert (2004): Inversion technique for optical remote sensing in shallow water. *Ph.D. thesis, University of Hamburg. http://www.sub.uni-hamburg.de/opus/volltexte/2005/2325/*

A. Albert, P. Gege (2005): Inversion of irradiance and remote sensing reflectance in shallow water between 400 and 800 nm for calculations of water and bottom properties. *Applied Optics (accepted).*

A. Bricaud, A. Morel, L. Prieur (1981): Absorption by dissolved organic matter of the sea (yellow substance) in the UV and visible domains. *Limnol. Oceanogr. 26, 43-53 .*

H. Buiteveld, J. H. M. Hakvoort, M. Donze (1994): The optical properties of pure water. *SPIE Vol. 2258, Ocean Optics XII, 174-183.*

M. S. Caceci, W. P. Cacheris (1984): Fitting Curves to Data. *Byte May 1984: 340-362.*

K. L. Carder, G. R. Harvey, P. B. Ortner (1989): Marine humic and fulvic acids: their effects on remote sensing of ocean chlorophyll. *Limnol. Oceanogr. 34: 68-81.*

C. Cox, W. Munk (1954): Statistics of the sea surface derived from sun glitter. *J. Marine Res., 13, 198-227.*

C. Cox, W. Munk (1956): Slopes of the sea surface deduced from photographs of sun glitter. *Bulletin Scripps Inst. Oceanogr. Univ. Calif., 6,* 401-488.

P. Gege (1994): Gewässeranalyse mit passiver Fernerkundung: Ein Modell zur Interpretation optischer Spektralmessungen. *PhD thesis. DLR-Forschungsbericht 94-15, 171 p.*

P. Gege (1995): Water analysis by remote sensing: A model for the interpretation of optical spectral measurements. *Technical Translation ESA-TT-1324, 231 pp., July 1995.*

P. Gege (1998a): Correction of specular reflections at the water surface. *Ocean Optics XIV, November,10-13, 1998, Kailua-Kona, Hawaii, USA. Conference Papers, Vol. 2.*

P. Gege (1998b): Characterization of the phytoplankton in Lake Constance for classification by remote sensing. *Arch. Hydrobiol. Spec. Issues Advanc. Limnol. 53, p. 179-193, Dezember 1998: Lake Constance, Characterization of an ecosystem in transition.*

P. Gege (2000): Gaussian model for yellow substance absorption spectra. *Proc. Ocean Optics XV conference, October 16-20, 2000, Monaco.*

P. Gege (2001a): A software tool for simulation and analysis of optical in-situ spectra. *Proc. 4th Berlin Workshop on Ocean remote sensing, Berlin, Germany, May 30 to June 1, 2001.*

P. Gege (2001b): The water colour simulator WASI: A software tool for forward and inverse modeling of optical in-situ spectra. *Proc. IGARSS, Sydney, Australia, 9-13 July 2001.*

P. Gege (2002). Error propagation at inversion of irradiance reflectance spectra in case-2 waters. *Ocean Optics XVI Conference, November 18-22, 2002, Santa Fe, USA.*

P. Gege (2004): The water color simulator WASI: an integrating software tool for analysis and simulation of optical in situ spectra. *Computers & Geosciences, 30, 523-532.*

P. Gege, A. Albert (2005): A tool for inverse modeling of spectral measurements in deep and shallow waters. In: L.L. Richardson and E.F. LeDrew (Eds): *"Remote Sensing of Aquatic Coastal Ecosystem Processes", Kluwer book series: Remote Sensing and Digital Image Processing.* (accepted)

H. R. Gordon, O. B. Brown, M. M. Jacobs (1975): Computed Relationships between the Inherent and Apparent Optical Properties of a Flat Homogeneous Ocean. *Applied Optics 14, 417-427.*

H. R. Gordon (1989): Can the Lambert-Beer law be applied to the diffuse attenuation coefficient of ocean water? *Limnol. Oceanogr. 34(8), 1389-1409.*

T. Heege (2000): Flugzeuggestützte Fernerkundung von Wasserinhaltsstoffen am Bodensee. *PhD thesis. DLR-Forschungsbericht 2000-40, 134 p.*

N. G. Jerlov (1976): Marine Optics. *Elsevier Scientific Publ. Company.*

J. H. Jerome, R. P. Bukata, J. E. Bruton (1990): Determination of available subsurface light for photochemical and photobiological activity. *J. Great Lakes Res. 16(3), 436-443.*

J. T. O. Kirk (1984): Dependence of relationship between inherent and apparent optical properties of water on solar altitude. *Limnol. Oceanogr. 29, 350-356.*

J. T. O. Kirk (1991): Volumen scattering function, average cosines, and underwater lightfield. *Limnol. Oceanogr. 36, 455-467*

Z. P. Lee, K. L. Carder, C. D. Mobley, R. G. Steward, J. S. Patch (1998): Hyperspectral remote sensing for shallow waters. I. A semianalytical model. *Appl. Optics 37, 6329-6338.*

C. D. Mobley, B. Gentili, H. R. Gordon, Z. Jin, G. W. Kattawar, A. Morel, P. Reinersman, K. Stamnes, R. H. Stavn (1993): Comparison of numerical models for computing underwater light fields. *Appl. Optics 32, 7484-7504.*

C. D. Mobley (1994): Light and Water. *Academic Press, 592 pp.*

C. D. Mobley (1999): Estimation of the remote-sensing reflectance from above-surface measurements. *Appl. Optics 38, 7442-7455.*

