Radiometry, apparent optical properties: measurements and uncertainties

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The quest for "truth"



Why do we care about uncertainties?

We want to:

- Do good science
- Be useful for space agencies by providing them with high-quality validation data
- Be useful for other potential users who have to make some decision from the data we provide
- Be able to quantify long-term trends in satellite ocean colour radiometry data ("climate-quality data records")

That's all about metrology and deployment protocols and data processing techniques

The "Guide to the Expression of Uncertainty in Measurement" (GUM): <u>https://www.bipm.org/documents/20126/2071204/JCGM_100_2008_E.pdf/cb0ef43f-baa5-11cf-3f85-4dcd86f77bd6</u>





With:

p: water-air Fresnel reflection coefficient

n: refractive index of seawater

L_u(z): upwelling radiance at depth z

K: diffuse attenuation coefficient for Lu

Is it actually that "simple"?

Where the uncertainties come from?

Radiometer (Es), 3 solar panels and junctior. box, ARGOS beacon, wireless Ethernet link to the ship, and flashing light 4 m Radiometers (Ed, Eu, nadir Lu) Fluorometer, transmissometer 9 m 5 m Battery, computer, tilt and compass Radiometers (Ed, Eu, nadir Lu) Fluorometer, transmissometer, CTD, Backscattering meter Center of gravity (CG) at 6.8 m above the base of the buoy 8.2 m Center of buoyancy (CB) at 3.8 m above the base of the buoy 2.8 m 82 m

A practical example: the BOUSSOLE buoy

- $L_u(z)$, $E_u(z)$ and $E_d(z)$ measured at 2 depths
- E_s measured at +4.5 m above sea level
- Used to derive R_{rs}

 $K_{Lu} = \ln(\frac{L_u(z_1)}{L_u(z_2)})/(z_2 - z_1)$

Bialek, A., V. Vellucci, B. Gentili, D. Antoine, J. Gorroño, N. Fox and C. Underwood, 2020. Monte Carlo–Based Quantification of Uncertainties in Determining Ocean Remote Sensing Reflectance from Underwater Fixed-Depth Radiometry Measurements, J. Atmos. Ocean. Tech. 37, DOI: 10.1175/JTECH-D-19-0049.1

$$L_{\rm w} = \frac{1 - \rho}{n^2} L_{{\rm u}, z_1} \exp(-K_{\rm u} z_1) f_h + 0$$

Combining uncertainties

If x, ..., w are measured with independent and random uncertainties $\delta x, ..., \delta w$, and are used to compute q = x + ... + z - (u + ... + w), then the uncertainty in q is the quadratic sum:

$$\delta q = \sqrt{(\delta x)^2 + ... + (\delta z)^2 + (\delta u)^2 + ... + (\delta w)^2}$$

If x, ..., z are measured with independent and random uncertainties $\delta x, ..., \delta z$ and are used to compute q(x, ..., z) then the uncertainty in q is

$$\delta q = \sqrt{\left(\frac{\partial q}{\partial x}\delta x\right)^2 + \dots + \left(\frac{\partial q}{\partial z}\delta z\right)^2}$$

From R. Palmer, "Propagation of Uncertainty through Mathematical Operations" https://web.mit.edu/fluids-modules/www/exper_techniques/2.Propagation_of_Uncertaint.pdf

What do we do if uncertainties are not independent and random?

- One option is the "Monte Carlo" technique:
- 1- Define the "Probability distribution functions" of individual uncertainties (can be normal, log normal, rectangular, ...) and the sensitivity coefficients
- 2- Run the measurement equation multiple times, each time with a different subset of values for each of the uncertainty sources. These values are randomly "picked" from the PDFs, hence the "Monte Carlo" terminology
- 3- Produce enough outputs so that you end up with a distribution of the quantity of interest, e.g., L_w.
- 4- The average and stdev of this distribution will give you the uncertainty

Type A and B uncertainties

- Type A uncertainty:

- You can derive it from a series of measurements.
- This is essentially the variance of the mean

- Type B uncertainty (from the "GUM")

When the standard uncertainty is evaluated by scientific judgement based on all of the available information on the possible variability. The pool of information may include:

- previous measurement data;
- experience with or general knowledge of the behaviour and properties of relevant materials and instruments;
- manufacturer's specifications;
- data provided in calibration and other certificates;
- uncertainties assigned to reference data taken from handbooks.

