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Assessing Uncertainties in Satellite Ocean Color Bio-Optical Properties

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ABSTRACT

Uncertainties in retrievals of bio-optical properties from satellite ocean color imagery are related to a variety of factors, including errors associated with sensor calibration and degradation, atmospheric correction, and the bio-optical inversion algorithms. Here we examine the impact of uncertainties in the top-of-atmosphere (TOA) radiances and coefficients in the quasi-analytical algorithm (QAA) on the satellite estimation of the normalized water-leaving radiances (${}_nL_w$) and downstream bio-optical properties, such as the absorption and backscattering coefficients and chlorophyll. We use a Moderate Resolution Imaging Spectroradiometer (MODIS) image, free from clouds, covering the Gulf of Mexico, as our data set. We apply ensembles at each pixel in the image to simulate noise on the satellite TOA radiance values (randomly-distributed in the range of ±2.0%) at MODIS visible wavelengths, as well as the two near-infrared (NIR) wavelengths used for atmospheric correction. For each set of ensemble runs, we assess the effect of uncertainty on ${}_nL_w$ and bio-optical retrievals by analyzing the results spectrally for a coastal and open ocean region within our test image. In general, we found that as little as 2% uncertainty (noise) in the TOA radiances can significantly change ${}_nL_w$ retrievals, absorption and backscattering coefficients across the visible wavelengths, as well as derived chlorophyll values. We also use ensembles to analyze sensitivity of coefficients in the QAA algorithm. By varying coefficients in the algorithm, we can quantify the impact of uncertainties on the backscattering coefficient of suspended particles (b_{bp}). Within the QAA algorithm, we vary coefficients used in calculating remote sensing reflectance (R_{rs}) and the exponent used in calculating b_{bp}.

INTRODUCTION

TOA radiances from multi-spectral sensors used for remote sensing, such as MODIS and VIIRS, and the hyper-spectral sensor, HICO, are subject to frequent calibration. There are ongoing efforts to apply vicarious calibration and to generate new look-up tables used for creating new spectral TOA radiances [1,2]. Regardless of continuous calibration and adjustment of TOA radiances for the various sensors, there will always be a degree of uncertainty in the TOA measurements. Any uncertainty or adjustment in TOA radiances affects down-stream bio-optical properties. After the TOA radiances have been calibrated, they are atmospherically corrected, resulting in ${}_nL_w$ radiances, which are then converted into R_{rs}. Then, bio-optical properties, such as chlorophyll, and a and b_{bp}, are derived from R_{rs}. Small uncertainties (1 to 2 percent) in TOA radiances are enough to sometimes change ${}_nL_w$ radiances by as much as 20-30 percent, therefore changing down-stream bio-optical properties. Similarly to how uncertainty exists in the TOA radiances, uncertainty also exists in several stages of algorithms used for atmospheric correction and deriving bio-optical properties, such as the QAA algorithm, which is used in calculating absorption and backscattering coefficients [3]. Most uncertainties within the QAA algorithm have already been evaluated [4]. Here, we perform a sensitivity test on model constants used in calculation of R_{rs} and the b_{bp} exponent. These parameters have little effect on a; however, variation in b_{bp} is observed.

OBJECTIVES

Our objectives are to: (1) apply noise to satellite TOA radiances using an ensemble approach to quantify uncertainties in $_nL_w$ radiances and down-stream bio-optical properties; (2) assess results of uncertainty of TOA radiances by plotting each ensemble set spectrally, as well as ensemble mean and original values, for $_nL_w$, chlorophyll, *a*, and b_{bp}; (3) using an ensemble approach, adjust ranges used in calculating R_{rs} and the b_{bp} exponent to evaluate sensitivity in calculating spectral b_{bp}; (4) assess results of sensitivity tests in calculating R_{rs} and the b_{bp} exponent by plotting each ensemble set spectrally for b_{bp}.

BACKGROUND

The Naval Research Laboratory (NRL) at the Stennis Space Center (SSC) in Mississippi has developed an Automated Processing System (APS) that ingests and processes AVHRR, SeaWiFS, MODIS, MERIS, and OCM satellite imagery [5]. It has since been extended to also include HICO and VIIRS satellite imagery. APS is a powerful, extendable, image-processing tool. It is a complete end-to-end system that includes sensor calibration, atmospheric correction (with near-infrared correction for coastal waters), image de-striping, and bio-optical inversion. APS incorporates the latest NASA MODIS code and enables us to produce the NASA standard SeaWiFS and MODIS products, as well as Navy-specific products using NRL algorithms. We can readily test and validate new products and easily incorporate new algorithms from other investigators. In addition, as we make modifications to the algorithms, we can easily reprocess many data files (dozens of scenes/day) and compare to previous results. Furthermore, we can automatically extract image data from regions-of-interest to facilitate time-series analyses, and from specific locations for match-ups with *in situ* ship station data. We maintain compatibility with NASA/Goddard algorithms and processing code. All imagery was processed with consistent atmospheric correction and bio-optical algorithms using the NRL APS version 4.6, which is consistent with SeaDAS version 6.3.