A. Morel (1974): Optical Properties of Pure Water and Pure Sea Water. *In: Jerlov, N. G., Steemann Nielsen, E. (Eds.): Optical Aspects of Oceanography. Academic Press London, 1-24.*

A. Morel (1980): In water and remote measurements of ocean colour. *Boundary-Layer Meteorology 18, 177-201.*

A. Morel, Gentili (1991): Diffuse reflectance of oceanic waters: its dependence on Sun angle as influenced by the molecular scattering contribution. *Appl. Optics 30, 4427-4438.*

J. L. Mueller, R. W. Austin (1995): Volume 25 of Ocean Optics Protocols for SeaWiFS Validation, Revision 1. *S. B. Hooker, E. R. Firestone, and J. G. Acker, eds., NASA Tech. Memo. 104566. NASA Goddard Space Flight Center, Greenbelt, Md.*

J. A. Nelder, R. Mead (1965): A simplex method for function minimization. *Computer J. 7, 308-313*.

G. Nyquist (1979): Investigation of some optical properties of seawater with special reference to lignin sulfonates and humic substances. *PhD Thesis, Göteborgs Universitet, 200 p.*

K. F. Palmer, D. Williams (1974): Optical properties of water in the near infrared. *J. Optical Soc. of America 64, 1107-1110.*

N. Pinnel (2005): Spectral discrimination of submerged macrophytes in lakes using hyperspectral remote sensing data. *Ph.D. thesis. Limnological Institute of the Technical University Munich (in preparation).*

R. W. Preisendorfer, C. D. Mobley (1985): Unpolarized irradiance reflectances and glitter patterns of random capillary waves on lakes and seas, by Monte Carlo simulation. *NOAA Tech. Memo. ERL PMEL-63, Pacific Mar. Environ. Lab., Seattle, WA, 141 pp.*

R. W. Preisendorfer, C. D. Mobley (1986): Albedos and glitter patterns of a wind-roughened sea surface. *J. Phys. Ocean., 16, 1293-1316.*

L. Prieur (1976): Transfers radiatifs dans les eaux de mer. *Thesis, Doctorat d'Etat, Univ. Pierre et Marie Curie, Paris, 243 pp.*

L. Prieur, S. Sathyendranath (1981): An optical classification of coastal and oceanic waters based on the specific spectral absorption curves of phytoplankton pigments, dissolved organic matter, and other particulate materials. *Limnol. Oceanogr. 26, 671-689.*

T. Pyhälahti, P. Gege (2001): Retrieval of water quality parameters using different channel configurations. *Proc. ISPRS symposium "Physical measurements & signatures in remote sensing", Jan. 8-12, 2001, Aussous, France.*

T. I. Quickenden, J.A. Irvin (1980): The ultraviolet absorption spectrum of liquid water. *J. Chem. Phys. 72(8), 4416-4428.*

S. Sathyendranath, T. Platt (1988): Oceanic Primary Production: Estimation by Remote Sensing at Local and Regional Scales. *Science, 241, 1613-1620.*

S. Sathyendranath, L. Prieur, A. Morel (1989): A three-component model of ocean colour and its application to remote sensing of phytoplankton pigments in coastal waters. *Int. J. Remote Sensing 10, 1373-1394.*

S. Sathyendranath, T. Platt (1997): Analytic model of ocean color. *Applied Optics 36, 2620-2629.*

J. N. Schwarz, P. Kowalczuk, S. Kaczmarek, G. Cota, B. G. Mitchell, M. Kahru, F. Chavez, A. Cunningham, D. McKee, P. Gege, M. Kishino, D. Phinney, R. Raine (2002): Two models for absorption by coloured dissolved organic matter (CDOM). *Oceanologia 44(2), 209-241.*

M. M. Tilzer, N. Stambler, C. Lovengreen (1995): The role of phytoplankton in determining the underwater light climate in Lake Constance. *Hydrobiologia 316, 161-171.*

D. A. Toole, D. A. Siegel, D. W. Menzies, M. J. Neumann, R. C. Smith (2000): Remote-sensing reflectance determinations in the coastal ocean environment: impact of instrumental characteristics and environmental variability. *Applied Optics 39(3), 456-469.*

Appendix 1: Installation

WASI has no custom setup routine like most WINDOWS programs. However, installation is very easy.

Method 1:
The simplest method is to install WASI in the directory D:\WASI. The steps are:
- Create the directory D:\WASI
- Copy WASI.ZIP into D:\WASI
- Unzip WASI.ZIP

Method 2:
If you prefer to install WASI in another directory than D:\WASI, then installation needs a little bit more effort. The steps are:
- Create the desired directory
- Copy WASI.ZIP into that directory
- Unzip WASI.ZIP
- Edit WASI.INI: Replace with a text editor all occurences of "D:\WASI\" with your directory

To start WASI, execute the file WASI.EXE.

