- **1** A method to extrapolate the diffuse upwelling radiance attenuation coefficient
- 2 to the surface as applied to the Marine Optical Buoy (MOBY)
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- 19 Abstract: 250 words

20	The upwelling radiance attenuation coefficient (K_{Lu}) in the upper 10 m of the water
21	column can be significantly influenced by inelastic scattering processes, and thus
22	will vary even with homogeneous water properties. The Marine Optical BuoY
23	(MOBY), the primary vicarious calibration site for many ocean color sensors,
24	makes measurements of the upwelling radiance (L_u) at 1 m, 5 m, and 9 m and uses
25	these values to determine K_{Lu} and propagate the upwelling radiance directed
26	toward the zenith, L_u , at 1 m to and through the surface. Inelastic scattering causes
27	the K_{Lu} derived from the arm measurements to be an underestimate of the true K_{Lu}
28	from 1 m to the surface at wavelengths greater than 570 nm, thus the derived water
29	leaving radiance is underestimated at wavelengths longer than 570 nm. A method
30	to correct this K_{Lu} , based on a model of the upwelling radiance including Raman
31	scattering and chlorophyll fluorescence has been developed which corrects this
32	bias. The model has been experimentally validated, and this technique can be
33	applied to the MOBY data set to provide new, more accurate products at these
34	wavelengths. When applied to a 4 month MOBY deployment, the corrected water
35	leaving radiance, L_w , can increase by 5% (600 nm), 10% (650 nm) and 50% (700
36	nm). This method will be used to provide additional more accurate products in the
37	MOBY data set.

1. Introduction

40 The Marine Optical Buoy (MOBY) (Clark *et al.* 1997, 2002) has been the
41 primary vicarious calibration site for many, if not all, ocean color satellite

instruments since 1997 (Barnes et al. 2001, Eplee et al. 2001, Franz et al. 2007,
Wang et al. 2013). This data set provides the water leaving spectral radiance,
$$L_w(\lambda)$$
, and normalized water leaving radiance, $L_{wn}(\lambda)$, to satellite programs for use
in the vicarious calibration process (Clark *et al.*, 1997), and as such is required to
provide these parameters with the highest possible accuracy. MOBY has three
arms, at 1 m, 5 m, and 9 m depth, for measuring the upwelling radiance, $L_u(\lambda, z)$,
so the shallowest depth that MOBY measures L_u is at 1 m. To propagate this
measurement to the surface requires an estimate of $K_{Lu}(\lambda, 0, 1)$, the diffuse
upwelling radiance attenuation coefficient for the depths from 0 m – 1 m (hereafter
referred to as K01 for simplicity). The diffuse attenuation coefficient between

53
$$K_{Lu}(\lambda, z_1, z_2) = -\frac{\ln[L_u(\lambda, z_2) / L_u(\lambda, z_1)]}{z_2 - z_1}$$

54 Also needed are the transmission of the air-sea interface for upwelling radiance, 55 and the index of refraction of the water to account for refractive effects on the 56 radiance due to the air-sea interface. These latter two parameters are assumed to 57 be constant but K01 is variable and must be determined for each data set. 58 The current estimate of K01 is derived by using this upper arm measurement at 59 1 m, combined with either the measurement of $L_u(\lambda, z)$ at 5 m or 9 m. In general, the pair of measurements at 1 m and 5 m are used to form $K_{Lu}(\lambda, 1, 5 m)$ (K15) and 60 61 this is assumed to represent K01. For the MOBY products named $L_w l$, and $L_{wn} l$, 62 $L_{u}(\lambda, 1m)$ is propagated to the surface using K15. For wavelengths greater than 63 570 nm, in the clear water where MOBY is located, because of inelastic processes, 64 both due to Raman scattering (Sugihara et al. 1984) and due to chlorophyll

65	fluorescence (Gordon 1979), $K_{Lu}(\lambda)$ is not constant with depth. In general, for these
66	wavelengths K15 will be less than K01 due to the increasing fraction of light that
67	has been inelastically scattered from the blue region of the spectrum, where energy
68	is abundant, to the red region, where the incoming light is rapidly attenuated. It
69	has been pointed out that using K15 in place of K01 in the region above 570 nm
70	causes the $L_w(\lambda)$ and $L_{wn}(\lambda)$ derived from MOBY to be an underestimate of their
71	true values. (Li et al., 2016). This paper will describe a method to estimate the
72	correct K01 using a validated model of K01 in terms of K15 and K19 along with
73	the measured K15 and K19

75 **2. Model and validation**

As described above, the goal is to develop a model for estimating K01 given K15, K19, or K59 or some combination of these. The model is derived by simulating the in-water light field utilizing radiative transfer computations.

