

Web Appendix 2

Measurement uncertainty analysis

Kevin G. Ruddick,¹ Vera De Cauwer,² and Young-Je Park

Management Unit of the North Sea Mathematical Models (MUMM), Royal Belgian Institute for Natural Sciences (RBINS), 100 Gulledele, B-1200 Brussels, Belgium

Gerald Moore

Plymouth Marine Laboratory, Prospect Place, Plymouth PL1 3DH, United Kingdom

The uncertainty of measurements of $\rho_w(\lambda)$ and of the derived similarity spectrum $\bar{\rho}_{\text{wn } 780}(\lambda)$ arising from the method described in the main text is assessed here. This uncertainty is considered to arise from three main sources (Zibordi et al. 2002, 2004):

- Instrument calibration and performance,
- correction for air-sea interface reflection, and
- optical changes of the water induced by the measurement platform.

For validation of satellite measurements, further uncertainties arise from spatiotemporal differences between seaborne and satellite measurements. However, this is not relevant in the present context.

Instrument calibration and performance

The three instruments were calibrated at the Plymouth Marine Laboratory (PML) in August 2001 and June 2002 in the framework of the MERIS validation team. All three instruments were calibrated in the same laboratory conditions (lamp, straylight, etc.) within a 2-h period. Further checks were made during laboratory intercalibrations at GKSS in November 2002 and PML in December 2002, and since November 2002 further relative calibrations were made at the start of each cruise using the white LED-based portable TriOS-FieldCAL unit (Regeling and Wernand 2001), which proved stable at 450 nm and for the range 520–700 nm to within 2% (better stability could possibly be obtained for the range 450–520 nm with better thermal control). Calibration measurements were also made by the instrument manufacturers, TriOS, in April 2001 and July 2003.

Although differences of order 10% (spectrally rather flat and of the same magnitude for all three sensors) were found in some cases in the absolute calibration from the various laboratories and are thought to arise from uncertainties in lamp output, these uncertainties are greatly reduced when reflectances are calculated because of division of radiances

by irradiances calibrated from the same lamp. All calibrations showed that the two radiance sensors were extremely stable over the 2-yr period with relative drift of one sensor compared with the other of <1%.

According to estimates made here for the range 650–900 nm, the main instrument-related reflectance measurement uncertainties arise from (in order of decreasing importance) possible temporal change in sensitivity, especially for the irradiance sensor, estimated as up to 3% and spectrally correlated to within $\pm 0.5\%$; departure from cosine response of the irradiance sensor, evaluated as <1.5% for the range of sun zenith angles typical of most measurements (35–55°) and spectrally correlated to within $\pm 0.2\%$; uncertainty in the reflectance of the Spectralon plaque used for radiance calibrations estimated as 1%, spectrally correlated to within $\pm 0.25\%$; and polarization sensitivity of the radiance sensors, evaluated as <1% except for the range 800–850 nm (1.5%). These uncertainties, evaluated from data at 50 nm intervals, are combined by quadrature sum to give the relative uncertainty of reflectance measurements denoted as “instrument calibration” in Table 1. The effect of possible water droplets on the radiance sensors was assessed in the GKSS laboratory as of order 2%, thus justifying the careful procedure adopted for protecting lenses between stations and for checking absence of droplets before each measurement.

The impact of all these instrumental uncertainties on the normalized reflectance spectrum in the range 650–900 nm (“Instrument calibration” row of Table 2) is greatly reduced by their spectral correlation because of partial cancellation when reflectance ratios are taken. For example, the temporal change in radiometer sensitivities gives an absolute error of <0.01 in calculation of $\Delta\rho_{\text{wn } 780}(\lambda)$ because of cancellation of near-white uncertainties.

Air-sea interface reflection

Correction for reflection of sky radiance at the air-sea interface reflection, as represented by the term $\rho_{\text{sky}}L_{\text{sky}}^{0+}/E_{\text{d}}^{0+}$, is made here by

$$\rho_{\text{sky}} = 0.0256 + 0.00039W + 0.000034W^2$$

$$\text{for } \frac{L_{\text{sky}}^{0+}(750)}{E_{\text{d}}^{0+}(750)} < 0.05 \quad (1)$$

¹ Corresponding author (K.Ruddick@mumm.ac.be).

² Present address: Polytechnic of Namibia, P/Bag 13388, Windhoek, Namibia.