Appendix 2: WASI.INI

WASI.INI is the initialization file of WASI. It is read automatically during program start. All program settings are stored in this file. The following is an example listening.

```
Initialization file for the program WASI - water colour simulator
-----------------------------------------------------------------
WASI.INI version 25 August 2005
WASI.EXE Version 3 - Latest update: 11 June 2005

[ Spectrum of x-values ]
d:\wasi\data\ch_meris.prn
3    = Header lines
1    = Column with x-values

[ E0 = Spectrum of solar constant ]
d:\wasi\data\E0_sun.prn
11   = Header lines
1    = Column with x-values
2    = Column with y-values

[ tA = Spectrum of transmission of atmosphere ]
d:\wasi\data\ta.t
7    = Header lines
1    = Column with x-values
2    = Column with y-values

[ tC = Spectrum of transmission of clouds ]
d:\wasi\data\tc.t
7    = Header lines
1    = Column with x-values
2    = Column with y-values

[ aW = Absorption of water ]
d:\wasi\data\water.a
10   = Header lines
1    = Column with x-values
2    = Column with y-values

[ dadT = Temperature dependence of water absorption ]
d:\wasi\data\dawdt.prn
10   = Header lines
1    = Column with x-values
2    = Column with y-values

[ aP[0] = Specific absorption spectrum of phytoplankton class no. 0 ]
d:\wasi\data\phyto.a
12   = Header lines
1    = Column with x-values
2    = Column with y-values

[ aP[1] = Specific absorption spectrum of phytoplankton class no. 1 ]
d:\wasi\data\cry-lo.a
10   = Header lines
1    = Column with x-values
2    = Column with y-values

[ aP[2] = Specific absorption spectrum of phytoplankton class no. 2 ]
d:\wasi\data\cry-hi.a
11   = Header lines
1    = Column with x-values
2    = Column with y-values

[ aP[3] = Specific absorption spectrum of phytoplankton class no. 3 ]
d:\wasi\data\dia.a
10    = Header lines
1    = Column with x-values
2    = Column with y-values

[ aP[4] = Specific absorption spectrum of phytoplankton class no. 4 ]
d:\wasi\data\dino.a
10   = Header lines
1    = Column with x-values
2    = Column with y-values

[ aP[5] = Specific absorption spectrum of phytoplankton class no. 5 ]
d:\wasi\data\green.a
10   = Header lines
1    = Column with x-values
2    = Column with y-values

[ aX = Absorption of non-chlorophyllous particles ]
d:\wasi\data\x.a
```

```
7    = Header lines
1    = Column with x-values
2    = Column with y-values

[ aY = Specific absorption of Gelbstoff ]
d:\wasi\data\y.a
12   = Header lines
1    = Column with x-values
2    = Column with y-values

[ bL = Scattering coefficient of large particles ]
d:\wasi\data\eins.prn
2    = Header lines
1    = Column with x-values
2    = Column with y-values

[ albedo[0] = Bottom albedo #0 = const ]
d:\wasi\data\bottom.r
15   = Header lines
1    = Column with x-values
2    = Column with y-values

[ albedo[1] = Bottom albedo #1 = sand ]
d:\wasi\data\sand.r
21    = Header lines
1    = Column with x-values
2    = Column with y-values

[ albedo[2] = Bottom albedo #2 = silt ]
d:\wasi\data\bottom.r
15    = Header lines
1    = Column with x-values
3    = Column with y-values

[ albedo[3] = Bottom albedo #3 = green makrophyte "Chara aspera" ]
d:\wasi\data\bottom.r
15   = Header lines
1    = Column with x-values
4    = Column with y-values

[ albedo[4] = Bottom albedo #4 = green makrophyte "Potamogeton perfoliatus" ]
d:\wasi\data\bottom.r
15   = Header lines
1    = Column with x-values
5    = Column with y-values

[ albedo[5] = Bottom albedo #5 = green makrophyte "Potamogeton pectinatus" ]
d:\wasi\data\bottom.r
15   = Header lines
1    = Column with x-values
6    = Column with y-values

[ Measurement ]
d:\wasi\data\demo\R\fwd.r
8       = Header lines
1       = Column with x-values
2       = Column with y-values

[ Measurement: Irradiance reflectance, R ]
d:\wasi\data\demo\R\fwd.r
8       = Header lines
1       = Column with x-values
2       = Column with y-values

[ Measurement: Downwelling irradiance, Ed ]
d:\wasi\data\demo\E_down\R2R.C1
30      = header lines
1       = column with x-values
2       = column with y-values

[ Measurement: Sky radiance reflected at surface, Ls ]
d:\wasi\data\demo\L_sky\Ls.fwd
8       = header lines
1       = column with x-values
2       = column with y-values

[ Measurement: Remote sensing reflectance R_rs ]
D:\WASI\DATA\DEMO\R_rs\s2am.c-o
27      = Header lines
1       = Column with x-values
2       = Column with y-values

[ Measurement: Attenuation for downwelling irradiance, Kd ]
d:\Wasi\data\demo\K_down\K.prn
5       = Header lines
1       = Column with x-values
3       = Column with y-values

[ Weighting function for inversion ]
d:\Wasi\DATA\EINS.PRN
```

```
2       = Header lines
1       = Column with x-values
2       = Column with y-values

[ Spectra inverted in batch mode ]
D:\WASI\TEMP\*.fwd
8       = Header lines
1       = Column with x-values
2       = Column with y-values

[ Directories: save FWD, save INV ]
D:\WASI\TEMP
D:\WASI\TEMP

[ General settings and parameters ]
380     = xu             = lowest  x-coordinate displayed
805     = xo             = highest x-coordinate displayed
3.9E-5  = yu             = lowest  y-coordinate displayed
0.050   = yo             = highest y-coordinate displayed
380     = xub            = lowest x-coordinate calculated
900     = xob            = highest x-coordinate calculated
1       = dxb            = wavelength interval for calculation
400     = Norm_min       = lower boundary for normalisation (nm)
800     = Norm_max       = upper boundary for normalisation (nm)
3.1416  = Ed_factor      = multiplicator of spectrum E_down
