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Spatial and Temporal Distributions of Pelagic Sargassum in the Intra-Americas Sea and Atlantic Ocean

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Spatial and Temporal Distributions of Pelagic *Sargassum* **in the Intra-Americas Sea and**

Atlantic Ocean

by

Mengqiu Wang

A dissertation submitted in partial fulfillment of the requirements for the degree of Doctor of Philosophy College of Marine Science University of South Florida

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Keywords: *Sargassum*, remote sensing, Atlantic, Caribbean, Gulf of Mexico, global change

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Dedication

This dissertation is dedicated to my father Yesheng Wang and my mother Mingxia Chen. Their unconditional love has always been my strongest support.

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Abstract

Pelagic *Sargassum* is one type of marine macroalgae that is known to be abundant in the Gulf of Mexico and Sargasso Sea. It is also known to serve as a critical habitat for many marine animals. In the past few years, large amounts of *Sargassum* have been reported in the Tropical Atlantic and Caribbean Sea (CS), causing significant environmental and economic problems. The goal of this study is to improve the understanding of *Sargassum* distributions, quantity, transport pathways, and bloom mechanisms in the CS and Tropic Atlantic through combining a variety of techniques including satellite remote sensing, field and laboratory measurements, and numerical modeling.

The first question is where and how much *Sargassum* is in the CS and Tropic Atlantic. Previous field observations revealed strong seasonal and spatial variations of *Sargassum*, yet these observations are all limited in their spatial and temporal coverage. Satellite observations offer an effective means to measure their distributions with synoptic coverage and high sampling frequency, yet it is technically challenging to extract and quantify the small *Sargassum* features in coarse-resolution satellite imagery. Chapter 2 focuses on *Sargassum* detection and quantification algorithm development using Moderate Resolution Imaging Spectroradiometer (MODIS) data (Appendix A). The algorithm is based on MODIS alternative floating algae index (AFAI), which examines the red-edge reflectance of floating vegetation. The algorithm includes three basic steps: 1) classification of *Sargassum*-containing pixels through correction of largescale gradient, masking clouds and cloud shadows, and removal of ambiguous pixels; 2) linear unmixing of *Sargassum*-containing pixels; and, 3) statistical analysis of *Sargassum* area coverage in pre-defined grids at monthly, seasonal, and annual intervals. The algorithm is applied to MODIS observations between 2000 and 2015 over the Central West Atlantic (CWA) region ($0 - 22$ °N, 38 – 63°W) to derive the spatial and temporal distribution patterns as well as the total areal coverage of *Sargassum*. Results indicate that the first widespread *Sargassum* distribution event occurred in 2011, consistent with previous findings from the Medium Resolution Imaging Spectrometer (MERIS). Since 2011, only 2013 showed minimal *Sargassum* coverage similar to the period of 2000 to 2010; all other years showed significantly more coverage. More alarmingly, the summer months of 2015 showed mean coverage of $>$ 2000 km², or about 4 times of the summer 2011 coverage and 20 times of the summer 2000 to 2010 coverage. Analysis of several environmental variables provided some hints on the reasons causing the inter-annual changes after 2010, yet further multi-disciplinary research (including *in situ* measurements) is required to understand such changes and long-term trends in *Sargassum* coverage.

To better understand the potential ecological and environmental impacts of *Sargassum*, field and laboratory experiments are conducted to link the *Sargassum* areal coverage observations to biomass per area (density) and measure the nutrient contents and pigment concentrations (Chapter 3, Appendix B). An AFAI-biomass density model is established to derive *Sargassum* biomass density from the spectral reflectance, with a relative uncertainty of ~ 12%. Monthly mean integrated *Sargassum* biomass in the CS and CWA reached > 4.4 million tons in July 2015. The average % C, % N, and % P per dry-weight, measured from samples collected in Gulf of Mexico and Florida Straits in summer 2017, are 27.16, 1.06, and 0.10, respectively. The mean chlorophyll-a concentration is ~ 0.05% of the dry-weight. With these parameters, the amounts of nutrients and pigments can be estimated directly from remotely-sensed *Sargassum* biomass. During bloom seasons, *Sargassum* carbon can account for ~ 18% of the total particulate organic carbon in the upper water column. This chapter provides the first quantitative assessment of the overall *Sargassum* biomass, nutrients, and pigment abundance from remote-sensing observations, thus helping to quantify their ecological roles and facilitate management decisions.

To investigate the *Sargassum* transport patterns and potential bloom sources, a Lagrangian particle tracking model is established to track the *Sargassum* transport driven by surface currents and winds

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(Chapter 4, Appendix C). The mean *Sargassum* distributions derived from MODIS observations are used to initiate and evaluate a Lagrangian particle tracking model that tracks *Sargassum* advection under surface currents and winds. Among the thirty-nine experiments, adding surface currents alone improves model performance (i.e., by reducing difference between modeled and observed *Sargassum* distributions) in 82% of the cases after tracking *Sargassum* for one month. Adding 1% wind forcing to the advection model also shows improved performance in 67% of the cases. Adding a time- and location-dependent *Sargassum* growth/mortality rate (i.e., change rate), derived from time-series of the MODIS-based *Sargassum* abundance and the corresponding environmental data via a Random Forest regression, leads to further improvement in model performance (i.e., by increasing the matchup percentage between modeled and observed *Sargassum* distributions) in 64% of the cases, although the modeled change rates only explain ~ 27% of the variance of the validation dataset, possibly due to uncertainties in such-derived change rates. The *Sargassum* transport model, with the mean currents, winds, and change rates acting as the forcing, is applied to track the mean *Sargassum* distributions forward and backward. The results demonstrate the model's capacity of simulating the *Sargassum* distribution patterns, with emphasis on the role of biological terms in determining the large-scale distributions. These tracking experiments also suggest that *Sargassum* blooms in the CS are strongly connected to the Central Atlantic regions, and blooms in the Tropical Atlantic show relatively weak connections to the Atlantic regions further north.

Although it is straightforward to apply the transport model to predict *Sargassum* blooms, such longterm prediction could suffer from large error accumulations and unable to achieve satisfactory performance. Therefore historical *Sargassum* distributions derived from MODIS are used to provide an alternative way to realize the bloom prediction. Chapter 5 proposes such a prediction based on a hindcast of 2000–2016 observations from MODIS, which shows *Sargassum* abundance in the CS and the CWA, as well as connectivity between the two regions with time lags (Appendix D). This information is used to derive bloom and nonbloom probability matrices for each 1° square in the CS for the months of May–

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August, predicted from bloom conditions in a hotspot region in the CWA in February. A suite of standard statistical measures is used to gauge the prediction accuracy, among which the user's accuracy and kappa statistics show high fidelity of the probability maps in predicting both blooms and nonblooms in the eastern CS with several months of lead time, with an overall accuracy often exceeding 80%. The bloom probability maps from this hindcast analysis will provide early warnings to better study *Sargassum* blooms and prepare for beaching events near the study region. This approach may also be extendable to many other regions around the world that face similar challenges and opportunities of macroalgal blooms and beaching events. Using this forecasting scheme, the summer blooms in the CS in 2017 were successfully predicted. Since February 2018, we have also generated monthly-updated 1-page *Sargassum* outlook bulletins to help these regions to better prepare for potential beaching events.

Currently, the mean *Sargassum* distribution statistics used in this study are derived from MODIS, which has been operating well beyond the designed mission life, arousing concerns as to whether the *Sargassum* observation statistics can be continued in the future. As a follow-on sensor, the Visible Infrared Imaging Radiometer Suite (VIIRS) has the appropriate spectral bands to detect and quantify floating macroalgae. Based on previous works on MODIS, Chapter 6 presents an improved procedure to extract floating algae pixels from VIIRS AFAI imagery, with image filtering used to suppress noise and adjusted thresholds used to mask sun glint, clouds, and cloud shadows. The overall extraction accuracy is about 85%. Simultaneous daily observations from MODIS and VIIRS over the CWA show consistent spatial patterns, but VIIRS estimations of the algae coverage (in km²) are consistently lower than MODIS (around – 19% mean relative difference or MRD), possibly due to lower sensitivity of the VIIRS near-infrared (NIR) bands than the corresponding MODIS bands. Similarly, at monthly scale VIIRS also shows lower coverage than MODIS, and their difference (around – 29% MRD) is larger than the difference between MODIS-Aqua and MODIS-Terra estimates (around – 14% MRD). Despite these differences, the spatial and temporal patterns between VIIRS and MODIS observed algae distributions match very well at all spatial and temporal scales. These results suggest that VIIRS can provide continuous and consistent observations of floating algae distributions and abundance from MODIS as long as their differences are accounted for, thus assuring continuity in the future.

In summary, this study has worked on four connected topics regarding *Sargassum* distributions, biomass and nutrients, transport pathways, and bloom predictions through combined efforts in satellite remote sensing, field and laboratory measurements, physical modelling, and statistical analyses. To my best knowledge, this is the first comprehensive and multi-disciplinary study to investigate pelagic *Sargassum* at synoptic scale in the Intra-Americas Sea (IAS) and Atlantic Ocean. Although several questions remain to be answered (e.g., "What cause the inter-annual variations of *Sargassum* blooms?" and "Where are the bloom origins?"), the outcomes of this study (remote sensing algorithms, *Sargassum* distribution and abundance maps, established bio-physical model, and a bloom forecast model) are expected to make significant contributions in both scientific research (including new critical baseline data) and management decision support.

Chapter 1:

Introduction

1. *Sargassum* and its significance in ocean ecology, biogeochemistry, and management

Pelagic *Sargassum* is one type of brown macroalgae (Phaeophyceae), which has been known to grow in the Gulf of Mexico and Sargasso Sea in the North Atlantic Ocean (Butler et al., 1983; Butler and Stoner, 1984). Two floating *Sargassum* species (*S. natans* and *S. fluitans*) dominate the neuston tow collections in shipboard investigations in these areas (Parr, 1939; Stoner, 1983; Schell et al., 2015). These two species can be discriminated based on their arrangement of stem, blades, and air bladders (Schell et al., 2015). Under different environmental conditions, *Sargassum* can form features of variable sizes, from small clumps that are only a few centimeters wide to rafts or patches large enough to be detectable by coarseresolution satellites (Huffard, et al., 2014). Under high wind, large patches can be dissipated into smaller mats and may sink to the deep ocean floor, contributing the particulate organic matter (POM) in the deep sea (Johnson and Richardson, 1977). It is estimated that the sinking of pelagic *Sargassum* accounts for approximately 10% of the total POM transferred to the deep-sea community (Rowe and Staresinic, 1979).