79 The site where MOBY is located, off of the island of Lanai, Hawaii, can typically 80 be considered Case 1 waters, meaning that the inherent optical properties 81 (absorption and scattering coefficients, etc.) covary with the concentration of 82 Chlorophyll a (Chl) (Morel and Prieur 1977), and can be modeled using the single 83 parameter Chl. At the site, the range of Chl is also quite limited and is between 0.05 mg/m^3 and 0.15 mg/m^3 over 98% of the time. In addition, since the MOBY 84 85 measurements are made for the specific purpose of satellite vicarious calibration, 86 the measurements are usually performed within 3 h of solar noon, which results in

87 a somewhat limited range of solar zenith angles (<50°). Thus the parameter space 88 which must be filled with model results is limited. With these constraints, a 89 Monte-Carlo radiative transfer model, including Raman inelastic scattering was used to determine K01, K15 and K19 for four values of Chl (0 mg/m³, 0.05 mg/m³, 90 0.10 mg/m^3 , 0.15 mg/m^3), six solar zenith angles (SZA=10°, 20°, 30°, 40°, 50°, 91 92 and 60°), and for every 10 nm from 400 to 700 nm. 93 As expected, the results from this Monte Carlo model show that K_{Lu} depends 94 on the pair of depths used, Chl, and solar zenith angle. Figure 1 shows the Monte 95 Carlo results for 3 different Chl values for K01 as a function of wavelength at 10° 96 SZA. Also shown are K15/ K01, K59/ K01, and K19/ K01 for the 3 Chl values. 97 For wavelengths less than 575 nm, K01 is the same as K15 and K19 to within 3%. 98 Above 575 nm, the K_{Lu} 's rapidly diverge. The effect of using one of these K_{Lu} 99 values to provide K01 would be to underestimate L_w or L_{wn} in this spectral region. 100 Above 700 nm the values would continue to diverge, but because of issues such as 101 instrument self-shadowing (Gordon and Ding, 1992; Mueller, 2007) and very 102 small L_w , MOBY data above 700 nm are not used for vicarious calibration, and 103 will not be discussed in this paper. 104 Other features to note in Fig. 1 are that the best approximation for K01 is K15 105 followed by K19. K59 deviates the most from K01. When an error analysis is 106 carried out on the various environmental effects that can interfere with the 107 calculation of $K_{Lu}(\lambda)$, excluding inelastic effects, K19, because it spans a larger 108 depth range, has the least uncertainty. Thus, we will concentrate on the 109 relationship between K15 (because it is the closest to K01) and K19 (because it

theoretically should have the least uncertainty), and not discuss K59 until theappendix.

112	$K_{Lu}(\lambda)$ also depends on the solar zenith angle. Figure 2 shows the variation of
113	the modeled K01 with SZA, Chl is 0.10 mg/m^3 . As expected, particularly for
114	wavelengths above 600 nm, there is a stronger dependence on solar zenith angle at
115	angles greater than 30° than on Chl, for the range of Chl expected at the MOBY
116	site. Fortunately, for any specific measurement the solar zenith angle is known, so
117	an appropriate set of K_{Lu} 's can easily be determined.
118	To validate these model results, we used a dataset of hyperspectral $L_u(\lambda, z)$
119	measurements performed in the Hawaiian islands (Yarbrough et al., 2007a). It is
120	difficult to make measurements both near the surface, and in the region above 600
121	nm, where instrument self-shading is a large factor due to the high absorption of
122	water itself. A specialized instrument was developed to operate in this spectral
123	region, which was based on a Remotely Operated Vehicle (ROV) with a fiber
124	collector extending a meter in front of the ROV. (Yarbrough et al. 2007b). The
125	fiber extended from the ROV to the ship, where it was coupled to a spectrometer
126	with 1 nm resolution from 350 nm to 900 nm. The ROV was placed at several
127	different depths, so profiles of the near surface water column could be obtained. A
128	subset of data from this experiment was selected to validate these model results.
129	We selected profiles that were in deep water, had measurement depths within 10
130	cm of the surface paired with measurements at least 1 m and 5 m depths (but often
131	there was also a measurement at 9 m depth), and were performed in a reasonably
132	short period of time. As part of the criteria, the K_{Lu} 's derived from the