0.10000 = E0_factor      = multiplicator of spectrum E0
3.1416  = Rrs_factor     = multiplicator of spectrum R_rs
0       = calc_mode      = calculation mode: 1=invers, 0=2=batch
3       = spec_type      = type of spectrum: 0=E_d, 1=L_up, 2=R_rs, 3=R, 4=R_surf, 5=a, 6=K_d, 7=R_bottom
0       = Model_R        = R model: 0=f*bb/(a+bb), 1=f*bb/a
1       = Model_R_rsA    = R_rs above surface is a function of 0=R_rs(0-), 1=R, 2=both
0       = Model_R_rsB    = R_rs model below surface: 0=f_rs*bb/(a+bb), 1=f_rs*bb/a, 2=R/Q
4       = Model_f        = f model: 0=const, 1=Kirk, 2=Morel+Gentili, 3=Sath.+Platt, 4=Albert+Mobley
0       = Model_f_rs     = f_rs model: 0=Albert, 1=f/Q
-1      = bottom_fill    = bottom surface type adjusted to yield sum of weights = 1
$00E1FFFF = clPlotBk     = color of plot background

[ Flags: 0 = FALSE, 1 = TRUE ]
0       = flag_SubGrid   = draw subgrid
1       = flag_Grid      = draw grid
1       = flag_Autoscale = autoscale plot
1       = flag_ShowName  = display filename
1       = flag_ShowPath  = display path
0       = flag_INI       = save INI file automatically
0       = flag_sv_table  = save forward-spectra as table
0       = flag_save_t    = save calculation time
0       = flag_mult_Ed   = multiply spectrum Ed with factor
1       = flag_mult_E0   = multiply spectrum E0 with factor
0       = flag_mult_Rrs  = multiply spectrum R_rs with factor
0       = flag_x_file    = read x-values from file
0       = Par1_log       = Logarithmic steps of Parameter 1
0       = Par2_log       = Logarithmic steps of Parameter 2
1       = Par3_log       = Logarithmic steps of Parameter 3
0       = flag_b_SaveFwd = save all spectra of forward mode
0       = flag_b_SaveInv = save all spectra of invers mode
0       = flag_b_LoadAll = load spectra from files
1       = flag_b_Reset   = reset start values
0       = flag_b_Invert  = invert spectra
0       = flag_Res_log   = weight residuals logarithmically
1       = flag_Y_exp     = exponential Gelbstoff absorption
0       = flag_surf_inv  = wavelength dependent surface reflections (inversion)
0       = flag_surf_fw   = wavelength dependent surface reflections (forward mode)
0       = flag_use_Ed    = make use of Ed measurement
0       = flag_use_Ls    = make use of Ls measurement
0       = flag_use_R     = make use of R measurement
0       = flag_radiom    = reduce radiometric resolution
0       = flag_noise     = add noise
0       = flag_aW        = include water absorption in bulk absorption
1       = flag_above     = above water
0       = flag_shallow   = shallow water
1       = flag_autoiniR  = automatic determination of R start values
1       = flag_anX_R     = analytic determination X start value for R spectra
1       = flag_anX_Rsh   = analytic determination X start value for R spectra in shallow waters
1       = flag_anCY_R    = analytic determination C, Y start values for R spectra
1       = flag_anzB      = analytic determination of zB start value in shallow waters
0       = flag_Fresnel   = calculate Fresnel reflectance
1       = flag_bL_file   = large particle scattering spectrum from file
1       = flag_bL_linear = large particle scattering linear with C_L
0       = flag_CLisC0    = set C_L = C[0]
1       = flag_norm_X    = normalize SPM absorption spectrum from file at Lambda_0
1       = flag_norm_Y    = normalize Gelbstoff spectrum from file at Lambda_0

[ Settings for batch mode ]
0       = iter_type      = parameter that is iterated
2.0     = rangeMin       = first value of successive calculation
4.0     = rangeMax       = last value of successive calculation
1       = rangeDelta     = interval of successive calculation
1       = Par1_Type      = Parameter 1
0       = Par2_Type      = Parameter 2
0       = Par3_Type      = Parameter 3
```

```
1       = Par1_Min       = Minimum of Parameter 1
2.00    = Par2_Min       = Minimum of Parameter 2
0.100   = Par3_Min       = Minimum of Parameter 3
10.0    = Par1_Max       = Maximum of Parameter 1
8.00    = Par2_Max       = Maximum of Parameter 2
1       = Par3_Max       = Maximum of Parameter 3
10      = Par1_N         = Steps of Parameter 1
3       = Par2_N         = Steps of Parameter 2
10      = Par3_N         = Steps of Parameter 3

[ Settings for inverse mode ]
[ from  to  step  MaxIter ]
400    800     5   400   = fit of Ed
760    900    10   100   = fit of R and Rrs in IR region
380    450    10   100   = fit of R and Rrs in UV region
400    900     1  1000   = fit of R and Rrs
400    800     5   100   = fit of a (shallow water)
700    800     5   100   = fit of R and Rrs in IR region (shallow water)
400    500     5   100   = fit of R and Rrs in UV region (shallow water)
400    800     1  2000   = fit of R and Rrs (shallow water)
870    900               = LambdaLf  = wavelengths for C_L and f initialisation
5      0                 = dLambdaLf = wavelength intervals of LambdaLf
760                      = LambdaLsh = wavelengths for C_L initialisation (shallow water)
2                        = dLambdaLsh= wavelength interval of LambdaLsh (shallow water)
413    440    440        = LambdaCY  = wavelengths for C[0] and C_Y initialisation
5      5    870          = dLambdaCY = wavelength intervals of LambdaCY
625                      = LambdazB  = wavelength for zB initialisation (shallow water)
25                       = dLambdazB = wavelength interval of LambdazB (shallow water)
0.10                     = zB_inimin = zB   minimum during initial value determination (shallow water)
