

WASI – A software tool for water spectra

Peter Gege

German Aerospace Center (DLR), Remote Sensing Technology Institute, Wessling, Germany
Email: peter.gege@dlr.de

While satellite and aircraft sensors measure always one type of spectra, namely upwelling radiance, optical sensors on ship provide many different types: up- and downwelling radiance above and below the surface, irradiance of the upper and lower hemisphere in air and water for a flat or spherical surface (vector, scalar irradiance), irradiance reflectance, radiance reflectance, attenuation, absorption, scattering, backscattering, and others. Usually the data of each instrument are analysed with a software that is specifically tailored to that instrument or spectrum type. However, operating a fleet of programs is a potential source of errors, because the programs must be consistent to each others concerning the model and reference data used for data analysis. In addition, maintenance and data handling is time consuming. It is desirable to have one single integrating software. That was the motivation to develop WASI.

WASI is the acronym for "Water colour Simulator". It is a comfortable, WINDOWS based software tool for forward and inverse calculations of major types of spectra in aquatic environments. Experimental basis are data from Lake Constance (Bodensee). It is available as executable program free of charge [1]. Main applications are data analysis, data simulation, sensitivity studies, and student training. A screenshot of the opening window is shown in Fig. 1.

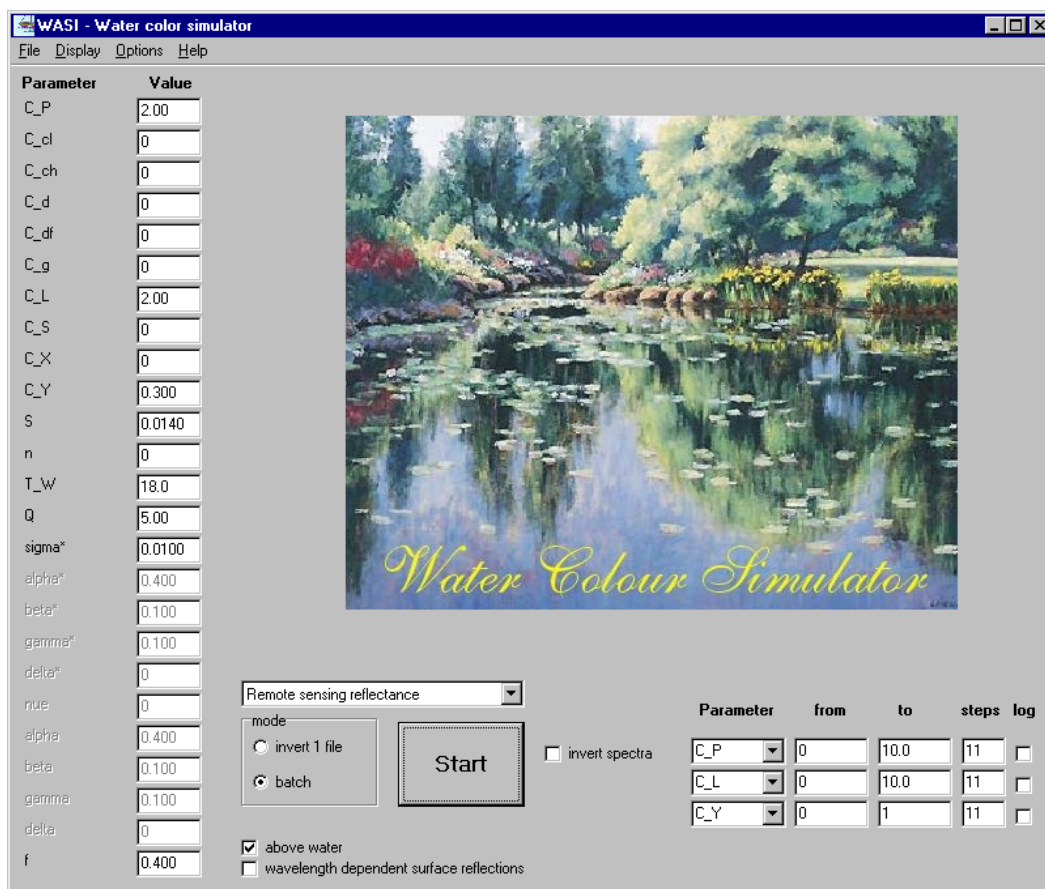


Fig. 1: Graphical user interface of WASI. During operation, the painting is replaced by a graphic showing loaded or calculated spectra.