In the open ocean, *Sargassum* serves as a critical ocean habitat and refuge for many marine organisms including fish, shrimp, crab, and sea turtles (Butler et al., 1983; Council, 2002; Rooker et al., 2006; Witherington et al., 2012; Lapointe et al., 2014; Doyle and Franks, 2015; Hardy, 2014; Casazza and Ross, 2008). For many pelagic fishes and seabirds, *Sargassum* rafts are important feeding and spawning grounds (Casazza and Ross, 2008; Trott et al., 2010). Although excessive *Sargassum* beaching resulted in various problems, it is noted that proper amount of *Sargassum* deposition could be conducive to coastal stabilization by providing nutrients to dune plants (Tsoar, 2005; Anthony et al., 2006). Through its ecological functions or releasing colored dissolved organic matter (CDOM), *Sargassum* can also affect the ocean biogeochemistry (Culliney, 1970; Carpenter and Cox, 1974; Phlips and Zeman, 1990; Lapointe, 1995; Turner and Rooker, 2006; Zepp et al., 2008; Lapointe et al., 2014). The role of nutrient limitation especially of reactive phosphorus, in the *Sargassum* growth was explored in relevant studies (Culliney, 1970; Carpenter and Cox, 1974; Phlips and Zeman, 1990; Lapointe, 1986; Lapointe, 1995; Lapointe et al., 2014). It was also found that nutrient-enhanced *Sargassum* productivity can occur in the neritic waters (Lapointe et al., 1995). Recent studies from Lapointe et al. (2014) revealed that mutualism with fishes may contribute to the *Sargassum* production in the neritic water of North Atlantic (Lapointe et al., 2014). Although field investigations have been made in the past few decades, the role of *Sargassum* in the carbon cycle and their total primary production remain largely unknown.

When excessive *Sargassum* is washed on to beaches, it can impose a burden to local management and needs to be removed. Local economy, especially the tourism industry and other directly or indirectly related businesses, can be greatly impacted since *Sargassum* will cover up the beaches and release unpleasant smells as it decays (Hu et al., 2016). Massive *Sargassum* deposition would clog harbors and attract insects, thus inhibit artisanal fishing and arouse public health concerns (Suida et al., 2016). Sea turtle population could also be impacted since the *Sargassum* accumulation may smother their nesting sites (Maurer et al., 2015; Hu et al., 2016). Long-term massive *Sargassum* deposition can also lead to coastal eutrophication (Suida et al., 2016), and induce unfavorable environments for the growth of nearshore corals and seagrass communities (van Tussenbroek et al., 2018). To physically remove the massive beached *Sargassum*, over 2.91 million dollars was spent annually in Texas (Webster and Linton, 2013). During the extreme beaching event in 2015, the Mexican Navy was called to help with the beach cleanup activities (Partlow and Martinez, 2015). All these positive and negative impacts call for a better understanding of the *Sargassum* and the *Sargassum* biological community.

2. *Sargassum* studies: current status

Sargassum **monitoring: field and satellite measurements**

Currently, investigations of *Sargassum* communities' spatial and temporal variabilities are from either ship-based or remote sensing-based observations. The first set of comprehensive studies of *Sargassum* abundance were conducted between 1933 and 1935 (Parr, 1939). As shown in Fig. 1a, their sampling sites cover the Caribbean Islands, the eastern Gulf of Mexico (GOM), and the western Sargasso Sea. Fifty years later, based on shipboard surveys in the same region, no significant decline was found in the *Sargassum* biomass (from 1977 to 1981) compared to the 1930s' study in most areas (Stoner, 1983; Butler and Stoner, 1984). Between 1939 and 1984, studies were more focused on the physiology, sinking rates (Johnson and Richardson, 1977; Woodcock, 1950), and the ecology of associated biota (Adams, 1960; Fine, 1970). Since 1992, the Sea Education Association (SEA, http://www.sea.edu) has been conducting quarterly *Sargassum* surveys (Schell et al., 2015; Siuda et al., 2016) to document *Sargassum* abundance and distributions over the western Sargasso Sea, the GOM, and the Caribbean Sea areas (see Fig.1b). The species compositions were also identified and recorded for future analyses. Considering the significant seasonal and inter-annual variations of *Sargassum* abundance and spatial distributions, field measurements based on sporadic sampling are likely biased due to the lack of coverage in both time and space. Such a drawback may be overcome through more synoptic and frequent remote sensing measurements, once appropriate algorithms are developed and used.

Because *Sargassum* has distinctive reflectance spectral characteristics, remote sensing data have been used to observe their spatial and temporal distributions in several recent studies (Gower et al., 2006; Gower and King, 2011; Gower et al., 2013; Wang and Hu, 2016). Gower et al. (2006) is the first proof-ofconcept study that demonstrates the potential of satellite measurements for synoptic mapping of *Sargassum*, followed by the mapping effort for the GOM and north Atlantic between 2002 and 2011 using

MEdium Resolution Imaging Spectrometer (MERIS) observations (Gower and King, 2011; Gower et al., 2013). However, MERIS stopped functioning in 2012, leading an information gap on *Sargassum* abundance and distributions in more recent years. In addition to such an information gap, the algorithms applied to MERIS are preliminary, requiring further refinement to reduce uncertainties.

Figure 1.1: Past ship-based investigations over the Caribbean Sea, GOM, and Atlantic Ocean. a) Stations where neuston tows were made (Parr, 1939). b) Sampling sites for quarterly *Sargassum* surveys by SEA via the SSV Corwith Cramer between 1992 and 2013 (Schell et al., 2015; Siuda et al., 2016). The black dots and blue dots in the figures both represent the location of *Sargassum* tows.

Sargassum **bloom hypotheses and driving factors**

For the recent *Sargassum* blooms in the Tropical Atlantic, several hypotheses have been proposed to explain their origins, nutrient supplies, and bloom conditions (Franks et al., 2011; Johnson et al., 2012; Franks et al., 2014; Lapointe et al., 2015):

- Tropical Atlantic, rather than the Sargasso Sea, is likely to be the bloom origin.
- Nutrient enrichment from either atmospheric dust deposition, river inflow, or upwelling processes provides favorable bloom conditions.
- Large-scale climate variability related to the North Atlantic air-sea interactions may have induced environmental conditions favorable for *Sargassum* growth and accumulation.

Specifically, several studies have hypothesized that *Sargassum* blooms could first occur in the North Equatorial Recirculation Region (NERR) of the North Atlantic between the North Equatorial Counter Current and the equator (Franks et al., 2011; Johnson et al., 2012; Franks et al., 2014). This hypothesis is supported by the speciation analysis results from the 2015 SEA cruise survey (Schell et al., 2015). Satellitederived *Sargassum* distributions (Gower et al., 2013; Wang and Hu, 2016) show that large *Sargassum* patches detectable from satellites first appeared in the Tropical Atlantic and were then transported elsewhere. Although satellite observations can only represent the detectable proportion of the total *Sargassum* abundance (Wang and Hu, 2016), they may also serve as indirect evidence to test this hypothesis.

From previous laboratory experiments, *Sargassum* shows higher growth rate under high nutrient and suitable temperature (Hanisak and Samuel, 1987). Some studies attribute the recent increases of blooms events to nutrient enrichments(Lapointe, 1995; Smetacek and Zingone, 2013), where the nutrient sources include major rivers, dust plumes over the Atlantic, or enhanced upwelling (Johnson et al., 2012; Franks et al., 2014). Several climate indexes including the EI-Nino-Southern Oscillation (ENSO), North Atlantic Oscillation (NAO), and Atlantic Multi-decadal Oscillation (AMO) have also been investigated for their possible linkages with bloom events (Franks et al., 2014). Northward displacement of the Inter Tropical Convergence Zone (ITCZ), higher North Atlantic air pressure, and sea surface heating have been assumed to be related to the observed *Sargassum* distribution variability (Johnson et al., 2012). However, more data need to be collected and analyzed to test these hypotheses.

3. Research objectives

The goal of this study it to achieve a better understanding of the *Sargassum* abundance, distributions, transport pathways, and bloom mechanisms in the Caribbean Sea and Tropic Atlantic. Specifically, the

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study has the following research objectives, where field and laboratory measurements, remote sensing observations, statistical analyses, and physical modelling are used to achieve these objectives.

Objective 1: Design, test, and evaluate *Sargassum* detection and quantification algorithms to be used for existing ocean color sensors.

Objective 2: Investigate the spatial distributions, temporal changes, and connectivity and transport pathways of *Sargassum* in the IAS and Atlantic Ocean.

Objective 3: Determine the environmental factors responsible for the inter-annual variations of *Sargassum* abundance.

Objective 4: Establish a forecasting capacity to predict *Sargassum* blooms in the Caribbean for management decision support.

Note that while most chapters that follow will focus on the Caribbean Sea and Central West Atlantic, the study domain covers the entire IAS and Atlantic, where subregions are defined to help study connectivity and to delineate targeted studies. Fig. 1.2 shows the study domain and several important subregions.

Figure 1.2: The study region and several important subregions defined in this study, where *Sargassum* community distributions and their connectivity are investigated. The entire study region is from 20° S to 40° N and 98° W to 15° E.

4. Dissertation outline

To fulfill the research goals described above, the dissertation is composed of five major components focusing on remote sensing algorithm development (Chapter 2 and Chapter 6), *Sargassum* biomass estimations (Chapter 3), *Sargassum* transport modeling (Chapter 4), and *Sargassum* bloom prediction (Chapter 5). Many of these have been published or submitted in peer-reviewed journals, and for those cases the chapter will provide a brief summary of the published or submitted paper where the paper is presented in the Appendix.

In Chapter 2, *Sargassum* detection and quantification algorithms (Objective 1) are designed to extract *Sargassum* features from Moderate Resolution Imaging Spectroradiometer (MODIS) imagery, with its areal coverage quantified based on field-measured *Sargassum* reflectance spectra. Application of these algorithms to MODIS observations over the central West Atlantic Ocean leads to the derivation of the long-term *Sargassum* areal distributions, which serve as the basis to estimate *Sargassum* biomass and nutrients (Chapter 3) and to understand *Sargassum* transport across different regions (Chapter 4 and 5)*.* Several environmental factors are also investigated to discuss potential environmental conditions that may be conducive for bloom initiation and development (Objective 3).

In Chapter 3, based on results from field and laboratory experiments, *Sargassum* biomass, nutrients, and pigments are quantified from MODIS observations (Objective 1) to help understand the potential ecological and biogeochemical impacts of *Sargassum* on the ocean environment. A *Sargassum* biomass density model is established to estimate biomass density (weight per area) from *Sargassum* reflectance characteristics. The biomass density distributions are used to estimate *Sargassum* nutrients and pigments distributions based on calibration relationships determined from laboratory experiments. Despite of the estimated ~ 12% relative uncertainties, results suggest that *Sargassum* biomass can reach several million

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tons in bloom seasons in the Caribbean and adjacent waters, and that *Sargassum* carbon contributes a significant amount to total phytoplankton carbon.

To investigate *Sargassum* transport in the Atlantic Ocean (Objective 2), Chapter 4 uses a Lagrangian particle tracking model to simulate *Sargassum* transport and distributions in the Tropical Atlantic, where the model is primarily driven by ocean currents and surface winds. MODIS-derived *Sargassum* distributions (results from Chapter 2) are used for particle initiation, model evaluation, and for estimating *Sargassum* growth/mortality (change) rates. Long-term (6-month) particle tracking experiments are subsequently conducted to study bloom formations and regional connectivity (Objectives 2 and 3). It is concluded that *Sargassum* growth/mortality rate is a key parameter to modeling and understanding *Sargassum* distributions and their inter-annual variability, yet field experiments to determine this rate are lacking.