measurement pairs had to agree to within 0.03 m⁻¹ for the wavelength range from
400 nm to 550 nm.

135 Figure 3 shows the comparison between the model and ROV data for 4 representative data sets. The model results here assume a Chl value of 0.10 mg/m^3 136 137 and the model results are interpolated to match the SZA of the data. It shows that 138 the model represents the measured K15 and K01 reasonably well except for the 139 region between 660 and 700 nm where chlorophyll fluorescence (which was not 140 included in the original model) is important. Making a model which includes this 141 fluorescence from first principles is difficult because, as opposed to Raman which 142 depends on the physical properties of water (Bartlett et al., 1998), chlorophyll 143 fluorescence depends not only on the amount of chlorophyll in the water, but also 144 on the physiological status of the phytoplankton containing the chlorophyll (Keifer, 145 1973). The light history, packaging, and many other factors can affect the 146 quantum efficiency of fluorescence, η , and thus, the depth of the feature, or "Dip", 147 in K_{Lu} . To include the Dip in our model requires that we use more information 148 from each individual data set.

To determine the magnitude of the Dip in K_{Lu} we went back to our ROV data set and relaxed the selection criteria to include more data. In this case we allowed measurements that varied less than 0.1 m⁻¹ in the region between 400 and 550 nm, and additionally required that $K_{Lu} < 1 \text{ m}^{-1}$ between 660 and 700 nm. This had the effect of excluding data that had larger variations of surface irradiance during measurement than we could handle with the typical downwelling sky irradiance, *Es*, normalization procedures. We then formed a baseline using measurements at

156	660 nm and 700 nm, and found the difference between this baseline and the
157	measured K_{Lu} for each K_{Lu} (K01, K15, K19, and K59). Each data set was then
158	normalized to the value at 681 nm, to derive an overall shape for the Dip. The
159	average shape and standard deviation is shown in Fig. 4. The sharp feature in the
160	data at 687 nm is caused by an atmospheric oxygen absorption band at this
161	wavelength, and the associated line filling, similar to Fraunhofer line filling (Ge et
162	al., 1995). This is illustrated by including results of modeling this chlorophyll Dip
163	with and without the oxygen feature, as shown in Fig. 4. In this figure the model
164	assumed Chl = 0.1 mg/m ³ , SZA= 10°, and η =0.045. What can be seen, however, is
165	that the average of the data is a very good representation of the Dip (the standard
166	deviation is small) and we use this average to develop our correction to K01 for
167	this feature.
168	To handle the variation of the Dip with the physiological parameters of the
169	phytoplankton, we investigated the data and found there was a consistent
170	relationship between the depth of the Dip at 681 nm in K15 (Dip15) and K19
171	(Dip19) as shown in Fig. 5. We also found that while there was a relationship
172	between Dip15 and Dip19 ($r^2 = 0.69$), there was not a relationship between either
173	Dip15 and Dip01 ($r^2=0.003$) or between Dip19 and Dip01 ($r^2=0.019$). There was
174	also not a relationship between Dip05 and Dip59. There was also no dependence
175	of Dip01 with Chl or incident irradiance (although all the data, as with MOBY data,
176	were collected within ± 2 h of solar noon). Thus we were forced to assume a
177	constant value of -0.10 $\text{m}^{-1} \pm 0.02 \text{ m}^{-1}$ for the Dip01 at 681 nm.
178	3. Correction algorithm

We now have validated all of the steps necessary to form a correction

algorithm for the inelastic effects. The steps in the correction algorithm for eachdata set are:

182 1) Interpolate the model K_{Lu} tables to get the correct model K_{Lu} 's for the

183 specific solar zenith angle of that data set. The model was also interpolated to the

184 MOBY wavelengths using a spline interpolation.

185 2) Use the solar zenith interpolated tables to find which Chl (used as an index)

186 forms the best match between measured and modeled K15 and K19 at 500 nm.