Table 1. Estimation of relative reflectance measurement uncertainty $\Delta\rho_w/\rho_w$ for (a) $\rho_w(780) = 0.001$ and (b) $\rho_w(780) = 0.007$.

	Wavelength (nm)					
	650	700	750	800	850	900
Instrument calibration	0.035	0.033	0.034	0.035	0.033	0.029
Air-sea interface (a)	0.229	0.192	0.165	0.145	0.129	0.114
Air-sea interface (b)	0.033	0.027	0.024	0.021	0.018	0.016
Total $\Delta\rho_w/\rho_w$ (a)	0.232	0.195	0.169	0.149	0.133	0.118
Total $\Delta\rho_w/\rho_w$ (b)	0.048	0.043	0.042	0.041	0.038	0.033

derived from model simulations by Mobley (1999). This correction is a critical problem for above-water reflectance measurements (Hooker et al. 2002) for the following reasons:

- Wave slope statistics: Eq. 1 supposes that the statistics of the wave slopes forming the air-sea interface can be modeled using wave statistics (Cox and Munk 1954) as a function of locally observed wind speed. However, wave slope statistics in reality depend on many more factors, including wave orientation (Hooker and Morel 2003); spatial distribution of wind speed (e.g., for swell waves generated remote from the test site); air-sea temperature difference; time history of wind (young vs. well-developed sea); local wave-current interactions; presence of surface films, etc.

- Integration time: Eq. 1 supposes also that the integration time of sea-viewing measurements is sufficiently long that averaging over all wave slopes is valid. For the current measurements the integration time is adapted by the instrumentation to give optimal signal:noise ratio with no sensor saturation and corresponds to 1–2 s for most measurements reported here. The effect of sampling frequency is assessed for much faster instruments but for a viewing geometry with sunglint contamination by Hooker et al. (2002).

- Sky radiance distribution: Eq. 1 is based on model simulations that use an idealized clear blue sky radiance distribution (Harrison and Coombes 1988). With this model the whole sky radiance distribution can be modeled from the sky radiance, L_{sky}^{0+} , measured within the field of view of the instrument. ρ_{sky} represents an integration over wave slopes taking account of both the varying Fresnel reflectance and the varying sky radiance for waves that reflect from portions of the sky not directly measured. Although reasonable for clear, blue skies, this parameterization of ρ_{sky} can be seriously inaccurate if clouds just outside the portion of the sky directly measured as L_{sky}^{0+} are reflected at the air-sea interface into the sea-viewing sensor. In such cases the effective ρ_{sky} could be much larger (e.g., factor 2) than that estimated here and will also be wavelength-dependent (Mobley 1999).

- Instrument deployment: further uncertainties in ρ_{sky} arise from deployment issues (ship roll, tilt and yaw) relating to variation of viewing angles from the specified zenith of 40° and azimuth of 135° with respect to sun and from measurement of wind speed.

A complete discussion of these issues is beyond the scope of the present study but is considered in a number of the above-mentioned and other references (Carder and Steward 1985; Fougnie et al. 1999; Toole et al. 2000). However, it is clear that the measurement uncertainty is highly dependent on (1) the scan rejection criteria adopted, as noted by Hooker et al. (2002) but for instruments with faster sampling and a viewing geometry with more severe sun glitter; (2) the scan averaging procedure; and (3) the criteria used to select data for this study. In particular, the restriction of data to stations with clear sunny skies, as defined by the test used to evaluate ρ_{sky} , and the elimination of stations with high standard deviation over the scans used for averaging (usually relating to high wave conditions and hence highly variable ρ_{sky}) are crucial.

In view of the procedure adopted for scan and data selection, the overall measurement uncertainty associated with correction for air-sea interface reflection is estimated via an uncertainty for the air-sea interface correction coefficient of $\Delta\rho_{\text{sky}} = 0.003$, chosen arbitrarily but roughly equivalent to the difference in ρ_{sky} for W of 4 and 8 m s⁻¹. This gives an absolute uncertainty for estimation of water-leaving reflectance of $\Delta\rho_w = \pi\Delta\rho_{\text{sky}}L_{\text{sky}}^{0+}/E_d^{0+}$. Typical values of $L_{\text{sky}}^{0+}/E_d^{0+}$ for the sunny sky filtered measurements presented here are 0.0243, 0.0162, and 0.0121, respectively, at 650, 780, and 900 nm, giving corresponding $\Delta\rho_w$ errors of 0.00023, 0.00015, and 0.00011. This absolute error is independent of ρ_w and is, therefore, relatively less important for higher reflectances as shown by comparing cases (a) and (b) in Table 1. Uncertainties can be much greater (e.g., factor 10) for the rejected stations, where clouds are present in the sky-viewing direction, owing to greatly increased $L_{\text{sky}}^{0+}/E_d^{0+}$. Wind

Table 2. Estimation of absolute normalized (similarity) reflectance measurement uncertainty $\Delta\rho_{\text{wn } 780}$ for cases with (a) $\rho_w(780) = 0.001$ and (b) $\rho_w(780) = 0.007$.