METHODS

Uncertainty of TOA Radiances

To analyze the impact of uncertainty of TOA radiances and their effect on $_nL_w$ radiances and downstream bio-optical properties, we evaluate the application of ensembles consisting of simulated noise (randomly-distributed in the range of ±2.0% of the original TOA for a given pixel). For an individual ensemble member, noise applied to a particular wavelength is constant for all pixels throughout the scene. The following ensembles sets are analyzed here:

- Noise applied to all wavelengths, where {visible: 412, 443, 488, 547, 667 (nm)} and {near infrared (NIR): 748, 869 (nm)}.
- Noise applied to only visible wavelengths.
- Noise applied to only NIR.

We first compare the spectral $_nL_w$ radiances retrieved from each ensemble member and ensemble mean for each set of ensembles, to the spectral $_nL_w$ radiances from the original image. For this comparison, we have chosen two regions of interest within our MODIS Mississippi Bight image, April 13, 2008.

The first region is the mean value of a 5 km x 5 km area (25 total pixels, where each pixel is 1 km resolution) centered around the coastal location 28.75°N, 87.0°W, and the second region is the mean value of a 5 km x 5 km area centered around the open-ocean location 28.75°N, 87.0°W. We also calculate an ensemble mean image from each of the ensemble runs in a given ensemble set. We perform the same evaluation to examine how uncertainty in TOA radiances affects a and b_{bp}. We expect to see variation in retrieved ${}_nL_w$, a, and b_{bp} across all wavelengths and especially in the 412 nm and 443 nm wavelengths. We also expect the ensemble mean to correlate with the original ${}_nL_w$, a, and b_{bp} values (less than or equal to 5% correlation, where correlation = ((ensemble mean – original) / original) * 100).

Levels of Uncertainty in the QAA Algorithm

To analyze the sensitivity of model constants used in calculating r_{rs} and the b_{bp} exponent within the QAA algorithm, we evaluate ensembles consisting of ranges of coefficients. The following ensemble sets are analyzed here:

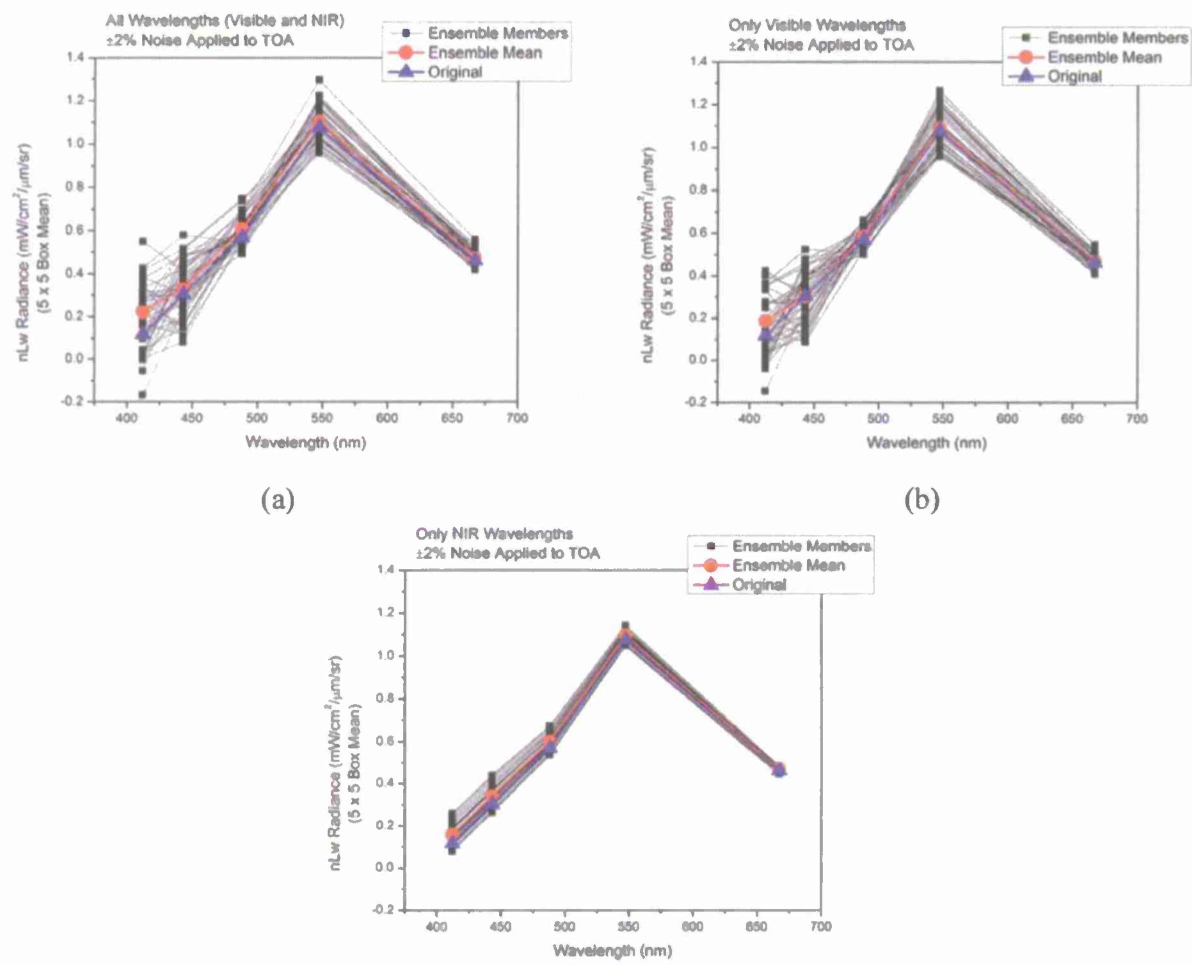
- Vary the coefficients used in calculating $r_{rs}(\lambda)$:
  $r_{rs}(\lambda) = R_{rs}(\lambda) / (T + \gamma Q R_{rs}(\lambda))$; $T = 0.52$, $\gamma Q = 1.7$
  T and γQ were calculated from HYDROLIGHT for optically deep waters and a nadir-viewing sensor. To demonstrate how an uncertainty in these values affects a and b_{bp}, we vary T from 0.47 to 0.57, in increments of 0.01, and we vary γQ from 1.2 to 2.2, in increments of 0.5.
- The exponent of bbp(λ), η, has changed from version 4 to version 5:
  $\eta = x (1 - 1.2 \exp (-0.9 (rrs(443) / rrs(555))))$, where $x = 2.2$ (version 4)
  $\eta = x (1 - 1.2 \exp (-0.9 (rrs(443) / rrs(555))))$, where $x = 2.0$ (version 5)
  To analyze the sensitivity of x on retrieved bbp, we vary x from 1.7 to 2.4, in increments of 0.1.