187 Using the average of these two retrieved values for Chl, interpolate the tables to188 find K01.

189 3) Add the average Dip01 scaled by -0.10 m^{-1} at 681 nm.

4) Below 500 nm K01_{final} is the average of the measured values K15 and K19.

191 5) Above 570 nm, K01_{final} is the modeled K01.

6) Because the measured K15 and K19 is a very good representation of K01 in
the region below 570 nm, see Fig. 1, the modeled K01 is blended into the average
of the measured K15 and K19 over the region from 500 to 570 nm using the

195 equation:

196
$$K01_{\text{final}}(\lambda) = \frac{(\lambda - 500 \,\text{nm})}{70 \,\text{nm}} K01 + \frac{(570 \,\text{nm} - \lambda)}{70 \,\text{nm}} (K15 + K19)/2$$
(3)

197 This K01_{final} can then be used in the data reduction process to propagate $L_u(\lambda, 1$ 198 m) to the surface to find $L_w(\lambda)$ and $L_{wn}(\lambda)$. Along with this, we can get an estimate 199 of the uncertainty in this value if we look at the differences between the correction 200 predicted from the two measured K_{Lu} 's. Note that this uncertainty only reflects the 201 uncertainty introduced by this process, and not the uncertainty in the fundamental

202values of K15 and K19. For the region below 500 nm, the uncertainty in the
$$K_{Lu}$$
203correction can be obtained by the difference in the measured K15 and K19.204Following section 4.3.6 of the GUM 2008 (JGCM, 2008) we estimate the205uncertainty below 500 nm to be:206 $\frac{|K15 - K19|}{2}$ (4)

. . .

.1

Above 570 nm this uncertainty is given by: 207

1 17 10 10 1

~ ~ ~

208
$$\frac{|K01(K15) - K01(K19)|}{2}$$
(5)

209 where K01(K15) refers to the K01 derived from the Chl found in the K15

210 measurement, and K01(K19) refers to the K01 derived from the Chl found in the 211 K19 measurement. The region between 500 nm and 570 nm blends these two 212 values, as in Eq. 3.

213 To show the effect this has on a set of MOBY data, Fig. 6 shows the original K_{Lu} used to propagate the $L_u(\lambda, 1 m)$ to the surface, along with the new modeled 214 K01_{final}. In addition, it shows the results of the uncertainty calculation as described 215 216 above. For most of the spectra, as expected, K01_{final} has not changed. However, 217 above 550 nm it starts to depart and rapidly becomes much larger than the original K_{Lu} . The uncertainty meanwhile is much less than 0.01 m⁻¹ through much of the 218 spectrum, but increases in the red to be on the order of 0.01 m^{-1} to 0.02 m^{-1} , much 219 smaller than the difference between the original and modeled K_{Lu} . 220 221 Figure 7 shows the effect of this change on the calculated L_w , which we call

222 $L_w 21$ to differentiate it from the heritage $L_w 1$. The major effect is in the red

223 wavelengths, where L_w is very small in either case. As can be seen in the right panel of Fig. 7, while there is no change below 550 nm, the percent difference between the old and new L_w grows to be on the order of 50% by 700 nm. For the region between 600 nm and 700 nm, this correction makes a significant difference to the data.

Figures 8 and 9 show the effect of using K01_{final} in the calculation of L_w when averaged over several bands of the Sentinel 3A Ocean Land Color Instrument (OLCI) (Donlon *et al.* 2012). In Fig. 8, there is little to no effect in the blue and green wavelengths as would be expected. However, Fig. 9 shows that there is a significant difference for the channels between 600 nm and 700 nm. This change is much larger than our uncertainty of the correction, and shows that this correction reduces a significant bias in the MOBY data set at these wavelengths.