Concept. WASI is designed as a sensor independent spectra generator and spectra analyser with well documented calculation steps and automatic visualisation of results. All input and output files are in text format (ASCII). This makes it easy to adapt the calculations to regional specifics by replacing some default input spectra. Spectral resolution, spectral data interval as well as number and positions of spectral channels are arbitrary and can be chosen by the user. The default input spectra provided with WASI are suited for calculating all implemented types of spectra at least from 390 to 800 nm at a spectral resolution of 1 nm.

All user settings are stored in an INI file (ASCII format), which is automatically read during program start. It contains file names, paths, model constants, parameter values and other data that may change. Whenever WASI creates output files, a copy of the INI file containing the actual settings is automatically stored for complete documentation. The INI file is furtheron the key for other programs to use WASI as a slave that generates or analyses data according to their inputs: WASI can be operated in a background mode, i.e. it reads the INI file, starts calculation as defined in that file, saves the results, and terminates, all "hidden" without opening a user interface. WASI was combined in that way with a radiative transfer simulation program for the atmosphere to estimate the influence of errors in atmospheric correction on the retrieval of water constituents from MERIS and MODIS data.

Models. The transfer of light in water depends on many factors: the optical properties of the water constituents, their spatial distribution in the water, and the illuminating radiation field of the sky. There exist numerically exact methods for calculation, but they are very time consuming, cannot be used for inversion, and the required input data are never completely known in practice. Furtheron, these methods require types of input data which are very rarely measured, for example phase functions and refractive indices. For these reasons mathematically simpler models have been developed, based on analytic equations which use parameters that can relatively easy be measured. These models have been optimised by comparison with numerically exact methods and experimental data. They require little computing time and can be used for inversion. WASI is based on such analytical models. Most of the implemented algorithms are well established among "ocean colour" modelers, some additional have been introduced by the author. The types of spectra which can be calculated with WASI are listed in the following table.

Spectrum type	Options
Downwelling irradiance	Above / below surface
Upwelling radiance	Above / below surface Surface reflections wavelength dependent / constant
Remote sensing reflectance	Above / below surface Surface reflections wavelength dependent / constant
Irradiance reflectance	Below surface
Specular reflectance	Wavelength dependent / constant
Absorption	Include / exclude pure water
Bottom reflectance	-

Table: Spectrum types supported by WASI.

For several spectra types different analytical models are implemented, allowing the user to select the desired model. An example of a corresponding user interface is shown in Fig. 2.