Example at BOUSSOLE





Antoine D, Vellucci V, Banks AC, Bardey P, Bretagnon M, Bruniquel V, Deru A, Hembise Fanton d'Andon O, Lerebourg C, Mangin A, Crozel D, Victori S, Kalampokis A, Karageorgis AP, Petihakis G, Psarra S, Golbol M, Leymarie E, Bialek A, Fox N, Hunt S, Kuusk J, Laizans K, Kanakidou M. ROSACE: A Proposed European Design for the Copernicus Ocean Colour System Vicarious Calibration Infrastructure. Remote Sensing. 2020; 12(10):1535. https://doi.org/10.3390/rs12101535

Confidence intervals

0.1% 0.5%

-2.5

-1.5

-1

-2

-0.5

0

Standard deviation

0.5

1.5

Uncertainty is given with respect to a given confidence interval:

 $u(y) = \pm 3 \text{ cm}$ at the 68.2% coverage probability (1 σ or k = 1) at the 95.4% confidence level $u(y) = \pm 6 \text{ cm}$ at the 95.4% coverage probability (2 σ or k = 2)

0.5% 0.1%

2.5

Slide from A. Bialek, 2016 6th IOCCG Summer Lecture Series, INCOIS, Hyderabad, India, 4-15 November 2024

More on uncertainties

Lectures by Agnieska Bialek, IOCCG SLS 2016

https://www.ioccg.org/training/SLS-2016/Bialek-L1.pdf https://youtu.be/V4bCOCnu3cQ

https://www.ioccg.org/training/SLS-2016/Bialek-L2.pdf https://youtu.be/rYyzVCId7FI

The "Guide to the Expression of Uncertainty in Measurement" (GUM): https://www.bipm.org/documents/20126/2071204/JCGM 100 2008 E.pdf/cb0ef43f-baa5-11cf-3f854dcd86f77bd6

Uncertainty sources

-Instrument itself

-How it is deployed in the field

-How quantities of interest (e.g., R_{rs}) are derived from the measurements

Instrument-related uncertainty sources

Radiant Flux and its conversion

Quantity	Symbol	SI units	Abbreviation	Notes
Radiant Energy	Q	joule	J	energy
Radiant Flux	Φ	watt	W	radiant energy per unit time, so called radiant power
Radiance	L	watts per square metre per steradian	W/m^2/sr	power per unit solid angle per unit projected source area
Irradiance	E	watts per square metre	W/m^2	power incident on a surface

Radiant Flux (Power) joules (energy) time

 $\Phi = \frac{dQ}{dt}$

Measured by Quantum (photon) Detectors



Light Detectors

Photomultiplier tube (PMT)

- photoelectric effect electron dislodged from the metal cathode amplified by successive dynodes to produce electron 'cascade'
- extremely sensitive light detectors
- degradation of dynodes due to electron bombardment
- stable, high voltages needed (power consumption)
 - thermal effects



http://learn.hamamatsu.com/articles/photomultipliers.html

Semiconductors (i.e., silicon photodiodes used in PAR sensors, OCRs etc.)

 photon-induced excitation of electrons to the conduction band of the silicon, producing a current

Diode Arrays (like HOCR, DALEC, Ramses)

- Linear or 2D area arrays of small photodiode 'pixels' i.e., 256 pixels @ ~10um spacing
- Allows direct alignment with a diffracted beam (spectral resolution) or imaging (2D)
- Pixels usually need to be 'read out' sequentially lower sampling rate

Current to Voltage Converters



Transimpedance Amp

- Sensitivity defined by gain resistor
- Instantaneous voltage output, directly proportional to photocurrent
- Feedback capacitor acts as temporal "smoother" filter
- Common approach used in individual photodiode-based sensors i.e. PAR and multispectral where signal is strong



Switched Integrator Amp

- Sensitivity defined by storage **capacitance value** AND the **duration** that the Reset switch is open
- Time discrete voltage 'readouts'
- This is where spectrometer "Integration Time" comes from
- Used for diffraction-based devices where signal is low (diode array spectrometers)

Analog (V) to Digital Conversion

Converts analog (continuous) voltage data into discretised "counts"



There are many different (~15) types of ADC architecture.