4. Conclusion

We have shown that there is a significant bias in the MOBY L_w and L_{wn} data set for wavelengths above 570 nm due to the influence of Raman scattering and Chl fluorescence in the estimation of K_{Lu} . With a validated model, we can use the existing measurements of K15 and K19 to adjust the model for K01 for each data set. We can also use this to estimate the uncertainty in the K01 used to propagate $L_u(\lambda, 1 \text{ m})$ to the surface to produce $L_w(L_w21)$ and $L_{wn}(L_{wn}21)$ for satellite

242 vicarious calibration.

243 While we have concentrated this work on illustrating the effect and developing 244 a correction algorithm specifically for the MOBY sensor, this work may be 245 generalized in that all in-water measurements must account for this non-linear K_{Lu}

246 near the surface for wavelengths greater than approximately 550 nm. This is

247	applicable both to systems that have fixed measurement depths and profiling
248	systems. It is obvious from this work, that for fixed measurement depth systems,
249	such as MOBY, a correction, using models must be made. Note that for a similar
250	system, the BOUSSOLE site, the modeled Lw includes the effect or Raman, but
251	not Chl flouresence. (Antoine et al., 2008) However, it is also true that for
252	profiling systems the effect of Raman scattering must be taken into account.
253	Seldom, in real world situations, can accurate measurements of the upwelling
254	radiance be made in upper 1 m of the water column. It is often the case that, to
255	reduce noise, the measurements in the upper 10 m of the water column of a profile
256	are accumulated to extrapolate the measurements to the upwelling radiance just
257	below the surface (Zibordi et al., 2011). Often this extrapolation is done assuming
258	a logarithmic decay of the radiance with depth, which is similar to assuming that
259	the K_{Lu} is constant with depth. As has been shown, this is not the case at these
260	longer wavelengths and either modeling must be done to extrapolate the
261	measurements to the surface, or, at the least, the extrapolation must be done
262	allowing for a non-linear decay of the log transformed radiance with depth.
263	

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267 Appendix A

268	The preferred MOBY data product for vicarious calibration of ocean color
269	satellites is the $L_w l$ or $L_{wn} l$ product. As discussed earlier, this product uses $L_u(\lambda, \lambda)$
270	1m) and K15 to generate $L_u(\lambda, 0)$, the upwelling radiance just below the sea
271	surface, which is then transmitted through the surface to form $L_w I$ or $L_{wn} I$, the
272	latter after normalization by the downwelling surface irradiance.
273	While MOBY has arms, and measurements, at 1 m, 5 m, and 9 m, at times the
274	measurements from one of the arms is not available, limiting the options for
275	deriving $L_u(\lambda, z)$ or K_{Lu} . When the 5 m arm is unavailable, we must use K19 to
276	propagate $L_u(\lambda, 1m)$ to the surface and this product is named $L_w 2$ (or $L_{wn} 2$). In this
277	case the technique described in the text can be used, but the estimation of K01
278	must depend only on K19, and will be called L_w22 (or $L_{wn}22$) to differentiate it
279	from $L_w 21$. This does not have a large effect on the processing, as in general the
280	K01 predicted from K15 and K19 agree quite well. Unfortunately, it is more often
281	the case that if an arm is not available, it is the upper arm that is missing. In this
282	case one is left with K59 and propagating $L_u(\lambda, 5m)$ to the surface to form $L_u(\lambda, 0-)$,
283	this product is called L_w7 and $L_{wn}7$. As was shown in Fig. 1, K59 is affected much
284	more strongly than K15 or K19 by inelastic processes, and the propagation to the
285	surface of $L_u(\lambda, 5m)$ is very sensitive to the K_{Lu} used. In addition, we are not
286	modeling K01, but rather K05. However, we can still generate an algorithm that
287	can improve our $L_w 7$ and $L_{wn} 7$ product.

In this variation of the algorithm we use K59 to generate a model K05, in a manner similar to the method described earlier. The Dip05, derived from an average of experimental data, as before, has a magnitude of $0.085 \text{ m}^{-1} \pm 0.009 \text{ m}^{-1}$ at 681 nm.