RESULTS

Effect of Simulated Noise Applied to TOA Radiances on ${}_nL_w$, a, b_{bp}, and chlorophyll

To test the approach, we applied randomly-distributed simulated noise in the range of ±2.0% of the original TOA radiance for a given pixel, to our ensemble members in our ensemble sets. Each ensemble set consists of 40 ensemble members. We extract the spectral shape for ${}_nL_w$, a, and b_{bp}, and plot the data for our two regions of interest (coastal and open ocean) for our MODIS northern Gulf of Mexico image. This is performed for the original, unaltered image, each ensemble member, and the ensemble mean.

Figures 1 – 3 illustrate the effect of ±2.0% noise applied to the TOA radiances in ${}_nL_w$, a, and b_{bp} for our coastal region. For this discussion, we denote the all wavelengths, only visible wavelengths, and only NIR wavelengths to be ensemble sets 1, 2, and 3, respectively. In Figure 1, the ensemble mean for ${}_nL_w$ correlated (5% error or less) with the original image for the 547 and 667 nm bands in ensemble sets 1 and 3, and 443, 488, 547, and 667 nm bands for ensemble set 2. 412 nm has poor correlation for all three ensemble sets (correlation values for coastal ensembles can be seen in Table 1). Similar tendencies are observed for a in Figure 2, but b_{bp} achieved good spectral correlation for all wavelengths in all ensemble sets in Figure 3. Figures 4 – 7 are similar to Figures 1 – 3 but correspond to the open ocean region. In Figure 4, the ensemble mean for $_nL_w$ correlated with the original image for wavelengths 443 and 488 nm in ensemble set 1, all wavelengths except 667 nm in ensemble set 2, and only wavelength 488 nm in ensemble set 3. Wavelengths 412, 443, 488, and 547 nm achieved correlation less than 10% for all ensemble sets, but 667 nm had poor correlation, which is difficult to observe in the Figure because that wavelength has a very low $_nL_w$ value. Figure 5 demonstrates good correlation for *a* values in wavelengths 412, 443, and 488 nm for all ensemble sets, with correlation values just exceeding our target for the 547 nm wavelength for ensemble sets 1 and 2. The 667 nm wavelength exhibits some interesting results due to its increase in value compared to the other visible wavelength, but some of the individual ensemble members with elevated values could potentially be filtered when we better confine our ensembles in future work. Due to the linear nature observed in Figure 6, poor correlation is observed spectrally in ensemble sets 1 and 3. However, all wavelengths except for 667 nm meet our target correlation in ensemble set 2. All correlation values for the open ocean ensembles described in Figures 4 – 6 can be seen in Table 2.



(a) (b)

(c)

Figure 1. Spectral nLw Radiance for 5 x 5 Box Mean Centered Around Coastal Area (see text for location) for Ensemble Sets with ±2.0% TOA Noise Applied to (a) All Wavelengths (Visible and NIR), (b) Only Visible Wavelengths, and (c) Only NIR Wavelengths