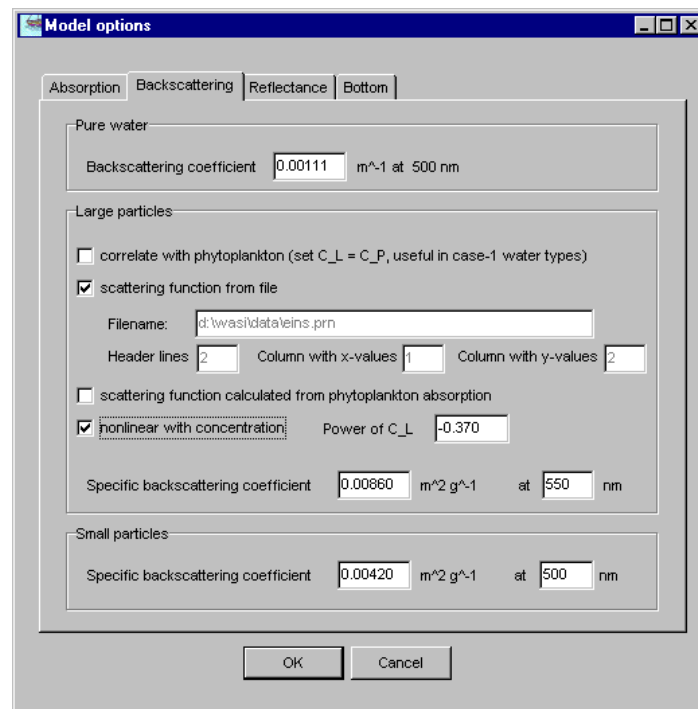


Fig. 2: Popup window for selecting the backscattering model.

Forward calculations. In the forward mode a spectrum or a series of spectra is calculated according to user-specified parameter values using a selected model. The spectra are automatically plotted on screen and can be saved as text files. In order to generate effectively a large number of spectra which cover a wide range of situations in nature, up to three parameters can be iterated simultaneously. For example, in Fig. 1 the user has selected that the concentrations of phytoplankton (C_P), suspended matter (C_L) and dissolved organic material (C_Y) shall be iterated from 0 to 10 $\mu\text{g/l}$, 0 to 10 mg/l and 0 to 1 m^{-1} (units of absorption at 440 nm), respectively. The number of steps is set to 11 for each water constituent, that means calculations will be performed for phytoplankton concentrations of 0, 1, 2, ... 10 $\mu\text{g/l}$, and similarly graduated for C_L and C_Y . Hence, $11^3 = 1331$ spectra will be calculated after the "Start" button is pressed. To give an idea about computing times: a notebook equipped with a 450 MHz Pentium III processor required 34 seconds to calculate and save these 1331 spectra, where each spectrum consisted of 801 data points in 1 nm steps from 200 to 1000 nm.

Main applications of the forward mode are generation of spectra for sensitivity studies and visualisation of spectral changes upon altered conditions. An example for the latter is given in Fig. 3. Two features are implemented which are useful to study the sensitivity of a sensor: statistical noise with user-defined standard deviation can be added, and the radiometric resolution can be defined arbitrarily.

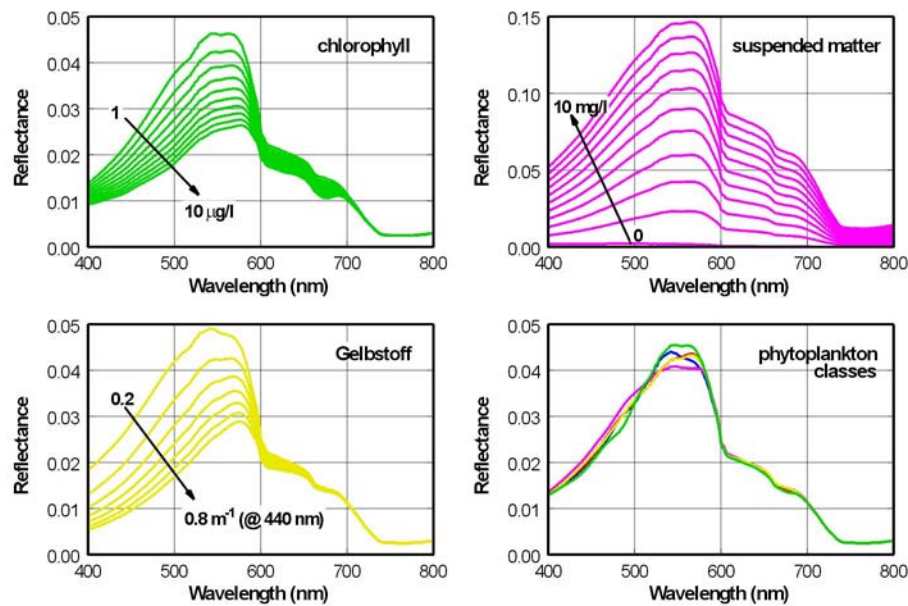


Fig. 3: Changes of the reflectance spectrum upon changes of concentrations of major water constituents and of the dominating phytoplankton class.