ADC Resolution defined as the number of digital numbers used to represent the converted analog photo current

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2-bit resolution = 2^2 = 4 Counts (as shown above)
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10-bit resolution = 2^{10} = 1024 Counts
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16-bit resolution = 2^{16} = 65536 Counts

ADC resolution does not necessarily equate to measurement resolution, might be digitizing noise.

https://commons.wikimedia.org/wiki/File:2-bit_resolution_analog_comparison.png

What to do about this?

- Instrument design adapted to what type of measurements are aimed at and in which environment
- Instrument laboratory characterization
- Instrument laboratory calibration

Instrument design

- Size, shape (self shading, ease of use)
- Heat dissipation (in-water or in-air instrument)
- Collectors design (in-water or in-air instrument)
- Design and quality of the optics
- Quality of the detectors (linearity, dynamic range, SNR, blooming?)
- Choice of electronics
- Internal temperature control
- Internal temperature measurement

Instrument lab characterisation

A number of instrument characteristics have to be assessed (quantified)

- Linearity of the detectors' response
- Spectral calibration
- Spectral band response functions (filters)
- Immersion coefficients
- Temperature dependence
- Sensitivity to polarization of the incoming (ir)radiance
- Straylight
-

Instrument lab calibration

Radiometric Calibration

- Need to compare the sensor's digital counts to a radiant flux standard so we can quantify light accurately.
- See Ocean Optics Protocols

Ocean Optics Protocols For Satellite Ocean Color Sensor Validation, Revision 4, Volume II:

Instrument Specifications, Characterization and Calibration

NASA/TM-2003-21621/Rev-Vol II

James L. Mueller, Giulietta S. Fargion and Charles R. McClain, Editors J. L. Mueller, C. Pietras, S. B. Hooker, R.W. Austin, M. Miller, K.D. Knobelspiesse, R. Frouin, B. Holben and K. Voss, Authors.

Radiometric Calibration

- Need (at minimum)
- a stable calibrated power supply
- a NIST-traceable FEL lamp (50h)
- Lambertian reflector for L (NIST)









Calibration Uncertainty

- Lamp calibration coefficients E_{50} are within 1% of NIST when less than 1 year old, and less than 50 hours burn time...
- Scale E₅₀ using distance "r" between plaque and lamp surface.
- Measure it accurately without touching the lamp or the lambertian reflector? +/- 1mm hopefully
- Delta-f. (distance between the filament and lamp surface) Which part of the filament?
- Spectralon Plaque Reflectivity / Cleanliness
- Power supply accuracy is important (8A)
- Buy a good (expensive) one
- Verify voltage over calibrated shunt resistors V=IR
- Relies on the wavelength calibration of detector
- use line emission source to verify and compensate if necessary, they do drift! i.e. 4nm in 15 years

Calibration source

The ocean environment



https://www.bsballasts.com/Workshop/N_Unzner/English/ Halogen_Curve_big2.htm



Morel/Antoine 1994, JPO

Independent checks



Intercomparison of instruments, useful to identify issues with the response of some of them

Cosine Response



Field Cosine Response









Also see, Zibordi et. al. 2017 jtech

Do not panic!

- The characterisation / calibration process is generally well performed by manufacturers (although you cannot necessarily blindly rely on this)
- Manufacturers will improve if we start discussing these issues in papers.
- Radiometric protocol documents to be updated to include new sensors?
- Add sensible error bars and move on !?
- The bigger the error bars, the easier disparate datasets can be said to "agree"

Deployment-related uncertainty sources

What makes radiometry measurement "special"?



The value of a radiometric quantity at a given point in the water column (e.g., the downward irradiance at a depth of 10 m) instantaneously results from the interaction of the light field (photons) with the atmosphere and water over a large spatial domain around the measurement point



Environment- and deployment-related

Uncertainty sources in measurement of radiometric quantities

What to consider?