0.10                     = CL_inimin = C_L  minimum during initial value determination (shallow water)
0.10                     = C0_inimin = C[0] minimum during initial value determination (shallow water)
0.010                    = CY_inimin = C_Y  minimum during initial value determination (shallow water)
5.0                      = a_ini     = start value of absorption for nested intervals  (shallow water)
1.0                      = da_ini    = initial absorption interval for a_ini (shallow water)
0.010                    = delta_min = threshold of spectrum change for nested intervals (shallow water}
0                        = res_mode  = type of residuum  (0=least squares)

[ Model constants ]
20.0    = T_W0           = Temperature of water absorption spectrum (°C)
1.33000 = nW             = refractive index of water
440     = Lambda_0       = Reference wavelength for Gelbstoff absorption (nm)
550     = Lambda_L       = Reference wavelength for scattering of large particles (nm)
500     = Lambda_S       = Reference wavelength for scattering of small particles (nm)
0.00111 = bbW500         = Backscattering coefficient of pure water (1/m)
0.00060 = bbL_A          = Multiplicative factor of C_L in scattering by large particles
-0.3700 = bbL_B          = Power of C_L in scattering by large particles
0.00860 = bbL_norm       = Specific backscattering coeff. of large particles (m^2/g)
0.00420 = bbs_norm       = Specific backscattering coeff. of small particles (m^2/g)
0.54000 = sigma_Eu       = reflection factor for upwelling irradiance
0.03000 = sigma_Ed       = reflection factor for downwelling irradiance
0.02000 = sigma_Lu       = reflection factor for upwelling radiance
0.00500 = dynamics       = radiometric resolution
0.00020 = noise          = noise level
1.05460 = K0             = coefficient of Kd
0.31800 = BRDF[0]         = BRDF of bottom type #0
0.31800 = BRDF[1]         = BRDF of bottom type #1
0.31800 = BRDF[2]         = BRDF of bottom type #2
0.31800 = BRDF[3]         = BRDF of bottom type #3
0.31800 = BRDF[4]         = BRDF of bottom type #4
0.31800 = BRDF[5]         = BRDF of bottom type #5

[ Model parameters ]
[ forward default    start      min      max  fit sv
    10.0       1     2.03    0.100      100   1  0   C[0]    = Concentration of phytoplankton class #0
       0       0        0        0     60.0   0  0   C[1]    = Concentration of phytoplankton class #1
       0       0        0        0     60.0   0  0   C[2]    = Concentration of phytoplankton class #2
       0       0        0        0     60.0   0  0   C[3]    = Concentration of phytoplankton class #3
       0       0        0        0     60.0   0  0   C[4]    = Concentration of phytoplankton class #4
       0       0        0        0     60.0   0  0   C[5]    = Concentration of phytoplankton class #5
    8.00   0.500     3.97    0.100      200   1  0   C_L     = Concentration large particles
       0       0        0        0      125   0  0   C_S     = Concentration small particles
   0.400   0.500    0.393   0.0500     10.0   1  0   C_Y     = Gelbstoff absorption
  0.0140  0.0140   0.0140  0.00400   0.0250   0  0   S       = Gelbstoff exponent
      -1   -1.00        0    -2.00     2.00   0  0   n       = Angström exponent of SPM backscattering
    18.0    18.0     18.0        0     35.0   0  0   T_W     = Water temperature (°C)
    5.00    5.00     5.00    0.500     10.0   0  0   Q       = Q-factor of Lu (1/sr)
  0.0200  0.0200   0.0201        0    0.500   0  0   sigma_L = reflection factor of sky radiance
   0.200   0.200    0.200    -5.00     50.0   0  0   alpha*  = fraction of Ls due to sun
   0.100   0.200    0.100    -5.00     50.0   0  0   beta*   = fraction of Ls due to blue sky
   0.100   0.200    0.100    -5.00     50.0   0  0   gamma*  = fraction of Ls due to aerosols
       0   0.200        0    -5.00     50.0   0  0   delta*  = fraction of Ls due to clouds
       1       0        0    -2.00     2.00   0  0   nue     = Angström exponent of aerosols
   0.200   0.200    0.200   -0.500     5.00   0  0   alpha   = fraction of Ed due to sun
   0.100   0.200    0.100   -0.500     95.0   0  0   beta    = fraction of Ed due to blue sky
   0.100   0.200    0.100   -0.500     5.00   0  0   gamma   = fraction of Ed due to aerosols
       0   0.200        0   -0.500     5.00   0  0   delta   = fraction of Ed due to clouds
   0.330   0.330    0.330    0.100    0.900   0  0   f       = f-factor of R
       0       0        0        0      100   0  0   z       = depth (m)
    3.00     100     3.00        0      100   0  1   zB      = bottom depth (m)
    47.0    30.0     47.0        0     89.9   0  0   sun     = sun zenith angle (°)
```

```
      0       0       0       0     89.9   0  0   view    = view zenith angle (°)
   20.0       0       0       0      180   0  0   dphi    = azimuth difference sun - observer (°)
      0       0       0       0     10.0   0  0   fA[0]   = fraction of bottom type #0
      0       0       0       0     10.0   0  0   fA[1]   = fraction of bottom type #1
      1       0       1       0     10.0   0  0   fA[2]   = fraction of bottom type #2
      0       0       0       0     10.0   0  0   fA[3]   = fraction of bottom type #3
      0       0       0       0     10.0   0  0   fA[4]   = fraction of bottom type #4
      0       0       0       0     10.0   0  0   fA[5]   = fraction of bottom type #5
      0       0       0       0      100   0  0   C_X     = Concentration non-chlorophyllous particles
0.00200       1       1       0     1000   0  0   test    = test parameter
```