Inverse modeling. Data analysis is done by inverse modeling, i.e. the actual values of model parameters are determined iteratively from a given spectrum or a series of spectra. In the first iteration a spectrum is calculated using initial values for the model parameters. This model spectrum is compared with the measured one by calculating the residual, which is a number that characterises the degree of correspondence. Several methods for calculating the residual are implemented, for example a spectral weighting function can be used. Then, in the further iterations, the parameter values are altered, resulting in altered model curves and altered residuals. The selection of the new parameter values in each step is done by the so-called Simplex algorithm. The choice depends on the previously calculated residuals. The procedure is stopped after the best fit between calculated and measured spectrum, or the minimum residual, has been found. The parameters that were used in the step with the smallest residual are the results.

Inverse modeling has to deal with two fundamental problems:

- Initial values problem. If the start values of the fit parameters are too different from the correct values, the inversion algorithm may not find the correct values. The problem occurs when different sets of model parameters yield similar spectra, i.e. the problem is model specific.
- Fit strategy problem. Since there exists an infinite number of possible parameter values, an effective strategy of the iteration process must be found to select a new set of parameters from the previous set.

For both problems exists no general solution, and consequently no inversion algorithm finds always the best solution. To obtain reliable results, model specific tuning of the algorithm is necessary. Methods which provide usually good results are implemented in WASI. Fine-tuning of these methods by the user is supported.