	Wavelength (nm)					
	650	700	750	800	850	900
Instrument calibration	0.0058	0.0044	0.0039	0.0026	0.0040	0.0095
Air-sea interface (a)	-0.5289	-0.3828	0.0099	-0.0301	0.0349	0.0519
Air-sea interface (b)	-0.0756	-0.0547	0.0014	-0.0043	0.0050	0.0074
Total absolute $\Delta\rho_{\text{wn } 780}$ (a)	0.5289	0.3828	0.0107	0.0303	0.0351	0.0527
Total absolute $\Delta\rho_{\text{wn } 780}$ (b)	0.0758	0.0549	0.0042	0.0050	0.0064	0.0121

Table 3. Estimation of relative normalized (similarity) reflectance measurement uncertainty $\Delta\rho_{\text{wn } 780}/\rho_{\text{wn } 780}$ for cases with (a) $\rho_{\text{w}}(780) = 0.001$ and (b) $\rho_{\text{w}}(780) = 0.007$.

	Wavelength (nm)					
	650	700	750	800	850	900
Normalized spectrum $\rho_{\text{wn } 780}$	4.953	3.757	1.013	1.145	0.616	0.409
Total relative $\Delta\rho_{\text{wn } 780}/\rho_{\text{wn } 780}$ (a)	0.107	0.102	0.011	0.026	0.057	0.129
Total relative $\Delta\rho_{\text{wn } 780}/\rho_{\text{wn } 780}$ (b)	0.015	0.015	0.004	0.004	0.010	0.030

speeds $>10 \text{ m s}^{-1}$ also generate higher measurement uncertainties because of the higher and more variable waves. Both the case of cloudy sky and high wind are excluded from the current data set.

The impact of this uncertainty on the similarity spectrum $\rho_{\text{wn } 780}(\lambda)$ is given by $\Delta\rho_{\text{wn } 780}(\lambda)$ as defined by

$$\Delta\rho_{\text{wn } 780}(\lambda) = \frac{\rho_{\text{w}}(\lambda) + \Delta\rho_{\text{w}}(\lambda)}{\rho_{\text{w}}(780) + \Delta\rho_{\text{w}}(780)} - \frac{\rho_{\text{w}}(\lambda)}{\rho_{\text{w}}(780)} \quad (2)$$

To first order in $\Delta\rho_{\text{w}}/\rho_{\text{w}}$, this gives

$$\Delta\rho_{\text{wn } 780}(\lambda) = \frac{1}{\rho_{\text{w}}(780)}[\Delta\rho_{\text{w}}(\lambda) - \rho_{\text{wn } 780}(\lambda)\Delta\rho_{\text{w}}(780)] \quad (3)$$

The uncertainty is thus inversely proportional to the measured water-leaving reflectance (i.e., as backscatter increases, the uncertainty in the NIR reflectance ratios associated with air-sea interface reflection becomes correspondingly smaller). This uncertainty is also smallest for wavelengths with $\rho_{\text{wn } 780}$ close to unity owing to approximate cancellation of the two terms in Eq. 3.

Taking the above-mentioned values for $\Delta\rho_{\text{w}}$ at 650, 780, and 900 nm gives, for a moderately turbid measurement with $\rho_{\text{w}}(780) = 0.001$, a corresponding absolute uncertainty for $\Delta\rho_{\text{wn } 780}$ of 0.529 at 650 nm and 0.053 at 900 nm. For highly turbid reflective water with $\rho_{\text{w}}(780) = 0.007$, these absolute uncertainties for $\Delta\rho_{\text{wn } 780}$ are correspondingly reduced to 0.076 at 650 nm and 0.007 at 900 nm as shown in Table 2.