Chapter 5 focuses on designing of a *Sargassum* bloom prediction scheme (Objectives 2 and 4) for the Caribbean Sea (CS). Through analyzing historical *Sargassum* distribution patterns and regional connectivity between the CS and Central West Atlantic (CWA), it is found that blooms in certain areas of the CWA in January – February can be used to predict blooms in the CS in May - August. Such a statisticsbased forecasting scheme is implemented to predict *Sargassum* blooms in the CS in May – August from MODIS observations in January – February in the CWA (> 2 months lead time). Results indicate relatively high accuracy (> 80%) for the eastern CS but lower accuracy further west. The forecasting scheme has been used to generate 1-page *Sargassum* outlook bulletins since February 2018. These bulletins have been distributed widely to, and used by, many stakeholders around the Caribbean to prepare for *Sargassum* blooms and potential beaching events.

In Chapter 6, algorithms to detect and quantify *Sargassum* developed for MODIS are further adjusted and tested with data collected by a newer satellite sensor, the Visible Infrared Imaging Radiometer Suite

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(VIIRS) (2012 – present). These algorithms are improved in an effort to develop a capacity for seamless *Sargassum* observations from multiple satellites. *Sargassum* areal coverages derived from MODIS and VIIRS are compared at different time scales, with consistent observations obtained after applying a correction factor to account for their differences in spectral band settings and signal-to-noise ratios. Because the U.S. National Oceanic and Atmospheric Administration (NOAA) has just put another VIIRS (VIIRS-II, on the NOAA-20 satellite) in orbit in November 2017 and will continue to operate a series of VIIRS-like sensors in the future, this work will form a basis to fine-tune the algorithms for future sensors, in order to form a multi-decadal data record to study *Sargassum* changes in response to climate variability and human activities.

The last chapter summarizes the major findings of this dissertation and their potential impacts to the science community and the public. Despite recent efforts of studying *Sargassum* by the research community and the findings from this dissertation, several important questions still remain to be addressed. For example, "What caused the sudden blooms in the Tropical Atlantic and CS in 2011?" and "What caused the inter-annual changes in subsequent years?" Potential ways for future improvements are outlined with respect to the research goals proposed in this study, specifically to understand *Sargassum* distributions, their quantity, transport, and bloom mechanisms.

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Chapter 2:

Sargassum **detection and quantification from MODIS observations**

1. Research overview

This chapter is focused on *Sargassum* feature extraction and quantification from MODIS imagery, from which long-term (2000 – 2015) *Sargassum* distributions in the Central West Atlantic are derived and analyzed. This work has been published in the journal, *Remote Sensing of Environment* (Wang and Hu, 2016). The paper is provided in Appendix A. A brief summary of this paper is provided below.

APPENDIX A - Mapping and quantifying *Sargassum* distribution and coverage in the Central West Atlantic using MODIS observations

This study develops a method to extract *Sargassum* features from Moderate Resolution Imaging Spectroradiometer (MODIS) Alternative Floating Algae Index (AFAI) imagery. The method uses surface-fitting to remove large-scale image gradients, median filtering to suppress noise, and threshold-based filtering to mask clouds and cloud shadows. The extraction accuracy is > 85%, ensuring its applicability to derive reliable long-term *Sargassum* distribution statistics. After extracting the *Sargassum*-containing pixels, their corresponding fractional coverages are quantified through linear spectral unmixing. The upper bound, representing 100% *Sargassum* coverage within a pixel, is determined from the field measured *Sargassum* reflectance spectra. The lower bound, representing 0% *Sargassum* coverage within a pixel, is determined from image statistics. This method is applied to the MODIS Aqua and Terra data from 2000 – 2015 covering

the Central West Atlantic (CWA) to map the spatiotemporal *Sargassum* distribution patterns. The estimated mean bloom coverage in the CWA during summer 2015 is $>$ 2000 km², much higher than the bloom size in 2011 when a bloom was firstly reported for this area. Several environmental variables (temperature, light, river discharge, etc.) are analyzed to investigate the potential causes of the unprecedented blooms in this region since 2011, yet the findings are not conclusive.

Chapter 3:

Remote estimation of *Sargassum* **biomass, nutrients, and pigments**

1. Research overview

This chapter has designed field and laboratory experiments to estimate *Sargassum* biomass, nutrients, and pigments directly from MODIS measurements. This work has been submitted to the journal, *Geophysical Research Letters* (Wang et al., 2018, accepted). The paper is provided in Appendix B. A brief summary of this paper is provided below.

APPENDIX B – Remote estimation of *Sargassum* biomass, nutrients, and pigments(Wang et al., submitted) Assessing the ecological and biogeochemical role of *Sargassum* requires a quantitative estimation of their total biomass, as well as the nutrient and pigment contents. The Alternative Floating Algae Index (AFAI) data derived from Moderate Resolution Imaging Spectroradiometer (MODIS) Rayleigh-corrected reflectance (Rrc) has been applied to estimate *Sargassum* areal coverages, but the associated biomass, nutrients, and pigments are unclear. This study has designed new field and laboratory experiments to derive all these parameters from MODIS observations through building an AFAI-biomass density model and quantifying the *Sargassum* nutrients and pigments concentrations. *Sargassum* reflectance spectra collected at various biomass density ranges (0.00 kg/m² to 7.03 kg/m²) are used to establish the AFAI-biomass density model, with the model's relative uncertainty estimated to be ~ 12%. The major *Sargassum* pigments and C, N, and P concentrations of *Sargassum* samples collected from the Gulf of Mexico and Florida Straits in summer 2017 are analyzed. Monthly distributions of *Sargassum* biomass, nutrients, and pigments are derived from MODIS observations between 2000 and 2017, based on the developed model and calibration relationships. During July 2015, *Sargassum* biomass in the Caribbean Sea and Central West Atlantic exceeded 4.4 million tons, higher than any reported macroalgae blooms in the world's oceans. The corresponding *Sargassum* carbon can account for \sim 18% of the total phytoplankton carbon in this region, thus should not be neglected in carbon cycle modeling. These estimations are expected to help understand the ecological and environmental impacts of massive *Sargassum* aggregations that occurred in the Central West Atlantic and Caribbean Sea in recent years, and to help guide local management agencies to make decisions for future occurrences.

Chapter 4:

Modeling *Sargassum* **transport in the Tropical Atlantic Ocean**

1. Research overview

This chapter is focused on developing a *Sargassum* transport model driven by physical factors (surface current and wind) and biological terms (growth and mortality), to model *Sargassum* transport in the Tropical Atlantic Ocean. This work has been prepared to be submitted to the journal, *Journal of Geophysical Research*. The paper is provided in Appendix C. A brief summary of this paper is provided below.

APPENDIX C – Modelling *Sargassum* transport in the Tropical Atlantic Ocean (Wang, Hu, and Mitchum, in preparation)

Sargassum clumps are floating on the ocean surface, thus treated Lagrangian particles in a Lagrangian trajectory model to understand their spatial distributions and temporal changes. In the model, surface currents and winds are used to drive the *Sargassum* transport in the Tropical Atlantic, while growth/mortality rate derived from MODIS-based statistics is used to modulate the *Sargassum* abundance. Compared to previous physical modeling efforts, this study improves the particle initiation and model evaluation by using the mean *Sargassum* distributions derived MODIS observations. These *Sargassum* abundance observations, along with the associated environmental variables, are used to build a model to estimate the time- and location-dependent *Sargassum* growth/mortality rate (change rate) via a Random Forest Regression. To test the

model performance, thirty-nine numerical experiments are conducted to track the *Sargassum* particles for one month. In most cases, adding surface currents and a 1% wind factor reduce differences between the modeled and MODIS-observed distributions, while adding the *Sargassum* change rate leads to better matchup percentage of the *Sargassum* abundances. The *Sargassum* transport model is applied to track mean *Sargassum* distributions forward and backward at longer time scales to investigate the formation of *Sargassum* distribution patterns and their regional connectivity. The results suggest that additional biological terms in the physicsbased transport model can help explain the observed *Sargassum* seasonal distribution patterns. Furthermore, strong connectivity is found between the Caribbean Sea and Central Atlantic, while a very weak connection is found between the Tropical Atlantic and the northern areas.

Chapter 5:

Sargassum **prediction based on historical** *Sargassum* **distributions**

1. Research overview

This chapter has proposed a *Sargassum* prediction method to accurately predict the spring-summer blooms in the Caribbean Sea based on statistical analyses of historical *Sargassum* distributions. This work has been published in the journal, *Geophysical Research Letters*. The paper is provided in Appendix D. A brief summary of this paper is provided below.

APPENDIX D - Predicting Sargassum blooms in the Caribbean Sea from MODIS observations (Wang and Hu, 2017)

Since 2011, *Sargassum* beaching events have induced serious problems to the coastal regions in the Caribbean Sea (CS). Long-term prediction helps to better prepare for the beaching events and to study *Sargassum* blooms. In this study, a hotspot region in the Central West Atlantic (CWA) has been identified to be indicative of the bloom conditions in the CS through time series analysis of the Moderate Resolution Imaging Spectroradiometer (MODIS) derived *Sargassum* distributions from 2007 – 2016. The overall prediction accuracy is > 80% in most eastern CS regions. Possibility of major blooms in the CS during the spring-summer months (May to August) can thus be predicted by the end of February with more than 2-months lead time. This forecasting approach successfully predicted the CS spring-summer bloom event in 2017 back in early February 2017, and predicted the CS spring-summer bloom event in 2018 back in early February 2018. The same

statistics and connectivity-based prediction approach might be of use in other regions experiencing similar blooms.

Chapter 6:

Looking forward – Observation continuity between multiple satellites

1. Research overview

This chapter has developed a *Sargassum* extraction and quantification algorithm to work on imageries obtained from VIIRS, a follow-on sensor of MODIS, and demonstrated the applicability of VIIRS data to provide continuous and consistent *Sargassum* statistics originating from MODIS measurements. This work has been published in the journal, *International Journal of Remote Sensing*. The paper is provided in Appendix E. A brief summary of this paper is provided below.

APPENDIX E – On the continuity of quantifying floating algae of the Central West Atlantic between MODIS and VIIRS (Wang and Hu, 2018)

Similar to the method developed for *Sargassum* extraction and quantification from Moderate Resolution Imaging Spectroradiometer (MODIS) observations, a refined procedure is proposed in this study to extract and quantify algae-containing pixels from the Visible Infrared Imager Radiometer Suite (VIIRS) observations. Comparable feature extraction accuracy (> 85%) is achieved after proper noise reduction and adjusting thresholds to mask clouds, cloud shadows, and sun glint. From simultaneous observations to monthly mean composites, VIIRS-derived *Sargassum* spatial and temporal distribution patterns match well with those from MODIS observations, although the VIIRS-derived *Sargassum* areal coverage is lower, due to mainly to its lower signal-to-noise ratios. The discrepancy, however, can be easily removed by applying a

calibration constant. This study therefore demonstrates the capacity of VIIRS to provide continuous and consistent *Sargassum* statistics originating from previous MODIS measurements to current VIIRS measurements. It also provides a methodology for dealing with discrepancies from other VIIRS-like sensors, either currently in orbit or being planned for the future, to form a seamless multi-sensor multi-decadal *Sargassum* data record.