291	To generate the uncertainty for this new product (called $L_w 27$ or $L_{wn} 27$) we can
292	look at how well $L_w 27$ agrees with these other products when we have all 3 arms
293	available. A similar situation occurs if we are missing either the 5 m or 9 m
294	measurement, the uncertainties have to be based on how well the final products
295	statistically agree with each other when all three arms are available. Figure 10a
296	shows a comparison between 4 products, $L_w 1$, $L_w 7$, $L_w 21$, and $L_w 27$ for Band 8
297	(665 nm) on the Sentinel 3 OLCI sensor. These products were generated for a
298	recent MOBY deployment (M253) for which all arms were operational. The OLCI
299	sensor is chosen as an example because it has several bands in the wavelength
300	range between 600 and 700 nm. As can be seen, the heritage products $L_w I$ and
301	L_w7 are significantly different than L_w21 and L_w27 , however the L_w21 and L_w27
302	agree with each other quite closely. To see this agreement more quantitatively, Fig.
303	10b shows a histogram of the percent difference between $L_w 21$ and $L_w 27$. There is
304	only a -1.2% bias (with a standard deviation of 7%) between these two products.
305	This can be compared to the 20% bias between $L_w 21$ and $L_w 1$, and 186% bias
306	between $L_w 27$ and $L_w 7$. $L_w 27$ is a significant improvement over $L_w 7$, and a good
307	substitute for $L_w 21$ when the top arm is unavailable.

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387 Figure Captions

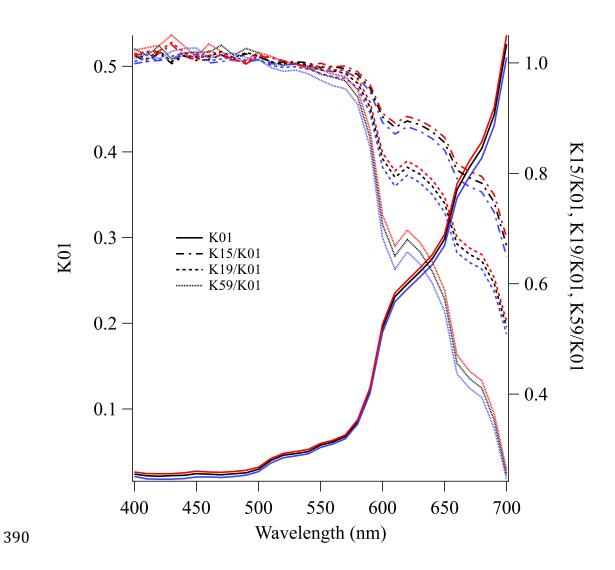


Figure 1) Modeled K01 (left axis) along with the modeled ratios K15/ K01 and K19/ K01 and K59/ K01 (right axis) for Chl = 0.05 mg/m^3 (blue), Chl = 0.10 mg/m^3 (black), and Chl = 0.15 mg/m^3 (red), all at 10° SZA.

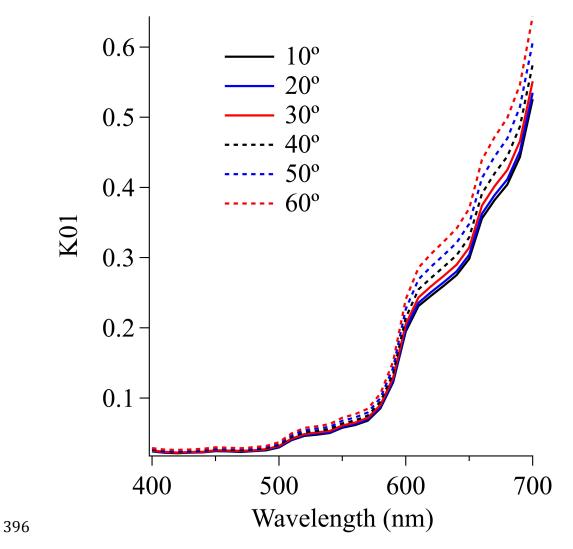


Figure 2) Variation in modeled K01 with wavelength and solar zenith angle, with Chl= 0.1 mg/m^3 .