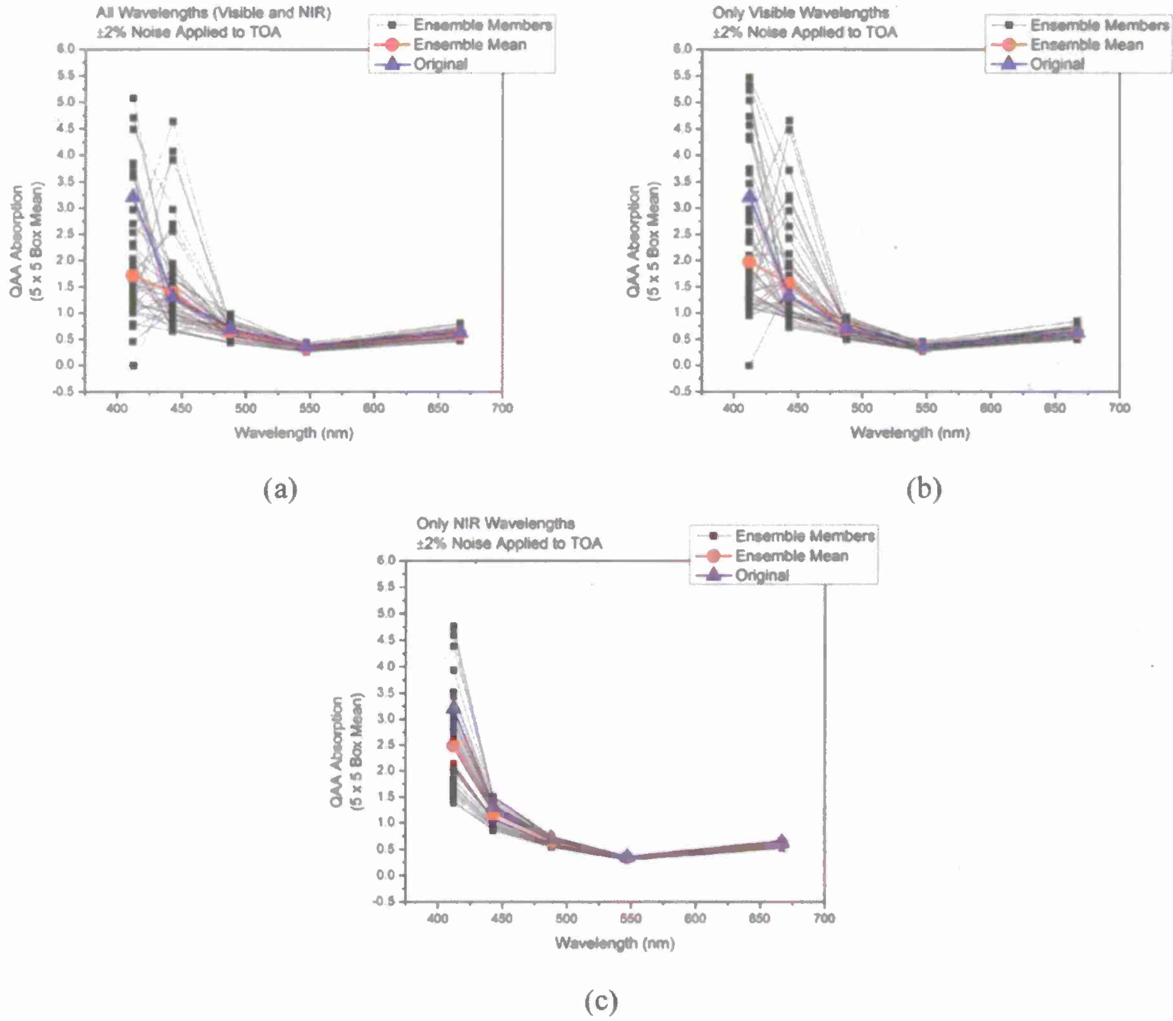
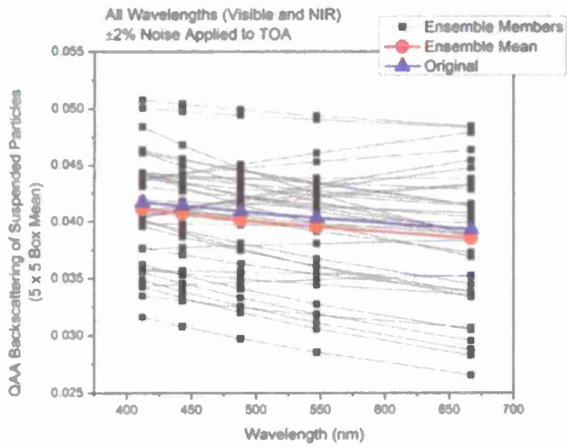
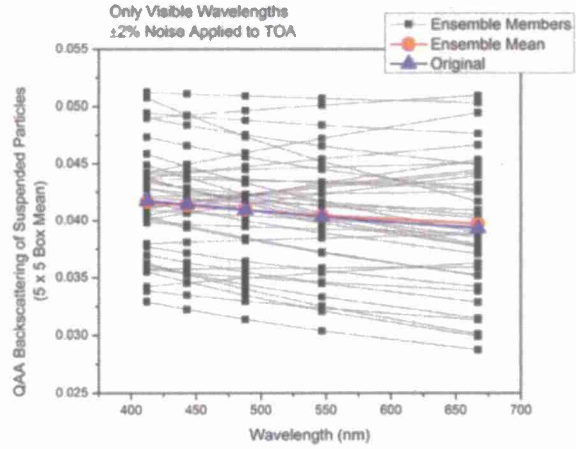


Figure 2. Spectral Total Absorption derived by the QAA Algorithm for 5 x 5 Box Mean Centered Around Coastal Area (see text for location) for Ensemble Sets with ±2.0% TOA Noise Applied to (a) All Wavelengths (Visible and NIR), (b) Only Visible Wavelengths, and (c) Only NIR Wavelengths