Chapter 7:

Summary and conclusions

1. Research overview

The goal of this study is to improve the understanding of the *Sargassum* abundance, distributions, transport pathways, and bloom mechanisms in the Caribbean Sea (CS) and Tropic Atlantic. Through the use of satellite remote sensing, field and laboratory measurements, and numerical models, most objectives under this overarching goal have been achieved, which has provided new findings available for other inter-disciplinary studies and to guide future research and management. Specifically, satellite observations from MODIS and VIIRS are used to map and quantify *Sargassum* distributions (areal coverages) at synoptic scales (Wang and Hu, 2016; Wang and Hu, 2018), to estimate distributions of their biomass, nutrients, and pigments (Wang et al., submitted). *Sargassum* transport in the Tropical Atlantic is studied using a Lagrangian particle tracking model (Wang, Hu, and Mitchum, in preparation), along with *Sargassum* growth/mortality rate derived from statistical analyses of MODIS observations and environmental data. Modeling results suggest that in addition to physical forcing by ocean currents and winds, biological factors also play an important role in determining *Sargassum* distributions and their regional connections among the CS, Central Atlantic, and North Atlantic. The connectivity study from the modeling and from long-term MODIS statistics suggests that *Sargassum* blooms in the CS in May – August can be predicted from bloom conditions in the CWA in January – February, providing at least a 2-month lead time to prepare for blooms and potential beaching events around the Caribbean (Wang and Hu, 2017). Finally, the observations, modeling, analyses, and forecasting can all be continued forward through

satellite continuity missions such as those from the VIIRS series (Wang and Hu, 2018), where a multisensor multi-decadal *Sargassum* data record may be established to help understand global changes and to help address research and management needs.

2. Research findings and impacts

The major findings of this study will benefit not only the science communities, but also local residents of the Caribbean. Below I summarize these research findings and their potential impacts.

Distributions: *Sargassum* **areal coverage maps**

The MODIS- and VIIRS-derived *Sargassum* distribution maps cover the period of 2000 – present, thus extending previous time-series of 2002 – 2011 from Medium Resolution Imaging Spectrometer (MERIS) observations(Gower et al., 2013; Gower and King, 2011). The new maps are based on an objective method for detection and quantification (Wang and Hu, 2016), thus providing improved data quality over previous results for analyzing the bloom characteristics, potential impacts, bloom origins, driving factors, and transport pathways. More importantly, although the targeted studies in the published papers and submitted manuscripts mainly focus on the CS and CWA, the monthly maps cover the entire Intra-Americas Sea (IAS, including the Gulf of Mexico) and Atlantic. Some examples for 2014-2015 are provided in Fig. 7.1. In these full-coverage maps, *Sargassum* mats can form a continuous "belt" in the Tropical Atlantic from the west coast of Africa to the Caribbean, and they can also enter the Gulf of Mexico via the Loop Current. Furthermore, blooms in the western Gulf of Mexico can be completely out of phase from blooms in the Caribbean, suggesting potentially different bloom origin that should be investigated in the future.

Figure 7.1: Monthly mean *Sargassum* areal coverage maps from 2014 to 2015. The region coverage is from 10° S to 32° N and 98° W to 15° E

In addition, the weekly *Sargassum* distribution maps for the CS and CWA regions, updated every day in the *Sargassum* Watch System (SaWS, [http://optics.marine.usf.edu/projects/saws.html\)](http://optics.marine.usf.edu/projects/saws.html), provide a general overview of the *Sargassum* distributions in these two regions for the research community and for the general public [\(http://optics.marine.usf.edu/cgi-bin/optics_data?roi=ECARIB¤t=1;](http://optics.marine.usf.edu/cgi-bin/optics_data?roi=ECARIB¤t=1) [http://optics.marine.usf.edu/cgi-bin/optics_data?roi=C_ATLANTIC¤t=1\)](http://optics.marine.usf.edu/cgi-bin/optics_data?roi=C_ATLANTIC¤t=1). Short-term predictions of beaching events can be made from these distribution maps when combined with ocean surface currents and wind data (Maréchal et al., 2017).

Abundance: *Sargassum* **biomass and nutrients**.

The AFAI-biomass density model established from field and laboratory experiments allows for the quantification of *Sargassum* biomass from satellite observations. Currently, *Sargassum* biomass estimations mostly rely on field observations using neuston tows. For practical reasons, the neuston tows have difficulties in sampling very dense *Sargassum* mats (Parr et al., 1939; Bulter et al., 1983; Bulter and Stoner, 1984), thus may provide biased observations. Moreover, considering the strong spatiotemporal variations, field samplings are likely biased due to their limited spatial and temporal coverage, calling for synoptic and repeated satellite measurements to better understand *Sargassum* biomass and associated major pigments and C, N, P concentrations. The study here fills this research needs by providing such estimates at synoptic scales every month for > 17 years, which can also be extended in the future.

These estimates can help understand the potential impacts of *Sargassum* on ocean biology, chemistry, and ecology. They can also help plan for *Sargassum* harvesting for both environmental and economic benefits.

Transport: Physics, biology, and connectivity

The *Sargassum* transport model presented here demonstratesthe roles of physical advection, winds, and growth/mortality rate in reproducing *Sargassum* distributions when the model is initiated with satellite observations. Although the results are limited by the lack of understanding on the *Sargassum* growth/mortality rate and lack of high spatial (e.g., sub-km) and temporal (e.g., sub-daily) *Sargassum* distribution maps, sensitivity analyses of different modeling scenarios still lead to several important findings: 1) *Sargassum* blooms in the Caribbean Sea are mainly a result of physical transport from the Central Atlantic regions; 2) Most of the *Sargassum* "particles" in the Central Atlantic region are selfretained, and thus unlikely to be linked to the North Atlantic areas (including the Sargasso Sea).

Predictions: Long-term versus short-term.

Based on MODIS observation statistics, the *Sargassum* forecasting model can provide warnings of possible blooms in the CS at least 60 days in advance, with > 80% overall accuracy in most eastern Caribbean areas. As significant *Sargassum* beaching events can impact tourism, artisanal fishing, and local

environments and economy, local management agencies and many other stakeholders can benefit from this prediction to better prepare for offshore blooms and beaching events (e.g., prepare equipment for physical removal). Researchers can also better plan their field sampling strategies from the early warnings. Indeed, based on MODIS and VIIRS observations and using this forecasting model, we developed 1-page bulletins every month since early February 2018 to provide a general outlook of *Sargassum* blooms across the entire Caribbean. Fig. 7.2 shows an example of the bulletins, generated and in early February 2018. These bulletins have been distributed widely to many user groups through emails and local news media, Very positive feedbacks were provided by the users of these bulletins. Indeed, similar to the successful prediction in early 2017, reports received from local groups confirmed the success of this year's prediction, where massive *Sargassum* blooms and many beaching events occurred a few months later in the Caribbean in 2018.

The approach of the prediction also has implications for other regions facing similar blooms and beaching events, for example coastal regions around Brazil and West Africa. Once regional connectivity is confirmed through analyses of historical *Sargassum* distributions, a similar model may be established for those areas.

While the statistics-based forecasting may provide a general outlook (e.g., Fig. 7.2) of possible bloom and beaching events several months in advance, predicting beaching events in the short term (days to 1- 2 weeks) is more technically challenging as such a prediction requires accurate knowledge on small-scale ocean and atmospheric conditions (currents and winds) several days or 1-2 weeks in advance. Such information is general not available for local regions. However, using the nowcast HYCOM ocean currents and real-time winds, short-term prediction is still possible with the near real-time MODIS and VIIRS based *Sargassum* observations (Maréchal et al., 2017). On the other hand, because the factors causing interannual changes of *Sargassum* blooms are not well understood, it is currently impossible to predict bloom conditions for the coming years.

Figure 7.2: An example of 1-page *Sargassum* bloom outlook bulletins, generated from MODIS and VIIRS observations and distributed to many user groups. This specific bulletin was generated in early February 2018, when it was predicted that major blooms and beaching events would occur in the Caribbean in the following months. Reports received during March to June 2018 from local groups confirmed this prediction.

3. Future research

Causes and origins: What's missing?

One of the objectives in this study is to understand what caused the inter-annual changes of bloom patterns, and what could be the origin of the *Sargassum* blooms. However, after extensive data analyses and modeling, there are still no answers to these questions. In Wang and Hu (2016), many environmental forcing factors are used in an attempt to understand inter-annual changes in bloom patterns. These include SST, Amazon River discharge, surface light availability, and precipitation. Although in some years one or two factors appear to explain the changes, in general the findings are not conclusive. Furthermore, because the entire IAS and North Atlantic are connective via ocean circulation, it is also difficult to pinpoint the bloom source(s). Addressing these challenges may require more process-driven studies than statistics and modeling driven approaches presented here. Unfortunately, such measurements are extremely scarce in the literature (Hanisak and Samuel, 1987). Clearly, more field measurements are required to quantify and understand *Sargassum* growth and mortality, with particular emphasis on what environmental factors may drive their changes.

Furthermore, because the IAS and the Atlantic are connected through ocean circulation, to understand the inter-annual variations of the *Sargassum* abundance in different regions, the IAS and Atlantic should be considered as a whole instead of being treated separately. More efforts are required to thoroughly investigate how *Sargassum* inter-annual changes are influenced by the various environmental factors, climate indexes, and regional connectivity through statistical analyses and physical and biogeochemical modeling.

Scales and uncertainties

As discussed in Chapter 2, *Sargassum* features have variable sizes, ranging from a few centimeters to hundreds of kilometers. The coarse-resolution sensors such as MODIS and VIIRS can only detect the dense Sargassum features of > 0.2% pixel size (Wang and Hu, 2016) or > 2.80 g/m² (Wang et al., 2018). In other words, all *Sargassum* results presented in this study represent only those that are *observable* by these satellites, while in reality many smaller *Sargassum* clumps and mats may exist in the ocean (Hu et al., 2015). One possible solution to fill this gap is to estimate the amount of MODIS-undetected *Sargassum* abundance using higher-resolution satellite data (such as Landsat-8 OLI (30-m resolution) or Sentinel-2

MSI (10-m resolution)). These higher-resolution data can help determine the uncertainties of our current *Sargassum* observations. However, reliable algorithms need to be developed to automatically extract and quantify *Sargassum* and to remove various confusing features such as thin clouds, cloud shadows, and sun glint. In the end, a multi-sensor multi-scale *Sargassum* quantification will provide a more comprehensive understanding of the total *Sargassum* abundance and their spatial/temporal changes in the IAS and Atlantic Ocean.

Sargassum **blooms and fishery**

As an essential marine habitat, *Sargassum* mats are often associated with many marine animals including a variety of fish and turtles (Casazza and Ross, 2008; Witherington et al., 2014; Lapointe et al., 2014; Hardy, 2014). It is natural to assume that increased *Sargassum* abundance may have a positive impact on fish populations in terms of total amount and diversity. The knowledge of *Sargassum* changes in response to natural and unnatural forcing is also relevant to the current restoration effort around the Gulf of Mexico. Future work will be dedicated to searching for possible linkage between *Sargassum* abundance and fish catch per unit effort and fish species compositions. The basin-wide *Sargassum* distribution maps from 2000 onward will serve as an important database for assessing the potential impacts of *Sargassum* changes to local fishery. Likewise, how *Sargassum* may affect ocean biology and chemistry and seafloor sediment record also remains to be further studied.