Appendix 3: Parameters

The following table summarizes the 36 model parameters of all 8 spectrum types. The No.'s are used program-internally as parameter indices. The parameters z and dϕ are included for future developments and are so far not used.

No.	WASI	Symbol	Units	Description
1-6	C[i]	C_i	µg/l	Concentration of phytoplankton class number i, i = 0..5
7	C_L	C_L	mg/l	Concentration of large suspended particles
8	C_S	C_S	mg/l	Concentration of small suspended particles
9	C_Y	Y	m^{-1}	Concentration of Gelbstoff (absorption at λ_0)
10	S	S	nm^{-1}	Exponent of Gelbstoff absorption
11	n	n	-	Exponent of backscattering by small particles
12	T_W	T_W	°C	Water temperature
13	Q	Q	sr	Anisotropy factor of upwelling radiation ("Q-factor")
14	sigma_L	σ_L	-	Reflection factor of sky radiance
15	alpha_s	α*	sr^{-1}	Fraction of sky radiance due to direct solar radiation
16	beta_s	β*	sr^{-1}	Fraction of sky radiance due to molecule scattering
17	gamma_s	γ*	sr^{-1}	Fraction of sky radiance due to aerosol scattering
18	delta_s	δ*	sr^{-1}	Fraction of sky radiance due to cloud scattering
19	nue	ν	-	Exponent of aerosol scattering
20	alpha	α	-	Fraction of irradiance due to direct solar radiation
21	beta	β	-	Fraction of irradiance due to molecule scattering
22	gamma	γ	-	Fraction of irradiance due to aerosol scattering
23	delta	δ	-	Fraction of irradiance due to cloud scattering
24	f	f	-	Proportionality factor of irradiance reflectance ("f-factor")
25	z	z	m	Depth
26	zB	z_B	m	Bottom depth
27	sun	θ_{sun}	°	Sun zenith angle
28	view	θ_v	°	Viewing angle (0 = nadir)
29	dphi	dϕ	°	Azimuth difference sun - view
30-35	fA[n]	f_n	-	Areal fraction of bottom surface type number n, n = 0..5
36	C_X	X	m^{-1}	Concentration of non-chlorophyllous particles (absorption at λ_0)

Forward mode. Each parameter can be set by the user. When a series of spectra is calculated, iteration can be performed over each of the parameters.

Invers mode. The user defines for each parameter if it should be treated as a constant or as variable to be fitted during inversion.

Appendix 4: Constants

The following table summarizes the model constants of all 8 spectrum types. They can be changed by editing the WASI.INI file.

WASI	Symbol	Units	Default value	Description
Lambda_R	λ_R	nm	calculated	Rayleigh scaling factor
Lambda_M	λ_M	nm	calculated	Mie scaling factor
Lambda_0	λ_0	nm	440	Reference wavelength for Gelbstoff absorption
Lambda_L	λ_L	nm	550	Reference wavelength for scattering of large particles
Lambda_S	λ_S	nm	500	Reference wavelength for scattering of small particles
T_W0	T_0	°C	20	Reference temperature of spectrum $a_W(\lambda)$
nW	n_W	-	1.33	Refractive index of water
bbW500	b_1	m^{-1}	0.00111	Backscattering coefficient of pure water at 500 nm
bbL_A	A	-	0.006	Multiplicative factor in scattering of large particles
bbL_B	B	-	-0.37	Factor of non-linearity in scattering of large particles
bbL_norm	$b_{b,L}$*	$m^2\ g^{-1}$	0.0086	Specific backscattering coefficient of large particles
bbS_norm	$b_{b,S}$*	$m^2\ g^{-1}$	0.0042	Specific backscattering coefficient of small particles
sigma_Eu	σ^-	-	0.54	Reflection factor of upwelling irradiance
sigma_Ed	σ	-	0.03	Reflection factor of downwelling irradiance
sigma_Lu	σ_L^-	-	0.02	Reflection factor of upwelling radiance
K0	κ_0	-	1.0546	Coefficient of attenuation
BRDF[n]	B_n	sr^{-1}	0.318	BRDF of bottom surface no. n, n=0..5

Appendix 5: Input spectra

The following table summarizes the 28 spectra which can be imported from files. For each, a default spectrum is provided in the WASI software package, and stored in the directory /WASI/DATA. The user can replace the default spectra by changing the corresponding file description in the WASI.INI file.