(a)



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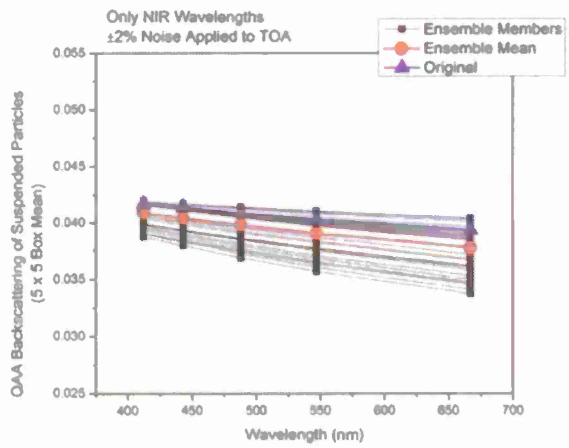
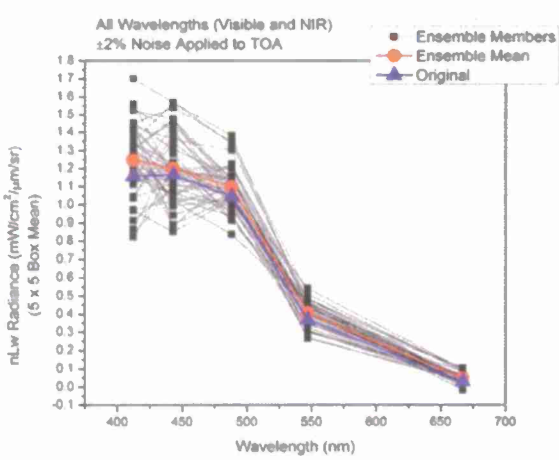


(c)

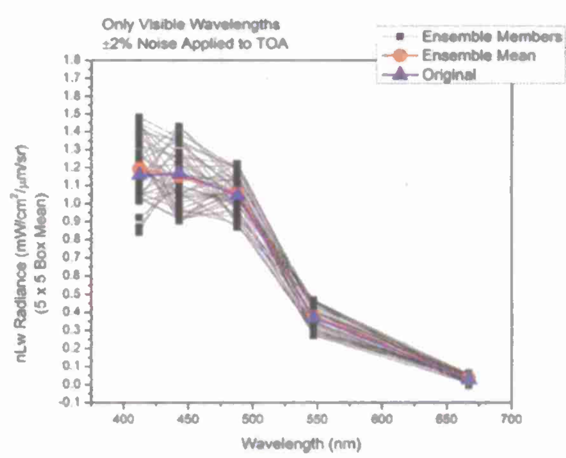
Figure 3. Spectral Backscattering of Suspended Particles derived by the QAA Algorithm for 5 x 5 Box Mean Centered Around Coastal Area (see text for location) for Ensemble Sets with ±2.0% TOA Noise Applied to (a) All Wavelengths (Visible and NIR), (b) Only Visible Wavelengths, and (c) Only NIR Wavelengths

Wavelength	412	443	488	547	667
			nLw		
All Wavelengths	87.5	8.9	7.2	2.6	2.6
Only Visible Wavelengths	57.7	1.0	3.0	1.1	1.3
Only NIR Wavelengths	35.2	12.9	5.5	1.9	1.5
			A		
All Wavelengths	46.5	6.3	6.4	4.0	3.9
Only Visible Wavelengths	38.4	19.0	1.5	0.3	0.3
Only NIR Wavelengths	22.8	10.7	6.7	4.6	5.2
			Bbp		
All Wavelengths	1.4	1.7	2.0	2.0	2.0
Only Visible Wavelengths	0.2	0.2	0	0.2	1.0
Only NIR Wavelengths	1.9	2.4	2.7	3.2	4.1

Table 1. Spectral Correlation for Coastal Ensembles for $_nL_w$, a, and b_{bp} for All Ensemble Sets



(a)



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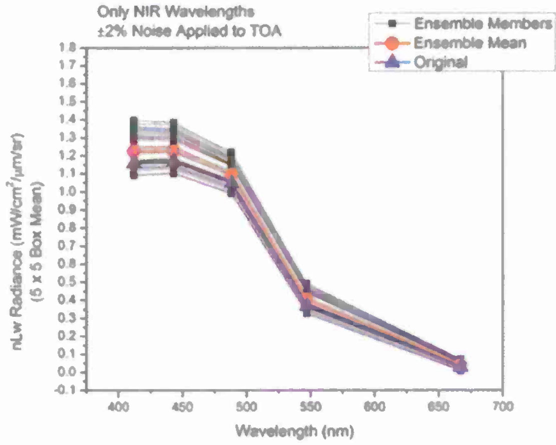
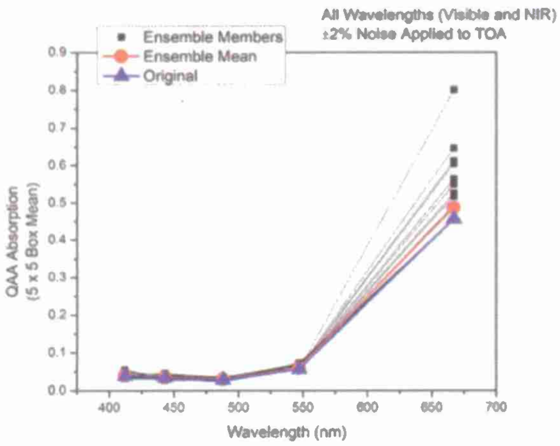