- Weather:
 - Is the sky could-free or overcast or cloudy? If the sky is cloud-free, how clear is it? Is the sea rough? Can I see white caps? Significant sea spray?
- Water:
 - How clear or turbid the water is?
 - Can I suspect strong vertical stratification?
 - How homogeneous are the waters around me?
- Platform and deployment:
 - How big is the ship I'm working from? Can I move my instrument far enough from it?
 - Where can I install my deck Es reference, if any? Is it gimbaled?
 - Can I easily communicate with the bridge? Do you have enough help on the deck?
- Instrument: (other than characterization/calibration considerations) Did I clean the optical surfaces?
 - Was the instrument properly stored, e.g., away from excessive heating source?
 - Cables and connectors have been checked?

Various techniques to get to AOPs



Ruddick, K.G.; Voss, K.; Boss, E.; Castagna, A.; Frouin, R.; Gilerson, A.; Hieronymi, M.; Johnson, B.C.; Kuusk, J.; Lee, Z.; Ondrusek, M.; Vabson, V.; Vendt, R. A Review of Protocols for Fiducial Reference Measurements of Water-Leaving Radiance for Validation of Satellite Remote-Sensing Data over Water. Remote Sens. 2019, 11, 2198. https://doi.org/10.3390/rs11192198



Ruddick, K.G.; Voss, K.; Boss, E.; Castagna, A.; Frouin, R.; Gilerson, A.; Hieronymi, M.; Johnson, B.C.; Kuusk, J.; Lee, Z.; Ondrusek, M.; Vabson, V.; Vendt, R. A Review of Protocols for Fiducial Reference Measurements of Water-Leaving Radiance for Validation of Satellite Remote-Sensing Data over Water. Remote Sens. 2019, 11, 2198. https://doi.org/10.3390/rs1119 2198

Measurement uncertainty

The platform

Hooker and Morel, JAOT, 2003





The platform

Hooker and Zibordi, Applied Optics 44(4), 2005





Data processing-related uncertainty sources

The following slides barely "scratch the surface" They are only a few examples of typical data processing steps that can lead to significant uncertainties

Data reduction

- Going from raw data to profiles (or time series) of the desired quantity (e.g., $L_u(z)$ or E_s). Applying calibration, and "filtering"



https://insitumarineoptics.com



Getting Es from a non-gimbaled sensor

The $E_s(\lambda)$ spectrum can be reasonably well simulated (need to know date, time, lat, long, and atmosphere parameters such as pressure, aerosol optical thickness, wind speed, ozone...)



An example for fixed-depth measurements (Antoine et al., JGR, VOL. 113, C07013, doi:10.1029/2007JC004472)



An example for profile measurements (unpublished data from BOUSSOLE)



Conclusion / message

-Extrapolation technique matters!

-There is definitely more to be done in that space to improve the quality of our data sets



(unpublished data from BOUSSOLE)





Method	Es	Kd
RRS1	Surface E _s measurements, corrected for cosine response. Spectral FOR loop median of data with less than 5 degree tilt	Full Cast model fit of E _d (z-)/(0.96*E _s) = exp(K _d *z)
RRS2	$\label{eq:surface} \begin{array}{l} \textbf{Surface} \ E_s \ measurements, \ corrected \ for \ cosine \ response, \ combined \ with \ subsurface \ data \ (corrected \ for \ transmission). \ Double \ parameter \ exponential \ fit \ yielding \ E_s \ and \ K_d \ using \ full \ cast \end{array}$	Full Cast model fit of $E_d(z-)=(0.96*E_s)*$ $exp(K_d*z)$
RRS3	Surface E_s measurements, corrected for cosine response, combined with subsurface data (corrected for transmission). Double parameter exponential fit yielding E_s and K_d using only R_{rs} depths for extrapolation (initial 1/K _d estimate)	Re-run model fit of $E_d(z-)=(0.96*E_s) *$ $exp(K_d*z)$ using data from 1/K _d or shallower
RRS4	Subsurface Irradiance data (corrected for transmission). Double parameter exponential fit yielding E _s and K _d using full subsurface cast	Full Cast model fit of $E_d(z-)=(0.96*E_s)*$ $exp(K_d*z)$
RRS5	Subsurface Irradiance data (corrected for transmission). Double parameter exponential fit yielding E _s and K _d (initial 1/K _d estimate)	Re-run model fit of $E_d(z)=(0.96*E_s) *$ exp(K_d*z) using data from 1/K_d or shallower