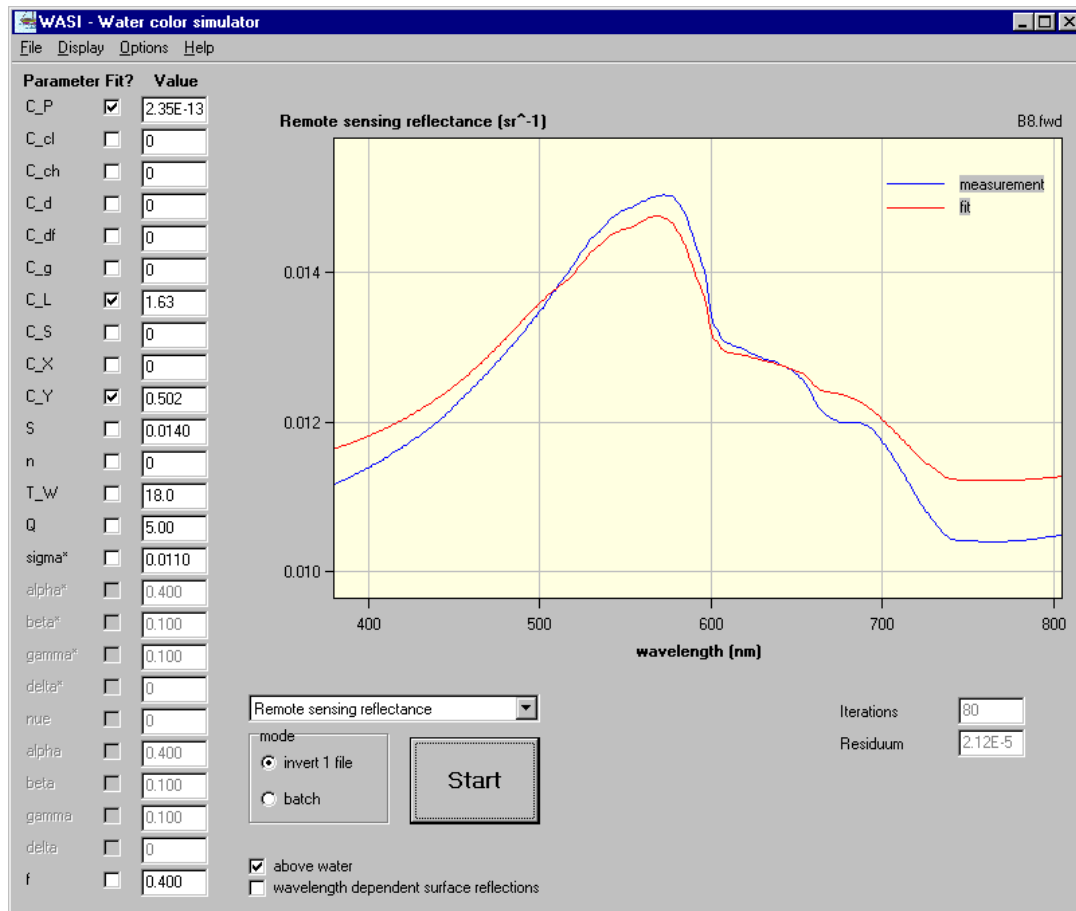


Fig. 4: User interface of the inverse mode.

An example of the user interface for the inverse mode is shown in Fig. 4. The symbols and values of all model parameters are listed on the left side. The parameter values are read from the INI file, they can be changed by editing the "Value" fields. Each parameter of the list can either be fitted or kept constant during inversion. Fitting is activated by checking the "Fit" box. In the example of Fig. 4 three parameters will be fitted (C_P, C_L, C_Y) after the "Start" button is pressed. Parameters not relevant in the actual mode of operation are disabled. There are 9 such irrelevant parameters in the example. They are relevant if the model for wavelength dependent surface reflections is chosen.

The graphic shows the input spectrum together with the resulting fit curve. In the example one of the 1331 spectra calculated in the forward mode has been inverted. If the model constants were set identical for forward and inverse modeling, the two curves were identical. Thus, the parameter sigma* was altered for illustration. This parameter is a wavelength-independent offset and characterises the Fresnel reflection of the water surface. In the forward mode it was set to 0.010, in the inverse mode to 0.011. With this error it is not possible to obtain a good fit curve by just fitting the concentrations of the water constituents. The best fit curve is shown, the corresponding fit parameters are listed on the left side. They are erroneous as a consequence of the sigma* error. If sigma* is also treated as fit parameter, all 4 parameters are correctly reproduced.

While single spectrum inversion allows to inspect in detail the results for a single spectrum, analysis of a large number of spectra is done effectively in the batch mode. Although the fit results are also in the batch mode automatically visualised on screen, there is normally not

much time for inspection because the screen is updated when the next result is available, and computing time is usually short. The required time depends on many factors like spectrum type, model, number of channels, number of fit parameters, fit strategy, initial values. To give an indication about the order of magnitude: all 1331 spectra calculated in the forward mode were read from file and then inverted fitting the three parameters C_P , C_L and C_Y . The start values of C_L (suspended matter concentration) were determined by pre-fitting the infrared spectral region (760 - 900 nm in 10 nm steps), the other start values were set to $C_P = 2 \mu\text{g/l}$ and $C_Y = 0.3 \text{ m}^{-1}$. The fit was performed from 400 to 700 nm in 1 nm steps. Under these conditions fitting of 1331 spectra required 224 seconds on a 450 MHz Pentium III notebook, i.e. the average computing time per spectrum was 0.17 sec.

The results are stored in a single text file, which tabulates the determined parameter values, the residual, and the number of iterations for each analysed spectrum. If desired, the fit curves can also be stored for later visualisation.

Conclusions. WASI is a software tool for analysing and simulating optical ship measurements. It summarises the experiences from 12 years of experimental and theoretical work performed at Lake Constance by DLR's Inland Water Group. These experiences are also part of the basis of software for processing multi- and hyperspectral airborne and satellite images, see the article of Heege et al. in this volume.

Work is not finished. In the moment, shallow water algorithms are under development. As soon as they are in operational stage, they will be included in WASI. It is planned to add further types of spectra, e.g. attenuation, further parameters, e.g. sun elevation and viewing angle, and further physical processes, e.g. fluorescence and Raman scattering. Furtheron, it is considered to include vertical profiles.

[1] WASI and a detailed manual can be downloaded from the directory [/pub/WASI](#) on the server <ftp.dfd.dlr.de>. Login: *anonymous*, password: *email address*.