(c)

Figure 4. Spectral nLw Radiance for 5 x 5 Box Mean Centered Around Open Ocean Area (see text for location) for Ensemble Sets with ±2.0% TOA Noise Applied to (a) All Wavelengths (Visible and NIR), (b) Only Visible Wavelengths, and (c) Only NIR Wavelengths



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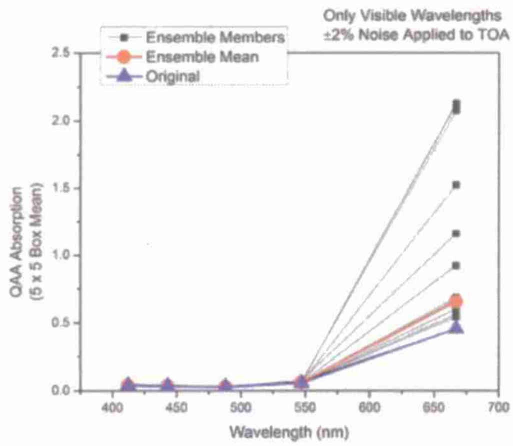

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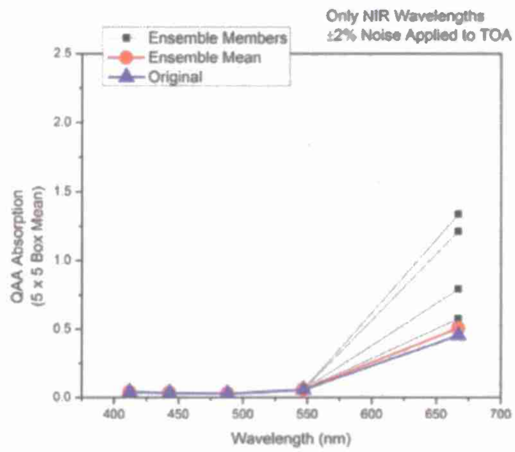
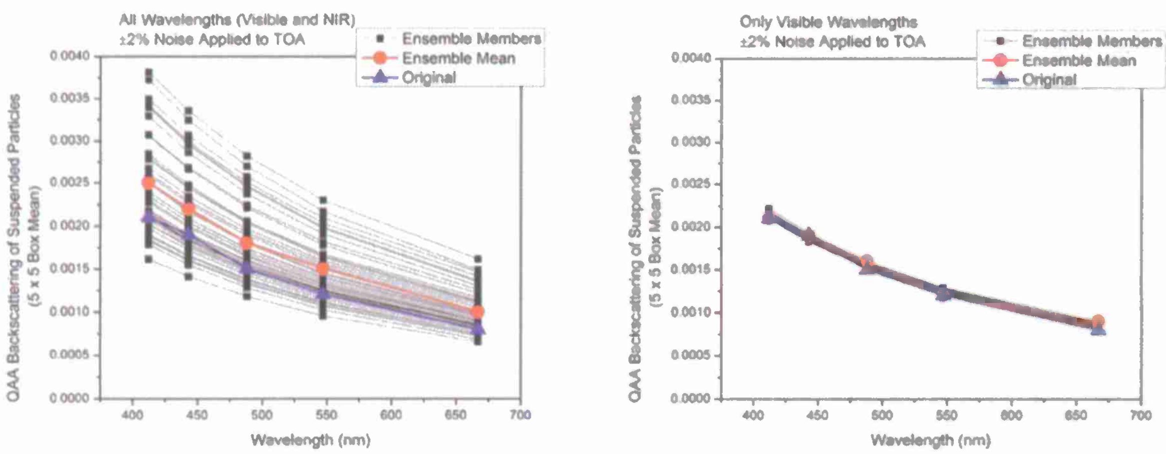
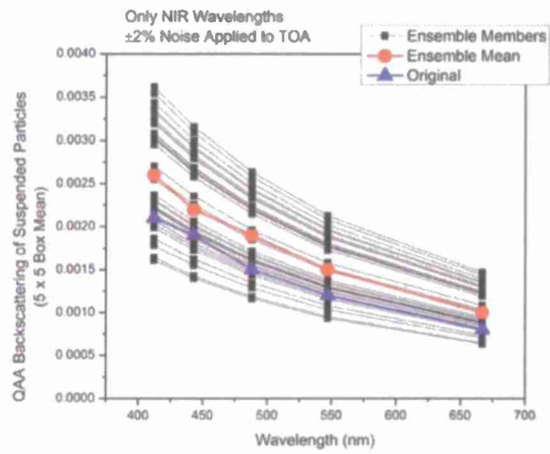


(c)

Figure 5. Spectral Total Absorption derived by the QAA Algorithm for 5 x 5 Box Mean Centered Around Open Ocean Area (see text for location) for Ensemble Sets with ±2.0% TOA Noise Applied to (a) All Wavelengths (Visible and NIR), (b) Only Visible Wavelengths, and (c) Only NIR Wavelengths



