ISUSPro The Satlantic ISUS Nitrate Processor Users Guide

Version 4.0

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1 Introduction

The Satlantic ISUS Nitrate Processor (**ISUSPro**) is a software utility to be used in conjunction with Satlantic's ISUS Nitrate Sensor. ISUSPro uses previously acquired data and provides a graphical representation of the data. Additionally, ISUS data can be reprocessed using different calibration data and processing parameters.

2 Software Installation

ISUSPro is available as a MS-Windows application. It requires MS-Windows NT, 2000, XP or higher operating system to run. A self-installing version of the program is available from Satlantic's website (<u>www.Satlantic.com</u>). In order to execute the program, the MatLab Component Runtime has to be installed. This component is present for all installations of MatLab 7 (R14). For users without a MatLab license, a stand-alone runtime is available from Satlantic.

Before installing ISUSPro, make sure that there is no other version installed. Otherwise, first uninstall the previous version. To install ISUSPro from CD, insert the CD into a CD drive and start the setup program. This can be done in Windows Explorer, or by selecting "**Run.**.." in the "**Start**" menu and typing "**D:\ISUSPro_4.0_Installer.exe**". (The CD drive letter may be different from D; the file name may differ for later software releases.) Follow the instructions on the screen. To install ISUSPro from the self-extracting install program, open the file in Windows Explorer or through the Start menu as described above.

3 Processing Data

3.1 Input Requirements

ISUSPro requires an **ISUS data file** as input. This file can be either logged by SatView (*.RAW) or internally by the ISUS instrument (*.DAT).

In order to read these files, **light and dark Telemetry Definition Format files** (* . TDF), which are distributed with the ISUS are needed.

Finally, a calibration **coefficient file** (ISUS*.CAL) is required for data processing.

Enter these input files either by typing the file names into the provided text boxes, or by using the three "Browse ..." buttons below the boxes. When browsing for the TDF files, enter both light and dark frame files at the same time.

When processing multiple data files, it is necessary to keep them all together with TDF and CAL files in a separate folder. All intermediate files and optional output files can then be found in sub-folders within that folder.

3.2 Preprocessing

Reading ISUS data files is a lengthy procedure for the ISUSPro software. For this reason, intermediate files are automatically generated in the 'tsn_files' sub-folder. These files can be deleted at any time. ISUSPro will regenerate them when needed.

3.3 Processing Parameters

Processing is done for one data file at a time.

A number of processing parameters can be adjusted, and it is possible to exclude selected extinction coefficients from the processing. In order to force the program to use the CAL file settings (only for Version 2 instruments), check the "Use CAL file as is" box.

Normally, a wavelength range of 216.5 to 240 nm should be used. Furthermore, the Baseline value should be set to "1" (linear baseline); other values are considered experimental and for troubleshooting purposes only. Average Darks are to be used; Seawater Darks can be used in ocean conditions when the instrument operates without its shutter.

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0.2			0.2					
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0.1 -			0.1 -					1
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Horizo	ntal Nitrate 💽	Single spectra		Coef1 Coef2	Coef3 Coef4	Coef5 Coef6	BL-0 B	L-1 BL-2
Vertic	al: Time <u>•</u>		Fit result:					

Figure 1: The ISUSPro graphical user interface.

3.4 Processing

Pressing the "Process" button starts processing. Depending on the size of the data file, processing may take a while. Progress reports are printed in the command window.

4 Viewing Data

Immediately after processing, two plots are displayed (Figure 2): The left panel displays the concentration of (initially) the first substance (usually nitrate) versus the acquisition time (vertical axis). The right panel displays averaged spectra and the absorbances of the different chemical species.

The user can select to display the concentration of other substances via selection in the 'Horizontal' Drop-down box.



Figure 2: The GUI after processing of the data.

4.1 Spectra

The right panel shows measured absorbance spectra and the components of its deconvolution: baseline, absorbance due to nitrate, bromide (salinity), optional third extinction coefficient, fitted absorbance spectra, and the difference between measured and fitted spectra (multiplied by a factor of 10 for easier viewing). Below the panel, the concentrations and baseline values corresponding to the displayed spectrum are displayed.

Immediately after selecting the "Process" button, an averaged spectrum is displayed. A single spectrum can be selected via the "Single spectra" buttons; a horizontal bar in the profile view indicates which spectra are displayed.

Using the "Fast Forward" or "Fast Backward" buttons ("<<" or ">>") causes the software to cycle through all spectra.

4.2 Change of Axis Limits

For both the profile and the spectra panel, the axis limits can be adjusted. For this purpose, there are two input text boxes at each axis of each panel. After entering the values, the respective "Rescale" button will redraw the plot using the new limits.

The vertical axis limits of the left plot show time (hours, minutes, seconds: in HH:MM:SS format) or depth (m). To edit seconds (if a profile is shown as a function of time) one has to first click on the required field using the left mouse button, then move to right using a keyboard button "->", and finally make the changes as required. Note that even if the starting time in hours is bigger than the end time (e.g. if measurements start at 23:59:00 and end at 00:05:00 of the next day) the indicated time series will be shown correctly since internally a year, month, and day are also considered.

4.3 Residuals

In order to get an overview of the quality of the entire data set, the residuals (i.e. the deviation of the fitted from the measured spectra) can be viewed for all acquired spectra in a 2-dimensional plot. To view the residuals, press the "Residuals (2-D)" button.

4.4 Saving Results

The processed data reside only in the program memory. For future use of processed data, for example within other applications, they can be written to an ASCII file using the "Save tofile" button. The name of the generated ASCII file will be identical to the selected MAT-file. The extension of the ASCII file will be CONC, and the *.CONC files will reside in an sub-folder asciifiles within the current data folder. The *.CONC files will contain only those data that were acquired by the ISUS; optional data will not appear via 'dummy' columns in the ASCII files.

5 Processing Parameters

The different processing parameters are explained in the ISUS manual and related literature. They are part of the ISSU setup, and it may be desired to 'rerun' an ISUS acquisition using a different set of processing parameters or an updated CAL file.

The **wavelength range** selects the part of the spectrum to be used for the calculations. All spectral values outside the given wavelength range are ignored. The default range from 216.5nm to 240.0nm was obtained by analyzing data acquired in different scenarios. Special environments may favor a slightly lower or higher range.

The default **baseline model** is linear. This is equivalent to the assumption that any wavelengthdependent instrument drift will be linear. In nearly all situations that were encountered, a linear model was sufficient to account for any drift. Using a quadratic baseline introduces an additional free parameter into the system of equations, and may adversely affect the stability of processing.

ISUS instruments generate better results using a **third thermal extinction coefficient**, which is present in all new CAL files. This coefficient can be turned off during processing by de-selecting the corresponding check-box in the processing pane.

Dark values of the instrument account for the thermal background noise of the sensors. The dark values are subtracted from the light values to correct for the thermal noise. Normally, the ISUS shutter blocks the path of light at regular intervals to measure the dark values. In the case of shutter failure, the shutter dark values can be replaced by the light values at very short wavelengths using the 'seawater darks' option. At these wavelengths, seawater completely absorbs UV radiation, thus providing an alternate source for the thermal noise correction. **This method does not work in freshwater.** Also, there is a slight difference between using a dark spectrum vs. a dark average when processing data. Assuming there is no shape to the dark spectrum, a dark average should prove more stable; if there is a shape to the dark spectrum, using an average introduces a bias.