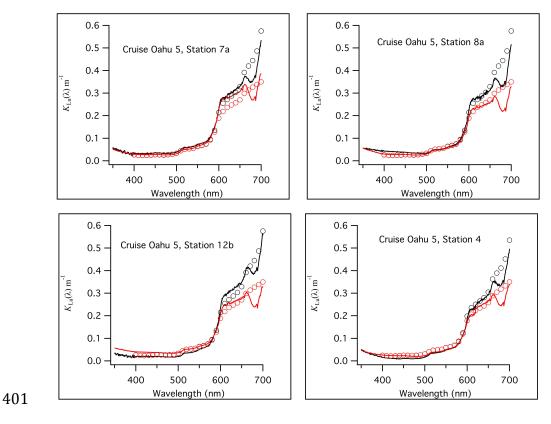


Figure 3) Comparison of modeled and ROV data. The model is displayed as
circles, data as solid lines. Red represents K15 while black is K01. Model data
were interpolated to appropriate solar zenith angle, but assumed a constant Chl
value of 0.10 mg/m³. Note in these graphs, the effect of Chl fluorescence has not
been included in the model results.

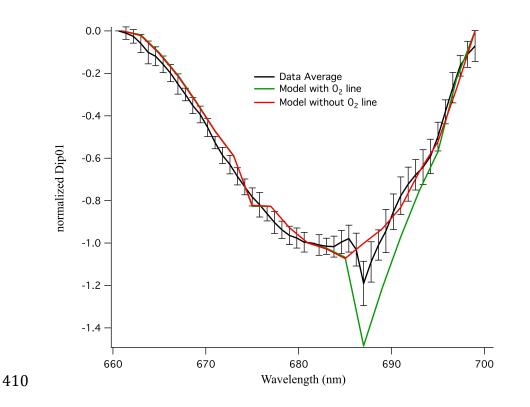


Figure 4) The deviation of K_{Lu} from a straight baseline between 660 nm and 700 nm, due to Chl fluorescence and an atmospheric oxygen absorption band at 687 nm. The average of the data is shown, along with the standard deviation of this average. Also shown are the model results with and without the oxygen band. In the model the Chl = 0.1 mg/m³, SZA= 10°, and η =0.45.

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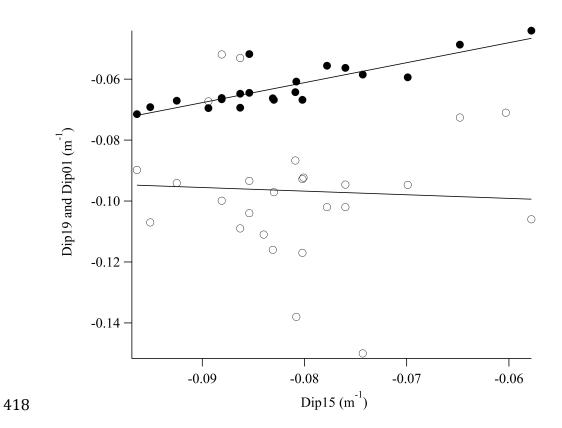
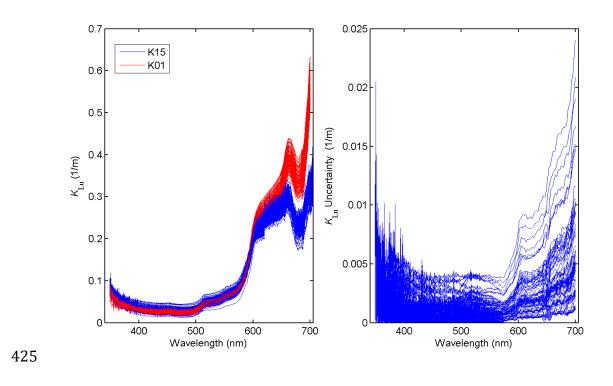


Figure 5) Dip19 and Dip01 versus Dip15 (all values for the Dip at 681 nm). The lines are a linear least square fit to the data. Dip19 are filled circles while Dip01 are open circles. As can be seen Dip15 and Dip19 have a relationship with each other ($r^2=0.69$) while Dip01 and Dip15 have no significant relationship ($r^2=0.003$).