(a) (b)



(c)

Figure 6. Spectral Backscattering of Suspended Particles derived by the QAA Algorithm for 5 x 5 Box Mean Centered Around Open Ocean Area (see text for location) for Ensemble Sets with ±2.0% TOA Noise Applied to (a) All Wavelengths (Visible and NIR), (b) Only Visible Wavelengths, and (c) Only NIR Wavelengths

Wavelength	412	443	488	547	667
			nLw		
All Wavelengths	7.7	3.0	4.9	9.9	63.0
Only Visible Wavelengths	2.9	1.4	1.1	1.9	15.9
Only NIR Wavelengths	5.7	5.2	4.4	9.5	47.4
			A		
All Wavelengths	1.0	0.2	4.2	5.5	6.7
Only Visible Wavelengths	0.5	3.5	0	5.5	43.8
Only NIR Wavelengths	1.8	2.9	4.6	0.4	11.5
			Bbp		
All Wavelengths	19.0	15.8	20.0	25.0	25.0
Only Visible Wavelengths	0	0	6.7	0	12.5
Only NIR Wavelengths	23.8	15.8	26.7	25.0	25.0

Table 2. Spectral Correlation for Open Ocean Ensembles for ${}_{n}L_{w}$, a, and b_{bp} for All Ensemble Sets

For chlorophyll, we plot all ensemble member samples for each ensemble set. We can compare the original value to the ensemble members of each ensemble set, as well as their respective ensemble mean values. The individual ensemble members higher variation in ensemble sets 1 and 2 than in ensemble set 3. This is due to the relationship between band ratios used in calculating chlorophyll in the oc3 algorithm, and those ratios will have a wider range of values when noise is applied to visible wavelengths than when noise is only applied to the NIR wavelengths, as in ensemble set 3. However, this does not imply that ensemble set 3 has better correlation than sets 1 and 2. Ensemble set 2 had nearly perfect correlation with the original chlorophyll value in the coastal region, having a correlation value of 0.4. Ensemble sets 1 and 3 had coastal correlation values of 5.2 and 9.8, respectively. For the open ocean region, correlation values were 12.9, 7.3 and 6.0 for ensemble sets 1 – 3, respectively.

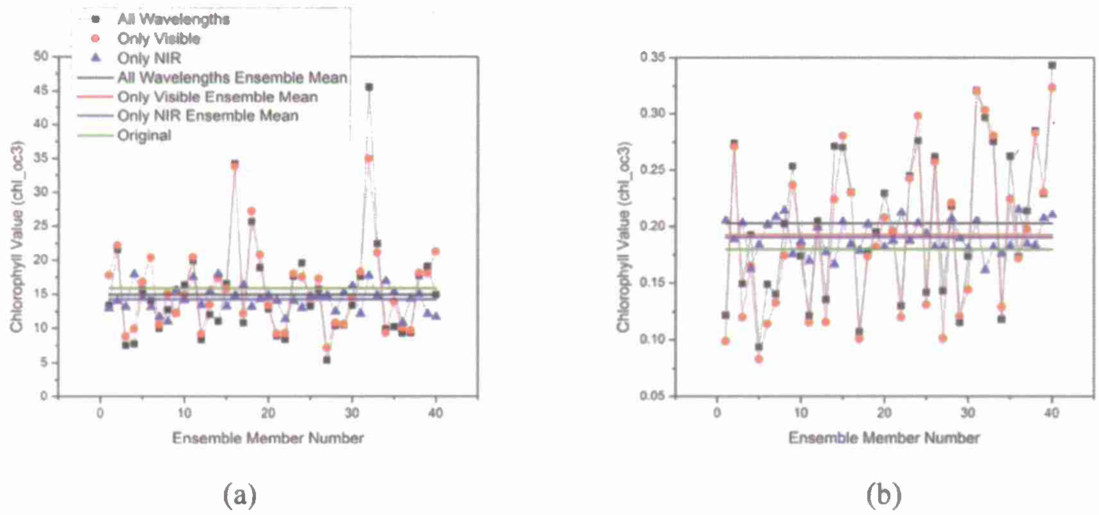
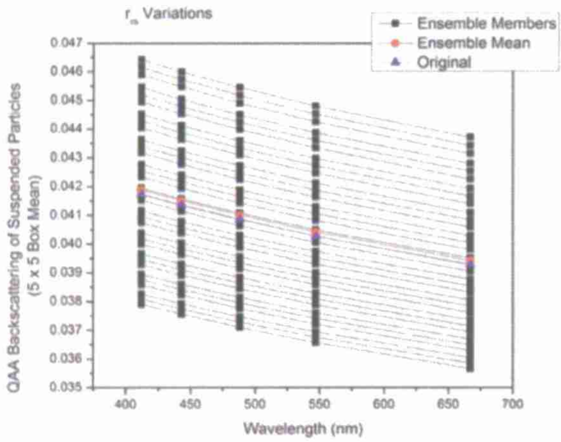