4. Conclusions

Despite significant *Sargassum* blooms and beaching events in recent years in the Caribbean Sea and Tropical Atlantic as well as in other regions, pelagic *Sargassum* has generally been understudied, especially when compared with studies of water column phytoplankton. Here, a comprehensive study of *Sargassum* in these regions has been conducted. The study combines satellite remote sensing, field and laboratory experiments, and numerical modeling to document and understand spatial distributions of *Sargassum*

abundance and their temporal changes since 2000. Several new findings are derived from this study, including the spatially continuous *Sargassum* aggregation in the Tropic Atlantic and the Caribbean, connectivity between the Caribbean and the Gulf of Mexico, large inter-annual changes of *Sargassum* abundance, and difficulty in understanding such inter-annual changes and in modeling *Sargassum* distributions without accurate knowledge of *Sargassum* growth/mortality rate. While several unanswered questions may be addressed from future follow-on efforts, the most significant outcomes of this study include the remote sensing algorithms, *Sargassum* distribution and abundance (including biomass, pigments, and nutrients) maps, established bio-physical model, and, more importantly, a forecast model to predict *Sargassum* bloom probabilities in the Caribbean with at least 2 months of lead time. These outcomes are expected to make significant contributions in scientific research and management decision support, and I anticipate continuing *Sargassum* studies along the outlined future directions.

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Appendix A:

Mapping and quantifying *Sargassum* **distribution and coverage in the Central West Atlantic using**

MODIS observations

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Mapping and quantifying Sargassum distribution and coverage in the Central West Atlantic using MODIS observations

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ABSTRACT

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Keywords: Sargassum Remote sensing **MODIS** FAI **AFAI** Cloud Cloud shadow Feature extraction Surface fitting

Sargassum washing ashore on the beaches of the Caribbean Islands since 2011 has caused problems for the local environments, tourism, and economies. Although preliminary results of Sargassum distributions in the nearby oceans have been obtained using measurements from the Medium Resolution Imaging Spectrometer (MERIS), MERIS stopped functioning in 2012, and detecting and quantifying Sargassum distributions still face technical challenges due to ambiguous pixels from clouds, cloud shadows, cloud adjacency effect, and large-scale image gradient. In this paper, a novel approach is developed to detect Sargassum presence and to quantify Sargassum coverage using the Moderate Resolution Imaging Spectroradiometer (MODIS) alternative floating algae index (AFAI), which examines the red-edge reflectance of floating vegetation. This approach includes three basic steps: 1) classification of Sargassum-containing pixels through correction of large-scale gradient, masking clouds and cloud shadows, and removal of ambiguous pixels; 2) linear unmixing of Sargassum-containing pixels; and, 3) statistics of Sargassum area coverage in pre-defined grids at monthly, seasonal, and annual intervals. In the absence of direct field measurements to validate the results, limited observations from the Hyperspectral Imager for the Coastal Ocean (HICO) measurements and numerous local reports support the conclusion that the elevated AFAI signals are due to the presence of Sargassum instead of other floating materials, and various sensitivity analyges are used to quantify the uncertainties in the derived Sargassum area coverage. The approach was applied to MODIS observations between 2000 and 2015 over the Central West Atlantic (CWA) region (0-22°N 63-38°W) to derive the spatial and temporal distribution patterns as well as the total area coverage of Sargussum. Results indicate that the first widespread Sargassum distribution event occurred in 2011, consistent with previous MERIS findings. Since 2011, only 2013 showed a minimal Sargassum coverage similar to the period of 2000 to 2010; all other years showed significantly more coverage. More alarmingly, the summer months of 2015 showed mean coverage of > 2000 km², or about 4 times of the summer 2011 coverage and 20 times of the summer 2000 to 2010 coverage. Analysis of several environmental variables provided some hints on the reasons causing the inter-annual changes after 2010, yet further multi-disciplinary research (including in situ measurements) is required to understand such changes and long-term trends in Sargassum coverage.

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1. Introduction

Since 2011, massive beaching events of the pelagic Sargassum macroalgae have occurred frequently on the Lesser Antilles Islands in the southern Caribbean (Fig. 1), significantly impacting local environments, tourism, fisheries, and economies (http://mission-blue.org/ 2014/10/sargassum-inundates-the-beaches-of-the-caribbean/; Gower, Young, & King, 2013; Maurer, De Neef, & Stapleton, 2015). Concurrent beaching events in western Africa and northern Brazil have also been reported (Oyesiku & Egunyomi, 2015; Széchy, Guedes, Baeta-Neves, & Oliveira, 2012). While pelagic Sargassum serves as an important habitat and refuge for many marine organisms in the open-ocean environment (Council, 2002; Rooker, Turner, & Holt, 2006; Witherington, Hirama, &

http://dx.doi.org/10.1016/j.rse.2016.04.019 0034-4257/0 2016 Elsevier Inc. All rights reserved. Hardy, 2012), excessive beaching poses significant environmental and profound economic problems. For example, over \$2.91 million have been spent annually on the deanup of Sargassum from Texas beaches (Webster & Linton, 2013). Despite the enormous efforts of local management in response to these beaching events, our knowledge about these blooms is limited. For example: Where do Sargassum blooms initiate? How much Sargassum is present in the oceans? What causes these blooms and their inter-annual changes? How do these blooms impact the ocean's biogeochemistry and ecology? Indeed, to date, the only published remote sensing works used Medium Resolution Imaging Spectrometer (MERIS) observations to document the Sargassum distributions and abundance in the Intra-Americas Sea and the central Atlantic between 2002 and 2011 (Gower & King, 2011; Gower et al., 2013). However, as MERIS stopped functioning in early 2012, there is virtually no information on the Sargassum distribution or abundance in the Caribbean, the greater Intra-Americas Sea, or nearby oceans after 2011

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Fig. 1. MODIS/Aqua AFAI image (a) on 1 January 2015 (17:05 GMT) over the CWA showing surface slicks (box 2) with enhanced near infrared (NR) reflectance. Black color indicates land or clouds or sunglint, representing no valid observation. The blue-colored features near the cloud edge (box 1), although easily identified as non-Sargussum through visual inspection, make accurate quantification of Sargassum coverage very difficult with automatic methods because they can be falsely treated as Sargassum-containing pixels. Red crosses mark the location of
the doud shadow and Sargassum pixels dimensionless) of Sargassum mats measured in the Gulf of Mexico and off Bermuda using a hand-held spectrometer are shown in (b). The thick solid line represents the mean of > 50 measurements while the dashed lines indicate 2 times of standard deviation. Also overlaid are the three MODIS bands centered at 667, 748, and 869 nm, which are used to calculate AFAI.

because of the loss of MERIS. Furthermore, the methods used in the MERIS-based study to detect and quantify Sargassum require refinements (see Section 2). Because these questions remain unanswered, the effort to broaden and continue further research, through the refinement of MERIS-based observations, and while exploring the possibility of using other satellite instruments, becomes crucial.

In 2009, Hu (2009) developed a floating algae index (FAI) using data collected by the Moderate Resolution Imaging Spectroradiometer (MODIS) to detect and trace the Ulva prolifera macroalgae blooms in the Yellow Sea near Qingdao, China (He, Liu, Yu, Li, & Hu, 2011; Hu et al., 2010a). Because FAI was designed using the vegetation red-edge reflectance in the near infrared, it can be used to detect any floating vegetation including Sargassum (Hu, Feng, Hardy, & Hochberg, 2015). In 2010, in order to help monitor potential Sargassum beaching events on the Lesser Antilles Islands in the southern Caribbean, FAI was implemented to generate MODIS FAI imagery covering the Central West Atlantic (CWA) region (0-22°N, 63-38°W) in near real-time through a Virtual Antenna System (VAS) (Hu, Barnes, Murch, & Carlson, 2014). The system has been running operationally with daily updates in near real-time (within 4-6 h of the satellite overpass). However, because there is no effective cloud-masking method for FAI, clouds are not masked in the imagery. Although Sargassum slicks can be visually differentiated from clouds in FAI imagery with a trained eye, it is difficult for visual interpretation by average users, as both Sargassum slicks and

clouds show high FAI values. To overcome this difficulty, an alternative FAI (AFAI) was developed (where clouds can be masked through band combinations), and data was produced over the whole MODIS time series (see below). Fig. 1 shows an example of the AFAI imagery generated and distributed in near real-time.

AFAI imagery allows for simple interpretation by a layperson to identify surface slicks of floating vegetation. When combined with surface current velocity estimates from the Hycom hydrodynamics model (all available through a simple click on a customized web portal http://optics.marine.usf.edu/projects/SaWS.html with full Google-Earth compatibility), the AFAI imagery has provided timely information on the location of large Sargassum slicks as well as their movement speed and direction to many local groups and individuals (Hu et al., 2014). However, several difficulties emerged when attempting to derive long-term statistics of Sargassum distribution and abundance using near real-time imagery: 1) frequent cloud cover made the valid data rather scarce (note the location of this region's proximity to the Inter Tropical Convergence Zone (ITCZ)) (Wylie, Jackson, Menzel, & Bates, 2005); 2) although it is relatively straightforward to identify Sargassum slides through visual in spection, because false positive detection often results from cloud shadow contamination it is difficult to automate such a detection; 3) the large-scale AFAI gradient across the image scene makes it difficult to apply threshold-based segmentation; and, 4) each identified Sargassum-containing pixel may contain varying

proportions of Sargassum, leading to biased statistics if each Sargassumcontaining pixel is treated equally.

Hence, given the challenges in quantitative assessment of Sargassum distributions, area coverage, long-term trends, and the pressing need of such knowledge in order to understand the potential causes of the trend and to help make management decisions, the objectives of this study, based on the existing MODIS AFAI imagery, are to:

- 1) develop a practical and objective method to quantify Sargassum distribution and area coverage in the Central West Atlantic using MODIS observations; and,
- 2) establish a long-term (2000-2015) time series of Sargassum distribution patterns and area coverage in the study region to quantify the long-term trend.

As this is primarily a methodology development paper, rather than following a traditional structure, the paper is organized in a way to first provide some background on Sargassum detection, then detail all steps in the method, and finally present a time series of Sargassum distributions. While the focus of this study is on the development of methodology and establishment of long-term time series, a preliminary analysis of several environmental variables is also undertaken in an attempt to understand these long-term patterns.