Ship perturbation

A further source of uncertainty is the perturbation of the light field induced by the measurement platform (ship) itself. For the turbid waters and viewing geometry considered, this will arise primarily from reflection of sunlight from the above-water ship hull and superstructure onto the water patch being viewed. Thus, for part of the downwelling radiance field reaching the water target, the diffuse sky radiance measured by the downwelling irradiance sensor will effectively be replaced by radiance reflected from the ship. Such effects have been assessed experimentally for underwater reflectance measurements (Zibordi et al. 1999) and for above-water reflectance measurements in nonoptimal side-viewing geometry and case 1 waters (Hooker and Morel 2003). For the present data set the ship perturbation is thought to be small compared with other measurement uncertainties because of the optimal mounting of the sea-viewing sensor at the prow facing forward (Hooker and Morel 2003). This viewing geometry minimizes the solid angle

subtended by the ship at the measured water volume and ensures that any reflection of direct sunlight from the ship hull into the water near the measured water volume occurs for high incidence angle and thus contributes very little to the underwater downwelling irradiance (Deschamps et al. 2004).

Total uncertainty

The total measurement uncertainty is given by the quadrature sum of the uncertainties detailed in the first two sections of this Appendix, which are assumed independent. The relative uncertainty of reflectance measurements is given in Table 1 for two cases of moderate and high reflectance. The air-sea correction uncertainty is clearly very high for low reflectances, whereas the instrument-related error becomes dominant for high reflectances. Spectral correlation of the various uncertainties gives an effective reduction when the uncertainties are calculated for the similarity spectrum, $\rho_{\text{wn } 780}(\lambda)$ as given in absolute and relative terms in Tables 2 and 3.

References

- CARDER, K. L., AND R. G. STEWARD. 1985. A remote-sensing reflectance model of a red-tide dinoflagellate off west Florida. *Limnol. Oceanogr.* **30**: 286–298.
- COX, C., AND W. MUNK. 1954. Measurements of the roughness of the sea surface from photographs of the sun's glitter. *Journal of the Optical Society of America* **44**: 834–850.
- DESCHAMPS, P.-Y., B. FOUNGIE, R. FROUIN, P. LECOMTE, AND C. VERWAERDE. 2004. SIMBAD: A field radiometer for satellite ocean color validation. *Applied Optics* **43**: 4055–4069.
- FOUNGIE, B., R. FROUIN, P. LECOMTE, AND P.-Y. DESCHAMPS. 1999. Reduction of skylight reflection effects in the above-water measurement of diffuse marine reflectance. *Applied Optics* **38**: 3844–3856.
- HARRISON, A. W., AND C. A. COOMBES. 1988. An opaque cloud cover model of sky short wavelength radiance. *Solar Energy* **41**: 387–392.
- HOOKE, S. B., G. LAZIN, G. ZIBORDI, AND S. MCLEAN. 2002. An evaluation of above- and in-water methods for determining water-leaving radiances. *Journal of Atmospheric and Oceanic Technology* **19**: 486–515.
- HOOKE, S. B., AND A. MOREL. 2003. Platform and environmental effects on above-water determinations of water-leaving radiances. *Journal of Atmospheric and Oceanic Technology* **20**: 187–205.
- MOBLEY, C. D. 1999. Estimation of the remote-sensing reflectance from above-surface measurements. *Applied Optics* **38**: 7442–7455.
- REGELING, G. M., AND M. R. WERNAND. 2001. FieldCAL: A por-

- table field calibration unit for RAMSES hyperspectral radiometers, p. 22. NIOZ-TRIOS report.
- TOOLE, D. A., D. A. SIEGEL, D. W. MENZIES, M. J. NEUMANN, AND R. C. SMITH. 2000. Remote-sensing reflectance determinations in the coastal ocean: Impact of instrumental characteristics and environmental variability. *Applied Optics* **39**: 456–469.
- ZIBORDI, G., J. P. DOYLE, AND S. B. HOOKER. 1999. Offshore tower shading effects on in-water optical measurements. *Journal of Atmospheric and Oceanic Technology* **16**: 1767–1779.
- ZIBORDI, G., S. B. HOOKER, J. F. BERTHON, AND D. D'ALIMONTE. 2002. Autonomous above-water radiance measurements from an offshore platform: A field assessment experiment. *Journal of Atmospheric and Oceanic Technology* **19**: 808–819.
- ZIBORDI, G., F. MÉLIN, S. B. HOOKER, D. D'ALIMONTE, AND B. HOLBEN. 2004. An autonomous above-water system for the validation of ocean colour radiance data. *IEEE TGARS* **42**: 401–415.