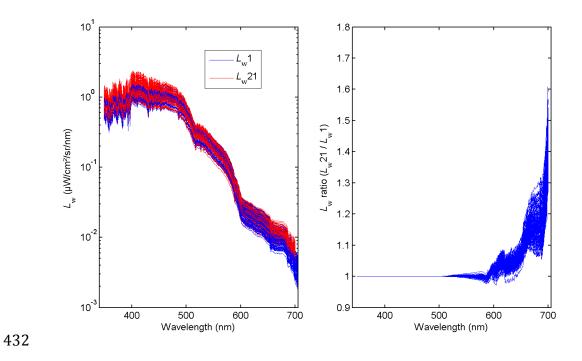




427 Figure 6) The modeled $K01_{final}$ along with the original K15 for a full MOBY

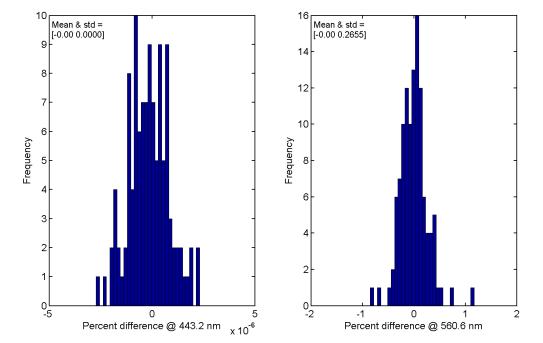
428 deployment (M253). The left panel shows the K_{Lu} values, while the right panel

429 shows our estimated uncertainty associated with the correction procedure.



433 Figure 7) Effect of using K01_{final} rather than K15 on the retrieved L_w . The left 434 panel shows the $L_w l$ and $L_w 2l$, while the right panel shows $L_w 2l/L_w l$. There is no

435 effect before 550 nm, above which the difference grows to 50%.



440 Figure 8) Histograms of the 100*($L_w21 - L_w1$)/ L_w21 for two bands of the Sentinel

3A, OLCI sensor. These are the 443 nm and 560 nm bands. The mean and

standard deviation of the change can be seen in the upper left of the figures. As

can be seen and as expected, there is a negligible change to $L_w I$ in these

wavelengths.

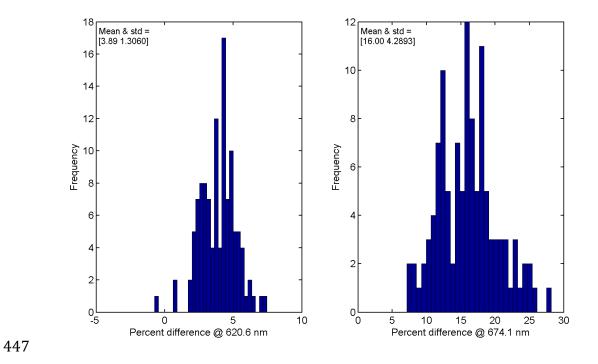


Figure 9) Similar to Fig. 8, but for the Sentinel 3A OLCI channels at 620 nm and
674 nm. As the wavelengths get longer, the effect of this change grows due to the
correction for the Raman scattering and Chl fluorescence.

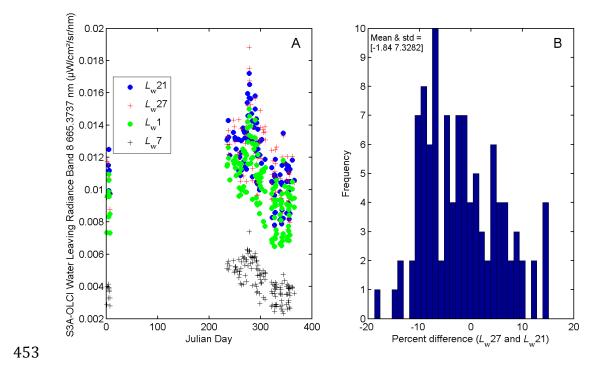


Figure 10) In panel (A) we show $L_w(665 \text{ nm})$ resulting from the different processing procedures, as described in the text, for a recent MOBY deployment that had all three arms operational for 665 nm. $L_w I$ is significantly different from $L_w 7$, $L_w 21$ and $L_w 27$, however the two new processing procedures ($L_w 21$ and $L_w 27$) agree quite closely. This is shown quantitatively in (B) where a histogram of the percent difference between $L_w 21$ and $L_w 27$ is presented. The bias between these products (-2%) and standard deviation (7%) are shown on the figure.