2. Sargassum remote sensing: What is available and what is not?

Gower, Hu, Borstad, and King (2006) first demonstrated that pelagic Sargassum (Sargassum natans and Sargassum fluitans) can be detected from satellite imagery based on elevated NIR reflectance (the red-edge effect, i.e., enhanced reflectance between 700 and 730 nm). This detection principle was applied to MERIS Maximum Chlorophyll Index (MCI (Gower, King, Borstad, & Brown, 2005)) (Gower et al., 2006), and later to MODIS FAI (Hu, 2009). Based on the MERIS MCI products, Gower and King (2011) first generated Sargassum distribution maps for the Gulf of Mexico (GOM) and Sargasso Sea between 2002 and 2008. They were later improved by extending coverage to include the central Atlantic with data up to 2011 in an attempt to explain the potential source of the 2011 Sargassum bloom in the Caribbean (Gower et al., 2013). When generating the monthly Sargassum distribution maps, for each of the pre-defined 5-km grids within the area of interest, the maximum MCI was used to represent that grid. Then, the maximum MCI value during the entire month was used to represent the monthly MCI value for that grid. Monthly maps derived in this manner potentially contain three error sources: 1) MCI was obtained from top-of-atmosphere (TOA) radiance, instead of atmospherically corrected reflectance, leading to uncertainties in deriving a universal threshold for Sargassum detection: 2) errors in TOA radiance-based cloud-masking; and 3) the use of maximum MCI instead of mean MCI within the 5-km grid during a month may overestimate Sargassum abundance.

Hu (2009) showed that MODIS FAI can also be used to detect macroalgae blooms. MODIS FAI and AFAI were implemented to detect and trace Sargassum blooms in near real-time over the CWA in 2010 (Hu et al., 2014) but has since been back processed to 2000 to include all MODIS data for the region, Compared to MERIS MCI, MODIS AFAI provides a comparable and potentially better alternative because MODIS is onboard both Aqua and Terra satellites (afternoon and morning passes, respectively) and each MODIS swath (2330 km) is approximately twice that of a MERIS swath (1150 km). Although the near real-time MODIS AFAI imagery has provided valuable information on the Sargassum location and movement, its interpretation was primarily based on visual inspection. Due to technical difficulties such as discriminating ambiguous pixels from clouds, doud shadows, cloud adjacency effects, and removing large-scale image gradients, there has not been any automatic detection, delineation, or use of MODIS AFAI to generate long-term statistics.

To date, most macroalgae delineation methods (through the use of MCI, FAI, Normalized Difference Vegetation Index (NDVI), or other similar data products) are threshold-based segmentation methods that all suffer from cross-scene large-scale image gradient. Several attempts have been made to use a global-scope threshold for image segmentation in recent studies. In 2009, Shi and Wang (2009) developed a floating macroalgae delineation method producing Normalized Difference Algae Index (NDAI) products which are similar to NDVI products, but a Rayleigh correction is applied to TOA reflectance to remove the molecular scattering effects before NDAI is calculated. The image is first classified into "algae" and "non-algae" classes using the median value of the NDAI scene, then the ocean background pixel value is determined from the mean value of the "non-algae" pixels in a 10×10 pixel window centered on the given "algae" pixel (Shi & Wang, 2009). The potential problems in this method are: 1) that the mean value may be affected by the high signal values of the algae pixels; 2) the 10×10 pixel window could be largely or even completely contaminated by algae pixels; and, 3) that the scene-wide NDAI median value may not be able to provide a good classification of the algae pixels (Garcia, Fearns, Keesing, & Liu, 2013). The main idea is to obtain the background ocean signal through image processing so that local macroalgae signals can be scaled against the cross-image gradient. To overcome these issues, a 'difference image' was proposed by Keesing, Liu, Fearns, and Garcia in 2011 and is computed by subtracting a background ocean image from the original image. Called the Scaled Algae Index (SAI) method, Keesing, Liu, Fearns, and Garcia (2011) proposed it to quantify U, prolifera macroalgae blooms in the Yellow Sea from MODIS NDVI images. The method used a 25×25 pixel median filter to determine the background water signal and applied a local threshold segmentation, based on the statistical distribution in the 25×25 pixel window, centered on the pixel of interest. The method was further modified in Garcia et al. (2013) to select the optimal window size and segmentation threshold. Due to variability of the feature distribution in the median filter window, the window size and the threshold often need to be tuned by a human expert to achieve satisfactory performance. In short, although visual detection is straightforward through one of the indexes, automatic detection and quantification of macroalgae blooms are still problematic when longterm time series data are desired. Another difficulty is that these indexes only detect the red-edge reflectance and thus not able to spectrally differentiate Sargassum from other floating materials (Dierssen, Chlus, & Russell, 2015; Hu et al, 2015). While the latter requires hyperspectral data that are mostly unavailable from currents satellites, the former is addressed using the approach developed in this study.

3. Data sources and processing methods

Although the near real-time monitoring of Sargassum slicks started in 2010 (Hu et al., 2014), the development of a complete time series MODIS data set, covering the CWA between April 2000 and October 2015, required downloading all relevant data from the U.S. National Aeronautics and Space Administration (NASA) Goddard Space Flight Center (http://oceancolor.gsfc.nasa.gov) which were subsequently processed using the software package SeaDAS (version 7.0.2) to generate Rayleigh-corrected reflectance (Rrc) data for each spectral band (Hu, 2009). Both MODIS/Terra (MODIST) and MODIS/Aqua (MODISA) data were downloaded and processed. The Rrc data were then used to calculate FAI for each pixel (Hu, 2009):

$FAI = R_{\pi,NIR} - R'_{\pi,NIR}$

 (1) $\overline{R}_{rcNR} = R_{rcRED} + (R_{rcSWR} - R_{rcRED}) \times (\lambda_{NIR} - \lambda_{RED}) / (\lambda_{SWR} - \lambda_{RED}),$

where the subscripts RED, NIR and short-wave infrared (SWIR) represent the spectral bands. FAI is the difference between R_{rcNIR} and the baseline reflectance R'_{rcNIR} derived from the linear interpolation between the red and SWIR bands. For MODIS FAI calculations, $\lambda_{\text{RED}} =$ 645 nm, λ_{NIR} = 859 nm, and λ_{SWIR} = 1240 nm. The FAI product provides a quick and easy way to visualize surface floating algae. However, due to lack of an effective doud-masking algorithm, only people with

training can differentiate floating algae slicks from cloud patches and other artifacts. This represents a major hurdle for an average person to interpret the images. To overcome this difficulty, the AFAI product was generated using the same FAI design but using different spectral bands ($\lambda_{\text{RED}} = 667$ nm, $\lambda_{\text{NIR}} = 748$ nm, $\lambda_{\text{SWIR}} = 869$ nm). Note that although 869 nm is in the NIR spectral range, for simplicity and consistency it is still termed as "SWIR".

Although AFAI has a lower spatial resolution (1-km) compared to FAI (250-m), the 1-km bands used in calculating AFAI have much higher signal-to-noise ratios (SNRs) than the 250-m bands for FAI (e.g., 995:1 for the 748-nm 1-km band compared to 157:1 for the 859-nm 250-m band, Hu et al., 2012), thus compensating for the reduction in resolution when detecting small Sargassum mats. While the disadvantage of AFAI is its saturation over bright targets such as clouds and strong sunglint (therefore leading to less data coverage), its advantage is relatively easy cloud-masking, making the resulting imagery simple to interpret even by a layperson. Such characteristics are particularly important for near real-time applications. One example of the AFAI imagery distributed online is shown in Fig. 1. The Sargassum slicks can be clearly visualized after cloud-masking. In total, 17,772 MODIS AFAI images from Terra and Aqua measurements between April 2000 and November 2015 were generated in order to develop a time series, corresponding to about 95 images per month.

To help understand the observed Sargassum distribution patterns, environmental data were obtained from several sources. Three data types were obtained from NASA's Giovanni online visualization and analysis system (http://giovanni.sci.gsfc.nasa.gov/giovanni/). These data included: 1) cloud fraction data from the Atmospheric Infrared Sounder (AIRS) AIRX3STM v006 between January 2009 and October 2015; 2) precipitation data from the Tropical Rainfall Measuring Mission (TRMM) TRMM_3b43 v7 between January 2009 and August 2015; and 3) aerosol optical depth (AOD, 500 nm) data from the Ozone Monitoring Instrument (OMI) OMAERUVd v003 between January 2009 and November 2015. In addition to Giovanni data, sea surface temperature (SST) anomaly data were derived from National Oceanic and Atmospheric Administration (NOAA) Optimum Interpolation (OI) SST V2 monthly mean products (provided by the NOAA/ OAR/ESRL PSD, Boulder, Colorado, USA, from their Web site at http://www.esrl.nogg.gov/psd/) from January 2009 to August 2015. Photosynthetically available radiation (PAR) data were obtained from the MODIS Aqua 4 km monthly mean products (http:// oceancolor.gsfc.nasa.gov/cgi/l3) from January 2009 to August 2015. And finally, Amazon River discharge data were acquired from the Brazilian National Water Agency at station Obidos (http://www2. ana.gov.br/Paginas/EN/default.aspx). The station is located 800 km upstream from the Atlantic Ocean and is above the tide's influence thus normal water-discharge fluctuations can be detected.

4. Technical approach

Given the available 17,772 AFAI MODIS images, the process for mapping and quantifying the Sargassum distribution and coverage is composed of three major steps:

- 1) Classification of individual image pixels into three classes:
	- A) no-observation (this class includes no satellite coverage, sunglint, douds, cloud shadows, and all other image artifacts);
	- B) Sargassum-free; and
	- C) Sargassum-containing.
- 2) Unmixing of the Sargassum-containing class using local thresholds for minimal (0%) and maximal (100%) sub-pixel coverage in order to estimate the fractional Sargassum coverage within a pixel.
- 3) Data binning of the individual image pixels into pre-defined grids at given time intervals (month, season, year) for the entire study

period (2000-2015), which leads to time series of area coverage and distribution maps.

Note that in reality the elevated AFAI signal can be from any floating vegetation, not just Sargassum. These floating vegetation include Trichodesmium mats (Hu et al., 2010b; Subramaniam, Brown, Hood, Carpenter, & Capone, 2002). This is actually where the name of floating algae index came from (Hu, 2009). However, in the context of Sargassum mapping the elevated AFAI signal is deemed to come from Sargassum mats based on both direct and indirect evidence (see Discussion).

The entire process is summarized in the flowchart in Fig. 2. Specifically, after masking clouds, sunglint and land, initial Sargassum pixel extraction is achieved by comparing the original AFAI image and a surface fitted image (generated by computing a four-degree polynomial fit to a surface with the valid AFAI pixels in each image). The extracted pixels are marked as potential Sargassum-containing pixels, and are excluded from the median filter used to calculate the Sargassum-free background ocean AFAI signal. The 'difference image' between the original AFAI image and background Sargassum-free ocean AFAI image is then segmented to extract the final Sargassum-containing pixels using a global scope (meaning within the CWA region in this work) threshold, T_0 . False-positives over cloud shadow pixels (e.g., Fig. 1) are masked as invalid data. For each Sargassum-containing pixel a linear unmixing scheme, based on locally-adjusted lower (0% sub-pixel) and upper (100% sub-pixel) bound coverage, is used to determine the fractional Sargassum coverage within a pixel. Finally, all valid pixels (both Sargassum-free and Sargassum-containing) within a pre-defined grid and a given time interval (month, season, year) are used to calculate the mean Sargassum fractional coverage for that grid and time interval. Statistical analyses of all grids lead to distribution and coverage maps. Below these steps are described in detail.

4.1. Step 1: Pixel classification into three classes: No observation (A), Sargassum-free (B), and Sargassum-containing (C)

4.1.1. No observation due to no satellite coverage, sunglint, clouds, or cloud shadows

All these conditions were treated as no observation, as no information on whether a pixel contains Sargassum can be determined.