ABOUT MISSIONS DATA DOCS SOFTWARE & TOOLS SERVICES GALLERY FORUM

CVO AOP Workshop Presentations

- Introduction Stanford Hooker
- Survey Summary Stanford Hooker
- Web-Based Processor Stanford Hooker
- GSFC Processor Stanford Hooker
- ODU Processor Richard Zimmerman
- UCSB Processor David Siegel
- USF Processor Dave English
- LOV Processor David Antoine
- SeaBASS Processor Jeremy Werdell
- SIO Processor (1) Mati Kahru
- Biospherical Processor John Morrow
- SIO Processor (2) Dariusz Stramski
- HOBI Labs Processor David Dana
- WHOI Processor Heidi Sosik
- FURG Processor Carlos Garcia
- NMFS Perspective Cara Wilson
- SIO Processor (3) Kozlowski
- MLML Processor Stephanie Flora, Carol Johnson
- Legacy Processors David Siegel
- Practical Cal/Val Sean Bailey
- Hyperspectral Processing David Dana
- Case2 Working Group Stanford Hooker
- ICESS Dave Menzies

https://oceancolor.gsfc.nasa.gov/community/meetings/aop 2009/presentations



Comparing data sets

Deriving the same quantity, e.g., R_{rs} , derived from simultaneous radiometry measurements using different techniques 10^{-2} MAD: 0.000151 / 0.000014 sr⁻¹





Comparison buoy-Free fall profiling (Antoine et al., JGR, VOL. 113, C07013, doi:10.1029/2007JC004472)

Comparison of 2 in-water profilers (Antoine et al., Optics Express, 2021, https://doi.org/10.1364/OE.412022)





Optical closure

What is this?

- Derive radiometric quantities and AOPs from radiative transfer using measured IOPs as inputs, and compare to the measured radiometric quantities and AOPs



- Total absorption, total scattering and the phase function (PF)
- Boundary conditions (sun elev., interface, bottom)

Main question is: do I have the required information to make it relevant?

- The particulate matter PF is generally unknown: the backscattering ratio must be known
- Typically: an AC-S would give you the required absorption and scattering data



An example from a "Thetis profiler", deployed off Rottnest Island, Western Australia

Example of programs addressing the uncertainty issue



FRM4SOC - Fiducial Reference Measurements for Satellite Ocean Colour



Eye of an algal storm. Copernicus Sentinel data (2015)/ESA

The FRM4SOC project, with funding from ESA, was structured to provide support for evaluating and improving the state of the art in ocean colour validation through a series of comparisons under the auspices of the Committee on Earth Observation Satellites (CEOS) Working Group on Calibration & Validation and in support of the CEOS ocean colour virtual constellation. FRM4SOC also strives to help fulfil the <u>International Ocean Colour Coordinating Group</u> (IOCCG) in situ ocean colour radiometry white paper objectives and contribute to the relevant IOCCG working groups and task forces (e.g. the working group on uncertainties in ocean colour remote sensing and the ocean colour satellite sensor calibration task force).

The project makes a fundamental contribution to the European

system for monitoring the Earth (Copernicus) through its core role of working to ensure that ground-based measurements of ocean colour parameters are traceable to SI standards. This is in support of ensuring high quality and accurate Copernicus satellite mission data, in particular Sentinel-2 MSI and Sentinel-3 OLCI ocean colour products. The FRM4SOC project also contributes directly to the work of ESA and EUMETSAT to ensure that these instruments are validated in orbit.

<u>https://frm4soc.org</u> <u>https://frm4soc2.eumetsat.int</u>

https://www.mdpi.com/journal/remotesensing/special issues/2nd_ocean_color_RS



Example of programs addressing the uncertainty issue



RESEARCH

NPL

Earth observation, climate and optical

We help to improve the quality of data collected through Earth observation systems and satellites

https://www.npl.co.uk/earth-observation



https://ioccg.org



Thanks for your attention