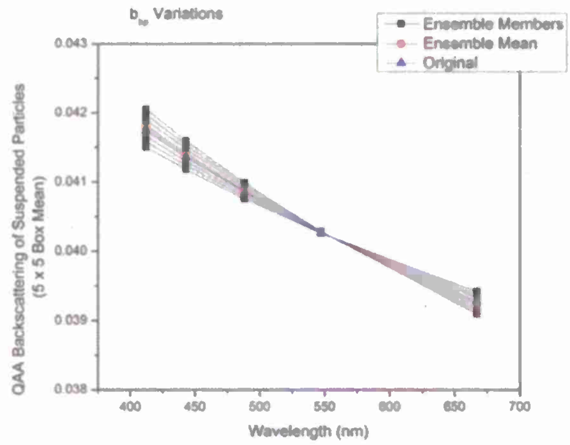
Figure 7. Chlorophyll Retrievals Using the OC3 Algorithm for All Ensemble Sets (±2.0% TOA Noise Applied to All, Only Visible, and Only NIR Wavelengths, and Their Individual Ensemble Members, for 5 x 5 Box Mean Centered Around (a) Coastal Area and (b) Open Ocean Area (see text for location)

Effect of Varying Coefficients in Stages of the QAA Algorithm

To test this approach, we varied model constants used in calculated R_{rs} and the b_{bp} exponent. We only want to observe the sensitivity of these constants in complex, coastal waters. T and γQ used in calculating Rrs were calculated from HYDROLIGHT for optically deep waters, so these constants may need to be modified for complex, coastal waters. In the QAA algorithm, x changed from 2.2 to 2.0. We created an ensemble set to adjust this constant in order to observe its sensitivity in calculating b_{bp} in coastal waters. In Figure 8a, we see that the individual ensemble members vary but good correlation is achieved for the ensemble mean value of b_{bp}, when compared to the original b_{bp} value. In Figure 8b, good correlation is also achieved for b_{bp}.



(a)



(b)

Figure 8. Spectral b_{bp} Retrievals Using the QAA Algorithm When (a) r_{rs}, and (b) the exponent of $b_{bp}(\lambda)$ are Varied, for 5 x 5 Box Mean Centered Around Coastal Area (see text for location)

DISCUSSION AND SUMMARY

We have examined how uncertainties in TOA radiances can impact $_nL_W$, a, and b_{bp} retrievals. Applying simulated noise to TOA radiances can have a substantial impact on $_nL_W$ and a retrievals in all wavelengths and especially in the 412 and 443 nm wavelengths. The ensemble mean $_nL_W$ and a values at the 412 nm wavelength, for all coastal ensemble sets, fail to correlate with their respective original values. Unlike $_nL_W$ and a, b_{bp} exhibits a linear spectral change in retrieved values and achieves good spectral correlation. In the open ocean region, better correlation is achieved spectrally in the blue wavelengths for $_nL_W$ and a, but b_{bp} has poor correlation. Chlorophyll retrievals (using the oc3 algorithm) show more variability when noise is applied to visible wavelengths (thus altering the relationship between band ratios) than when noise is only applied to NIR bands. The individual chlorophyll ensemble members show variation throughout the ensemble sets but their ensemble means correlate with the original chlorophyll value. A thorough study of ensemble effects on derived chlorophyll values can be seen in Dr. Richard Gould's research presented at this conference.

Most of the uncertainty in the stages of the QAA algorithm has been assessed by Lee *et al.* By producing two ensemble sets to test sensitivity, we demonstrated how model constants involved in computing R_{rs} and the b_{bp} exponent alter spectral b_{bp} for the coastal region in our MODIS image.

For most of the ensemble sets in this work, we achieved good correlation when compared to products in the original image. However, in this work we only used simple metrics to confine our ensemble sets, but we are currently working to only include ensembles that consist of natural variability. This is discussed within Dr. Richard Gould's research, but there are some individual ensemble members that should be dismissed. Some of our methods to better confine ensemble sets will include analyzing the spectral shape of $_nL_W$, a, and b_{bp}, and discarding ensembles that have spectral shapes that would not naturally occur. We can also perform statistical analyses to remove any ensembles that produce product values above or below a certain threshold, such as ±1 standard deviation from the ensemble mean.

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14. ABSTRACT

Uncertainties in retrievals of bio-optical properties from satellite ocean color imagery are related to a variety of factors, including errors associated with sensor calibration and degradation, atmospheric correction, and the bio-optical inversion algorithms. Here we examine the impact of uncertainties in the top-of-atmosphere (TOA) radiances and coefficients in the quasi-analytical algorithm (QAA) on the satellite estimation of the normalized water-leaving radiances (nLw) and downstream bio-optical properties, such as the absorption and backscattering coefficients and chlorophyll. We use a Moderate Resolution Imaging Spectroradiometer (MODIS) image, free from clouds, covering the Gulf of Mexico, as our data set. We apply ensembles at each pixel in the image to simulate noise on the satellite TOA radiance values (randomly-distributed in the range of ±2.0%) at MODIS visible and near-infrared wavelengths. We also use ensembles to analyze sensitivity of coefficients in the QAA algorithm to quantify the impact of uncertainties on absorption and backscattering coefficients.

15. SUBJECT TERMS

Uncertainties, ensembles, MODIS, QAA

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