4.1.1.1. No coverage. Each AFAI image was mapped to a rectangular projection, where some of the pixels in the projected image may not be covered by MODIS measurements. These pixels were assigned a value of -0.0999 during map projection. Pixels meeting the following criteria were identified as no satellite coverage:

$$
R_{rc}(667) = -0.0999 \text{ or } R_{rc}(748) = -0.0999 \text{ or } R_{rc}(869) = -0.0999.
$$
\n(2)

4.1.1.2. Sunglint and cloud-masking. Both sunglint and clouds lead to enhanced reflectance in all spectral bands. In this study, pixels meeting the following criteria were identified as sunglint or douds:

$$
R_{rc}(667) > 0.2 \text{ or } R_{rc}(748) > 0.2 \text{ or } R_{rc}(869) > 0.2. \tag{3}
$$

The criteria were determined through trial and error. Although SeaDAS processing generates a standard CLDICE (clouds or ice) flag (Patt et al., 2003), a comparison between CLDICE and the thresholdbased cloud-masking (Fig. 3) shows that CLDICE over-masked Sargassum-free pixels in some cases (Fig. 3e) while under-masked Sargassum-containing pixels in other cases (Fig. 3h). The former would reduce the number of valid observations while the latter would reduce the number of Sargassum-containing pixels, both leading to increased uncertainties in the Sargassum coverage estimation. Note that CLDICE M. Wang, C. Hu / Remote Sensing of Environment 183 (2016) 350-367

Fig. 2. Work flow to generate Sargossum distribution and coverage maps from MODIS AFAI images. They are generally grouped into three steps, as described in the text. Note that for simplicity and illustration purposes, cloud shadow masking is shown here as a preprocessing step before classification. Practically, cloud shadow masking has to rely on the preliminary classification results to improve the performance. Note that the illustration is to calculate a monthly mean, but the approach is the same for other time intervals. α_i represents the Sargassum subpixel cover

in SeaDAS was optimized for the processing of global ocean color data, with the ultimate goal of obtaining the highest-quality ocean color data products. In practice, to meet this goal CLDICE was determined in a conservative way, defined as R_{rc} (859) (after subtracting an estimated sunglint reflectance) > 0.027. This is why CLDICE masked
many non-cloud pixels (including Sargassum-free water pixels and Sargassum-containing pixels). Furthermore, some of the sunglint pixels were not masked by CLDICE (gray-reddish color in Fig. 3), and these pixels have high AFAI values, leading to false positive detection. Because threshold-based cloud-masking avoided all these problems, this method was selected to mask both sunglint and clouds in this study.

4.1.1.3. Cloud shadow screening. Cloud shadow pixels show high AFAI values and may be falsely identified as Sargassum (see Fig. 4a & b)), leading to overestimation of the Sargassum area coverage.

Due to the lack of direct solar radiation, cloud shadow pixels show low Rrc values as compared with the surrounding pixels. In this study, a local total Rayleigh corrected reflectance (LTR) was first defined as

$$
LTR = R_{rc}(469) + R_{rc}(555). \tag{4}
$$

Then, the difference between LTR of the current pixel and a reference LTR value, defined as the mean LTR of a 31 \times 31 pixel window centered at the current pixel, was examined. If the difference was lower than a predefined threshold, Tc:

$$
LTR-Ref_{LTR} < T_c. \tag{5}
$$

The current pixel was regarded as a cloud shadow pixel and masked as no observation. This cloud shadow masking is termed as local low

Fig. 3. Comparison between the threshold-based sunglint and cloud-masking (this study, (a)) and SeaDAS CLDICE masking (b). (c) and (f) are the enlarged regions from (a); (e) and (h) are the enlarged regions from (b); (d) and (g) are the corresponding RGB images to fadlitate interpretation. CLDICE over-masked water pixels in (e) and Sargussum pixels in (h) (red dashed circle). The color legend of the AFAI images is the same as the one in Fig. 1.

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Hg. 4. Comparison between SeaDAS LOWLW and the LIR cloud shadow masking (this study). (a) and (e) are the enlarged RGB images; (b) and (f) are the unmasked AFAI images; (c) and
(g) show the LOWLW flagged pixels in red; (d) In (g), some of the Sargassum-containing pixels are flagged as cloud shadows (yellow cirdes).

reflectance (LLR) masking, where T_c was determined to be -0.01 after trial and error and a sensitivity analysis.

Ideally, a cloud shadow mask should retain most Sargassum pixels and exclude most cloud shadow pixels. To select the optimal T_c in the LLR cloud shadow masking, we manually delineated several regions of interest for cloud shadow pixels ($N_c = 2573$) and Sargassum pixels $(N_s = 49.559)$. According to the cumulative and normalized histograms (Fig. 5a & b)), a selection of $T_c = -0.01$ served this purpose. Therefore, $T_c = -0.01$ was used as the threshold to detect and mask cloud shadow pixels.

Note that the LOWLW flag generated by SeaDAS processing has also been proposed to detect cloud shadows (Patt et al., 2003). It is based on a threshold of 0.15 mW cm^{-2} um⁻¹ sr⁻¹ in the derived normalized water-leaving radiance at 555 nm. However, a comparison between the LOWLW and LLR in Fig. 4 shows that LOWLW often missed some cloud shadow pixels (pink circles in Fig. 4c) while over-masked Sargassum-containing pixels (yellow circles in Fig. 4g). In contrast, both the under-masking of water pixels and the over-masking of Sargassumcontaining pixels are reduced by the LIR doud shadow masking method (Fig. 4).

Fig. 5. Cumulative and normalized frequency distributions of Sargussum pixels, cloud shadow pixels and adjacent ocean pixels in several regions of interest. (a) and (b) show the distribution of the (LTR - Ref_{LTR}) values of Sargassum pixels and cloud shadow pixels. (c) and (d) show the distribution of the (AFAI - Ref_{APAI}) values of Sargassum pixels and adjacent oce an pixels.

4.1.2. Class B and Class C: Sargassum-free and Sargassum-containing pixels Due to the presence of sunglint contaminated pixels (adjacent to sunglint masked pixels), the relatively large swath of MODIS, and incomplete atmospheric correction, there are large-scale gradient differences across AFAI images (e.g., Figs. 1 & 3) where AFAI values over Sargassum-free water are lower near the satellite scan edge than around the scan center. This makes it impossible to apply a global scope threshold to extract Sargassum-containing pixels in uncorrected images. Several steps were used to account for this across-image gradient, which are described below. Basically, a median filter (after excluding potential Sargassum-containing pixels determined first from surface fitting) was used to generate a background Sargassum-free AFAI image, which was then subtracted from the original AFAI image. Then, a global scope image based threshold was determined and applied to the entire image to extract the Sargassum-containing pixels.

4.1.2.1. Preliminary Sargassum pixel extraction based on surface fitting. To model the large-scale variability, a four-degree surface fitting is usually sufficient. Higher-degree surface fitting is likely to cause overfitting, which will hinder the extraction of local bright targets (i.e., Sargassum-containing pixels). The surface fitting was performed over pixels of valid observations only, with Sargassumcontaining pixels excluded. Because nearshore pixels tend to have high AFAI values, these pixels were also excluded before surface fitting. Pixels with AFAI values greater than the fitted value by a threshold T_s were identified as potential Sargassum-containing pixels, and were excluded from the median filter creation process used to determine the Sargassum-free ocean background.

The threshold T_s in the above process was determined from 8 representative AFAI images (4 in January and 4 in June). The Sargassum pixels were first manually delineated from the 8 images, which were then eroded using $a 5 \times 5$ pixel window to assure the exclusion of Sargassum-containing pixels when creating the median filter. A threshold of $T_s = 2.55 \times 10^{-4}$ was found to extract up to 95% of the Sargassumcontaining pixels (after erosion), and therefore was used for the entire dataset. Fig. 6a and d show the original AFAI image and resultant surface fitted image.

4.1.2.2. Median filtering to determine ocean background (RefAFAJ). The surface fitting derived background image still contains small-scale variance, therefore requiring a subsequent median filter to refine the background image. The median filter used a 51×51 pixel window to determine the median value of each pixel from the surface fitted image. This derived median image was used as the Sargassum-free ocean background, RefAFAI, to extract Sargassum-containing pixels by using a global scope threshold. To,

Adopting the use of a 51 \times 51 pixel window (W_{size} = 51 pixels) was based on several considerations. Because large Sargassum slicks do occur, a minimum W_{stze} of 31 pixels could be used to fill in the surface fitting derived bright targets to avoid data loss. In Garcia et al. (2013) the optimal W_{size} was obtained by comparing the standard error of the means (SEMs) from 10 randomly selected ocean regions. The SEMs would increase in a nonlinear fashion when W_{size} exceeded a certain value. In this study, randomly selected ocean regions within the CWA region from 6 representative images were analyzed to determine an optimal W_{size}. The SEMs of these selected ocean regions only decreased slowly with decreasing W_{size} when W_{size} was <51. This suggested that after excluding potential Sargassum-containing pixels from the surface fitting process, a median filter could be used effectively to remove small-scale variations providing a large-scale Sargassum-free ocean background (RefAFA), Fig. 6g). Considering the typical size of the potential Sargassum slicks and computational efficiency, Wsize = 51 was selected for use in the median filter.

4.1.2.3. Final Sargassum pixel extraction using a global scope segmentation threshold To. With the Sargassum-free ocean background (RefAFAI) obtained from the two processes above, a global scope threshold T₀ was determined and applied to the entire image to extract the Sargassumcontaining pixels whose AFAI values were higher than the background values of To:

AFAI-Ref_{AFAI}>T₀.

To was determined by comparing the cumulative frequency of manually delineated Sargassum-containing pixels and their adjacent pixels with a dilation of 5 pixels (11 \times 11 pixel window). The dataset used to

 (6)

Fig. 6. An example of the Sargassum pixel extraction process, (a) is the original AFAI image after masking sun glint, clouds, cloud shadows, and land; (b) and (c) are enlarged regions from the AFAI image in (a); (d) is the surface fitted image from (a); (e) and (f) are enlarged regions from the surface fitted image in (d); (g) is the median-filtered (RefAnn) image that is used as the reference; (h) and (i) are the enlarged regions from the $\text{Ref}_{\text{w}/\text{w}}$ image in (g); (j) is the difference image between (a) and (g); (k) and (l) are the enlarged regions from the AFA-Ref_{/*/} (difference) image in (i). Sorgassum-containing pixels are extracted from the difference image using the global sorpe threshold To. The color bar is for the difference image and the red arrow marked the global scope threshold To used in this study.

 $R_{\rm re}$

determine T₀ was the same as that used to determine the surface fitting threshold. The logic was also the same: T_0 should preserve most of the manually selected "ground truth" Sargassum-containing pixels while excluding most of the adiacent Sargassum-free pixels. As marked by the vertical line in the cumulative frequency distribution (Fig. 5c). when T₀ was selected to be 1.79×10^{-4} , about 95% of the Sargassumcontaining pixels were captured while only 10% of the adjacent Sargassum-free pixels were misdassified as Sargassum-containing. As with any threshold-based method, the choice of the threshold is always a compromise between false-positive and false-negative detections. The sensitivity test below shows that $T_0 = 1.79 \times 10^{-4}$ would lead to acceptable uncertainties in both categories, and would not impact the overall findings in the long-term trend of Sargassum distributions.