No.	WASI	Symbol	Units	Description
1	x	λ	nm	Wavelengths for which spectra are calculated
2	E0	$E_0(\lambda)$	mW m^{-2} nm^{-1}	Extraterrestrial solar irradiance
3	tA	$t_A(\lambda)$	–	Transmission of the atmosphere
4	tC	$t_C(\lambda)$	–	Transmission of clouds
5	aW	$a_W(\lambda)$	m^{-1}	Absorption of pure water
6	dadT	$da_W(\lambda)/dT$	m^{-1} °C^{-1}	Temperature gradient of pure water absorption
7	aP[0]	$a_0^*(\lambda)$	m^2 mg^{-1}	Specific absorption of phytoplankton class no. 0 Default: Mixture of species typical for Lake Constance
8	aP[1]	$a_1^*(\lambda)$	m^2 mg^{-1}	Specific absorption of phytoplankton class no. 1 Default: Cryptophyta type "L"
9	aP[2]	$a_2^*(\lambda)$	m^2 mg^{-1}	Specific absorption of phytoplankton class no. 2 Default: Cryptophyta type "H"
10	aP[3]	$a_3^*(\lambda)$	m^2 mg^{-1}	Specific absorption of phytoplankton class no. 3 Default: Diatoms
11	aP[4]	$a_4^*(\lambda)$	m^2 mg^{-1}	Specific absorption of phytoplankton class no. 4 Default: Dinoflagellates
12	aP[5]	$a_5^*(\lambda)$	m^2 mg^{-1}	Specific absorption of phytoplankton class no. 5 Default: Green algae
13	aX	$a_X^*(\lambda)$	–	Normalized absorption of non-chlorophyllous particles
14	aY	$a_Y^*(\lambda)$	–	Normalized absorption of Gelbstoff
15	bL	$b_L(\lambda)$	–	Normalized backscattering coefficient of large particles
16	albedo[0]	$a_0(\lambda)$	–	Albedo of bottom type no. 0. Default: Constant
17	albedo[1]	$a_1(\lambda)$	–	Albedo of bottom type no. 1. Default: Sand
18	albedo[2]	$a_2(\lambda)$	–	Albedo of bottom type no. 2. Default: Silt
19	albedo[3]	$a_3(\lambda)$	–	Albedo of bottom type no. 3. Default: Chara *aspera*
20	albedo[4]	$a_4(\lambda)$	–	Albedo of bottom type no. 4. Default: P. *perfoliatus*
21	albedo[5]	$a_5(\lambda)$	–	Albedo of bottom type no. 5. Default: P. *pectinatus*
22	meas	*variable*	*variable*	Current input measurement for inversion
23	R	$R(\lambda)$	–	Irradiance reflectance
24	Ed	$E_d(\lambda)$	mW m^{-2} nm^{-1}	Downwelling irradiance above water surface
25	Ls	$L_s(\lambda)$	mW m^{-2} nm^{-1} sr^{-1}	Sky radiance
26	R_rs	$R_{rs}(\lambda)$	sr^{-1}	Remote sensing reflectance
27	Kd	$K_d(\lambda)$	m^{-1}	Diffuse attenuation coefficient for downwelling irradiance
28	gew	$g(\lambda)$	–	Weights of channels at inversion

Appendix 6: Spectrum types

The following table gives for all spectrum types an overwiew which equation is used for calculation, and which parameters can be used as fit parameters. N = maximum number of fit parameters.

