Computation of Nitrate concentrations based on absorption spectra from OPUS / ProPS (TriOS)

Always take some reference samples for lab measurement, optics will support you to get high-resolution data, but can never replace reference sampling.

The data set of HE545 was collected with the UV sensor OPUS (TriOS). A matlab code to import data of the former instrument ProPS is also given. Here, only a set of spectra is provided to show how the data should look like. The CalculateNO3 script works with both sensors as long as it follows the format.

Step 1: Preparation in the laboratory

- Collect reference salinity spectra (“ReferenceSalinity”) with your instrument using low nutrient seawater with 35 psu.
- Measure the temperature of your salinity reference (you have to adapt the temperature in the CalculateNO3 script later, line 82 “calibrateTemperature”).
- Collect reference nitrate spectra (“ReferenceNitrate”) with your instrument with a defined concentration, e.g. 25 µmol/L (you have to adapt the nitrate concentration in the CalculateNO3 script later, line 127)

Step 2: Preparing raw data files

- Download absorption and reference data from your instrument
- Produce three text-files, as shown with the example data:
  - *'XXX_absorption.txt'*
  - *'ReferenceNitrate.txt'*
  - *'ReferenceSalinity.txt'*

Step 3: Load table of CTD based data

- Create a temperature- and a salinity-table from CTD data or from additional used sensors including date and time
- Use the ***ImportData_TS.m*** to import your CTD data table into MATLAB
- The MATLAB script automatically creates following variables:

  - *sampleSalinity.mat*
  - *sampleTemperature.mat*
  - *DateTime.mat*
  - *NitrateWetChem.mat*
- Import date/time, measured temperatures [°C] and measured salinities [‰] to your workspace (mat-files). Before running the “CalculateNO3” script these three variables have to be in your workspace

Step 4: Import raw data files into MATLAB

- Use the *ImportDataOPUS.m* / *ImportDataProPS.m*
- The MATLAB script automatically creates following variables:
  - *wavelength.mat*
  - *ReferenceNitrate.mat*
  - *ReferenceSalinity.mat*
  - *absorption.mat*

Step 5: Adapt own data to the CalculateNO3 script.

- Adapt the temperature (“calibrateTemperature”) of salinity reference (line 82)
- Adapt reference concentration of nitrate before calculating NO3 (line 127)
- Check and adapt the wavelength range of your instrument (line 99, 107, 121)

Step 6: Choose CDOM-Offset correction (function statements)

- 'Last': Last value will be subtracted from the spectrum
- 'Linear': Offset is determined using a linear interpolation
- 'Quadratic': Offset is determined using a quadratic interpolation

Step 7: MATLAB Input

```
k = length(absorption);
for i = 1: k
resultNO3(i,1)=CalculateNO3(absorption(:,i), sampleSalinity(i), sampleTemperature(i),
DateTime(i),'Linear',0);
end
```

Step 8: Check results

- As result you will receive nitrate concentrations in [µmol/L] for each observation
  - Column 1: Date and time
  - Column 2: Nitrate concentration
- Furthermore, results will automatically be exported to a .dat-file

- Compare calculated nitrate concentrations with reference samples measured in laboratory using wet-chemical methods (different plot functions are given in Matlab)
- Depending on region and composition of CDOM different functions for the correction can be chosen. Reference samples of nitrate should always be taken, chose for yourself how much is efficient.

For more details, check following reference publications:

Frank, C, Meier, D; Voß, D; Zielinski, O (2014): Computation of nitrate concentrations in coastal waters using an in situ ultraviolet spectrophotometer: Behavior of different computation methods in a case study a steep salinity gradient in the southern North Sea. Methods in Oceanography. Volume 9, April 2014, Pages 34-43. doi: 10.1016/j.mio.2014.09.002

Sakamoto, C M; Johnson, K S; Coletti, L J (2009): Improved algorithm for the computation of nitrate concentrations in seawater using an in situ ultraviolet spectrophotometer. Limnol.Oceanogr.: Methods 7, 132-143. doi: 10.4319/lom.2009.7.132

Zielinski, O; Voß, D; Saworski, B; Fiedler, B; Koertzinger, A (2011): Computation of nitrate concentrations in turbid coastal waters using an in situ ultraviolet spectrophotometer. J Sea Res 65: 456-460. doi: 10.1016/j.seares.2011.04.002

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