Spectrum type	Model options	Symbol	Equation	N	Fit parameters
Absorption	Exclude pure water	$a_{WC}(\lambda)$	(2.1)	9	$C_0 \ldots C_5$, X, Y, S
	Include pure water	$a_W(\lambda)$	(2.3)	10	$C_0 \ldots C_5$, X, Y, S, T
Attenuation	For downwelling irradiance	$K_d(\lambda)$	(2.5)	14	$C_0 \ldots C_5$, X, Y, S, T, C_L, C_S, n, θ_{sun}
Specular reflectance	Wavelength dependent	$R_{rs}^{surf}(\lambda)$	(2.13a)	10	α, β, γ, δ, $\alpha*$, $\beta*$, $\gamma*$, $\delta*$, ν, σ_L
	Constant	R_{rs}^{surf}	(2.13b)	1	σ_L
Irradiance reflectance	For deep water	$R(\lambda)$	(2.14)	14	$C_0 \ldots C_5$, X, Y, S, T, C_L, C_S, n, θ_{sun} or f
	For shallow water	$R^{sh}(\lambda)$	(2.16)	21	$C_0 \ldots C_5$, X, Y, S, T, C_L, C_S, n, θ_{sun}, $f_0 \ldots f_5$, z_B
Remote sensing reflectance	For deep water below water surface	$R_{rs}^{-}(\lambda)$	(2.17a)	15	$C_0 \ldots C_5$, X, Y, S, T, C_L, C_S, n, θ_{sun} or f, Q
		$R_{rs}^{-}(\lambda)$	(2.17b)	15	$C_0 \ldots C_5$, X, Y, S, T, C_L, C_S, n, θ_{sun}, θ_v
	For shallow water below water surface	$R_{rs}^{sh-}(\lambda)$	(2.19)	22	$C_0 \ldots C_5$, X, Y, S, T, C_L, C_S, n, θ_{sun}, θ_v or Q, $f_0 \ldots f_5$, z_B
	For deep water above water surface and wavelength dependent surface reflections	$R_{rs}(\lambda)$	(2.20a)	25	$C_0 \ldots C_5$, X, Y, S, T, C_L, C_S, n, θ_{sun} or f, Q, α, β, γ, δ, $\alpha*$, $\beta*$, $\gamma*$, $\delta*$, ν, σ_L
		$R_{rs}(\lambda)$	(2.20b)	26	$C_0 \ldots C_5$, X, Y, S, T, C_L, C_S, n, θ_{sun} or f, θ_v, Q, α, β, γ, δ, $\alpha*$, $\beta*$, $\gamma*$, $\delta*$, ν, σ_L
		$R_{rs}(\lambda)$	(2.20c)	25	$C_0 \ldots C_5$, X, Y, S, T, C_L, C_S, n, θ_{sun} or f, Q or θ_v, α, β, γ, δ, $\alpha*$, $\beta*$, $\gamma*$, $\delta*$, ν, σ_L
	For deep water above water surface and constant surface reflections	$R_{rs}(\lambda)$	(2.20a)	16	$C_0 \ldots C_5$, X, Y, S, T, C_L, C_S, n, θ_{sun} or f, Q, σ_L
		$R_{rs}(\lambda)$	(2.20b)	17	$C_0 \ldots C_5$, X, Y, S, T, C_L, C_S, n, θ_{sun} or f, θ_v, Q, σ_L
		$R_{rs}(\lambda)$	(2.20c)	16	$C_0 \ldots C_5$, X, Y, S, T, C_L, C_S, n, θ_{sun} or f, Q or θ_v, σ_L
	For shallow water above water surface and wavelength dependent surface reflections	$R_{rs}^{sh}(\lambda)$	(2.20a)	32	$C_0 \ldots C_5$, X, Y, S, T, C_L, C_S, n, θ_{sun}, $f_0 \ldots f_5$, z_B, Q, α, β, γ, δ, $\alpha*$, $\beta*$, $\gamma*$, $\delta*$, ν, σ_L
			(2.20b)	32	$C_0 \ldots C_5$, X, Y, S, T, C_L, C_S, n, θ_{sun}, θ_v, $f_0 \ldots f_5$, z_B, Q, α, β, γ, δ, $\alpha*$, $\beta*$, $\gamma*$, $\delta*$, ν, σ_L
			(2.20c)	31	$C_0 \ldots C_5$, X, Y, S, T, C_L, C_S, n, θ_{sun}, θ_v, $f_0 \ldots f_5$, z_B, α, β, γ, δ, $\alpha*$, $\beta*$, $\gamma*$, $\delta*$, ν, σ_L
	For shallow water above water	$R_{rs}^{sh}(\lambda)$	(2.20a)	23	$C_0 \ldots C_5$, X, Y, S, T, C_L, C_S, n,

	surface and constant surface reflections				θ_{sun}, f_0…f_5, z_B, Q, σ_L
			(2.20b)	23	C_0…C_5, X, Y, S, T, C_L, C_S, n, θ_{sun}, f_0…f_5, z_B, Q, σ_L
			(2.20c)	22	C_0…C_5, X, Y, S, T, C_L, C_S, n, θ_{sun}, f_0…f_5, z_B, σ_L
Bottom reflectance	For irradiance sensors	$R^b(\lambda)$	(2.21)	6	f_0…f_5
	For radiance sensors	$R_{rs}{}^b(\lambda)$	(2.22)	6	f_0…f_5
Downwelling irradiance	Above water surface	$E_d(\lambda)$	(2.23)	5	α, β, γ, δ, ν
	Below water surface for deep water	$E_d^-(\lambda)$	(2.25)	19	C_0…C_5, X, Y, S, T, C_L, C_S, n, θ_{sun} or f, α, β, γ, δ, ν
	Below water surface for shallow water	$E_d^{sh-}(\lambda)$	(2.25)	26	C_0…C_5, X, Y, S, T, C_L, C_S, n, θ_{sun}, f_0…f_5, z_B, α, β, γ, δ, ν
Upwelling radiance	Below water surface for deep water	$L_u^-(\lambda)$	(2.27)	20	C_0…C_5, X, Y, S, T, C_L, C_S, n, θ_{sun} or f, θ_v or Q, α, β, γ, δ, ν
	Below water surface for shallow water	$L_u^{sh-}(\lambda)$	(2.27)	27	C_0…C_5, X, Y, S, T, C_L, C_S, n, θ_{sun}, θ_v or Q, f_0…f_5, z_B, α, β, γ, δ, ν
	Above water surface for deep water and wavelength dependent surface reflections	$L_u(\lambda)$	(2.29)	26	C_0…C_5, X, Y, S, T, C_L, C_S, n, θ_{sun} or f, θ_v or Q, α, β, γ, δ, ν, σ_L^-, α*, β*, γ*, δ*, σ_L
	Above water surface for deep water and constant surface reflections	$L_u(\lambda)$	(2.29)	22	C_0…C_5, X, Y, S, T, C_L, C_S, n, θ_{sun} or f, θ_v or Q, α, β, γ, δ, ν, σ_L^-, σ_L
	Above water surface for shallow water and wavelength dependent surface reflections	$L_u{}^{sh}(\lambda)$	(2.29)	33	C_0…C_5, X, Y, S, T, C_L, C_S, n, θ_{sun}, θ_v or Q, f_0…f_5, z_B, α, β, γ, δ, ν, σ_L^-, α*, β*, γ*, δ*, σ_L
	Above water surface for shallow water and constant surface reflections	$L_u{}^{sh}(\lambda)$	(2.29)	29	C_0…C_5, X, Y, S, T, C_L, C_S, n, θ_{sun}, θ_v or Q, f_0…f_5, z_B, α, β, γ, δ, ν, σ_L^-, σ_L