To understand the uncertainties in the extraction results, 12 representative MODIS AFAI images (6 from January 2015 and 6 from June 2015), all independent from the dataset used in determining T_0 , were used to extract Sargassum-containing pixels following the above procedures, with their results compared to those with manual delineation (regarded as the "truth"). For the estimates of Sargassum area coverage using unweighted Sargassum-containing pixels, the false positive rate was 30.41% and the false negative rate was 15.67%. Due to these uncertainties, a linear unmixing method was developed (see below) and applied to Sargassum-containing pixels. After weighting the Sargassumcontaining pixels using this linear unmixing method, the false positive rate decreased to 18.97% and the false negative rate decreased to 7.42%. As shown in Table 1, the overall accuracy, defined by the Fscore (Chinchor & Sundheim, 1993) was 86.05% and thus acceptable for time series and trend analysis.

4.2. Step 2: Unmixing of Sargassum-containing pixels to determine fractional coverage (> 0 % but ≤ 100 %)

So far, for every AFAI image, each pixel was classified as noobservation (Class A), Sargassum-free (Class B), or Sargassumcontaining (Class C). For the Sargassum-containing pixels, the next step is required to determine the fractional coverage through unmixing, as Sargassum mats can rarely occupy the entire 1-km pixel. This linear unmixing scheme is used to quantify the percentage of Sargassum coverage within a given pixel. For each Sargassum-containing pixel, its fractional coverage was determined as

$$
AFAI_{U} = AFAI_{U0} - (AFAI_{I0} - AFAI_{L})
$$
\n(7)

$$
\alpha_i = (AFAI_{Ai} - AFAI_{Li})/(AFAI_{Li} - AFAI_{Li}) \times 100\%.
$$
 (8)

where α_i is the fractional (percentage) Sargassum coverage (ranging from 0.0% to 100.0%) for the ith Sargassum-containing pixel, AFAIA₁ is the AFAI value of the ith Sargassum-containing pixel ("A" in the subscript represents "algae", i.e., Sargarssum), AFAI_{Li} and AFAI_{Ui} are the lower (corresponding to 0.0% coverage) and upper (corresponding to 100.0% coverage) bounds for the ith Sargassum-containing pixel, respectively. AFAI_{LO} and AFAI_{UO} are the global scope lower and upper bounds (image and pixel independent constants) for 0% and 100% sub-pixel coverage, respectively. AFAI1 and AFAI_U and are the local lower and upper bounds, respectively, for the Sargassum patch containing the ith Sargassum-containing pixel, which may vary among Sargassum patches and images. Therefore, to determine α_i , four parameters are required: AFAI_{U0}, AFAI_{L0}, AFAI_U, and AFAI_L.

To determine AFAI_{U0}, which represents 100% Sargassum coverage within a pixel, surface reflectance measured from pure Sargassum mats in the GOM and off Bermuda (Fig. 1b) were used to simulate R., and AFAI as sensed by MODIS through radiative transfer simulations. The collection of these spectra was described in Hu et al. (2015). The simulation is the same as described in Hu (2009):

$$
=R_a+t_oTR_{s,avg}
$$

where R_a is the atmospheric path reflectance due to aerosols and aerosol-Rayleigh interactions, Rsarg is the mean Sargassum reflectance from field measurements (Fig. 1b), t_0 is the atmospheric diffuse transmittance from the sun to the Sargassum mat, and T is the atmospheric beam transmittance from the Sargassum mat to the satellite sensor, Because of the atmospheric effects, the same R_{sare} could result in different R_{rc} as measured by the satellite. Such effects were simulated in the following way.

Two solar/viewing scenarios were considered in the simulation, with one for image center and the other for image edge. Two aerosol types were considered: maritime aerosols with 90% relative humidity (m90) and coastal aerosols with 50% relative humidity (c50). representing both open ocean and coastal ocean scenarios. Aerosol optical thickness at 869 nm, T_a(869), was varied between 0.02 and 0.38 (the upper bound for aerosols, Robinson, Franz, Patt, Bailey, & Werdell, 2003). All variables in Eq. (9) (i.e., R_a , t_a , T) corresponding to these different scenarios were determined using the MODIS aerosol lookup tables from the SeaDAS data processing software package (Baith, Lindsay, Fu, & McClain, 2001), Table 2 presents a summary of the MODIS AFAI_{U0} values corresponding to all variable atmospheric conditions and solar/viewing geometry. The 2013-2015 climatological mean $\tau_a(869)$ for the CWA region was estimated to be 0.10. The mean value corresponding to $\tau_a(869) = 0.10, 4.41 \times 10^{-2}$, was used in this study to represent the global AFAI₁₁₀ for 100% Sargassum coverage within a pixel. Note that for an individual Sargassum slick, the local upper bound was adjusted using Eq. (7) to account for variable atmospheric and observing conditions.

To determine AFAI_{LO}, a histogram of AFAI values from all water pixels near these Sargassum slicks (6 pixels outward from the slickedges) was generated. The median value was determined to be -8.77×10^{-4} and was assigned to AFAI_{LO} to represent 0% Sargassum-containing coverage. Here the median value is selected to avoid noise interference in calculating the lower bound. For each Sargassum patch, the local AFAI, was also determined using the same method. The local AFAI_U was derived using Eq. (7) by normalizing the global AFAI_{U0} against the difference between AFAI_{LO} and AFAI_L. These values were then used in Eq. (8) to calculate sub-pixel coverage α_i for each of the Sargassum-containing pixels within a Sargassum patch. This method was applied in a loop through all Sargassum patches within an image. Fig. 7a, b, c, and d show an example of the process for extracting Sargassum-containing pixels and determination of sub-pixel coverage.

4.3. Step 3: Data binning to derive distribution and area coverage maps

After obtaining the sub-pixel coverage of each Sargassum-containing pixel from all images, the entire study region was divided into $0.5^{\circ} \times 0.5^{\circ}$ grids to generate mean distribution maps at different time intervals (monthly, seasonal, and annual). For each grid, mean fractional Sargassum coverage within a particular time interval was calculated

Table 1

 (9)

358 Table 2

MODIS AFAI upper bound values (i.e., corresponding to 100% Sorgossum coverage within a pixel) for various atmospheric conditions (aerosol type and optical thickness) and solar/viewing geometry, based on Eq. (9) and radiative transfer simulations.

m90	$T_s(869)$									
	0.02	0.06	0.10	0.14	0.18	0.22	0.26	0.30	034	0.38
$0 = 4^{\circ}$ $0 = 57^{\circ}$	0.052 0.049	0.050 0.046	0.048 0.042	0.045 0.039	0.043 0.036	0.041 0.033	0.040 0.030	0.038 0.028	0.036 0.026	0.034 0.024
c50	$T_s(869)$									
	0.02	0.06	0.10	0.14	0.18	0.22	0.26	0.30	0.34	0.38
$\theta = 4^\circ$	0.052	0.049	0.046	0.044	0.042	0.039	0.037	0.035	0.033	0.031
$0 = 57^{\circ}$	0.049	0.045	0.041	0.037	0.033	0.030	0.027	0.025	0.022	0.020

Note: Two aerosol types are selected for open and mastal oceans: maritime aerosols with 90% relative bumidity (m90) and coastal aerosols with 50% relative humidity (c50). Two solar/ viewing scenarios are applied; near satellite nadir (satellite zenith $\theta = 4^{\circ}$, solar zenith $\theta_0 = 18.4^{\circ}$, relative azimuth $\phi = 22^{\circ}$) and near scan edge $(\theta = 57^{\circ}, \theta_0 = 29^{\circ}, \phi = 21^{\circ})$. $\tau_n(869) =$ 0.10 corresponds to the mean aerosol optical thickness over the study region between 2013 and 2015 as derived from MODIS. The average of these values for $\tau_a(869) = 0.10$ is $441 \times$ 10⁻², (bold font), which was used in this study as the global upper bound for pure Sargassum coverage.

from all Sargassum-containing (NA) and Sargassum-free pixels (Nw) falling in that grid as

$$
f = \frac{1}{N} \left[\sum_{i=0}^{N} \alpha_i \right] \tag{10}
$$

$$
N = N_A + N_W \tag{11}
$$

where the summation was for all Sargassum-containing and Sargassumfree (i.e., water) pixels in that grid within the time interval, with $\alpha_i =$ 0.0 for water pixels. The mean area coverage maps were generated after integrating all grids. The general process is illustrated in Fig. 7.

5. Results: Long-term Sargassum distribution and coverage

The above methods were applied to the entire time series between 2000 and 2015, where 17,772 MODIS AFAI images (9013 between 2009 and 2015) were used to generate the Sargassum distribution and coverage maps over the CWA region at monthly, seasonal, and annual intervals. The threshold values were selected as: T₀ = 1.79×10^{-4} , AFAI_{U0} = 4.41×10^{-2} , and $AFAI₁₀ = -8.77 \times 10^{-4}$.

Fig. 8 presents the distributions of monthly mean coverage of Sargassum in the study region between 2000 and 2015. The color-coded value represents the monthly mean percentage of Sargassum coverage for a

Fig. 7. The process used to generate the monthly mean Sargassum area coverage maps using original AFAI images. The AFAI image in (a) is used to extract Sargassum-containing pixels in (b). These pixels are dilated to find the nearest water pixels (dark blue color around the Sargassum patches in (c)) to be used to calculate AFAL for each Sargassum patch (b) and (c) are used to calculate (d), the required illustrated

Fig. 8. Monthly mean distribution maps show Sargussum area coverage in the CWA region between 2000 and 2015, derived from MODS AFA1 images using the approach developed in this paper. Land is masked to black and coastline i

Fig. 8 (continued).

given grid, varying from 0% to about 0.4%. Because the results for 2000 through 2009 are very similar and they all show minimal Sargassum coverage, for clarity the distribution maps between 2001 and 2008 are

omitted here, During that period, small numbers of Sargassum slicks occasionally appeared off the Amazon River mouth between August and October, and the daily time sequence indicated northward movement.

Table 3

Annual mean Sarvassum coverage over the CWA region between 2009 and 2015. The annual mean coverage between 2000 and 2008 was similar to those in 2009, thus not listed la tha talda

However, they did not develop into large-scale blooms during those periods.

Large amounts of Sargassum slicks did not appear until April 2011 when they were captured in MODIS AFAI imagery around 3.0° N and 40° W. These Sargassum slicks then developed and advected to the Lesser Antilles Islands in the southern Caribbean from May to July. This agrees well with the timing of the reported Sargassum beaching events in those islands. From August to September, massive Sargassum slicks started to decrease. Some Sargassum slicks still appeared off the Amazon River mouth later in October and November, but their sizes were much smaller.

In 2012, Sargassum distribution patterns closely resembled those found in 2011 except for the scattered slicks in the first months of 2012 around 18°N which were apparently left over from the 2011 bloom. During July, most of Sargassum slicks appeared between 5°N and 10°N, Unlike 2011, August 2012 experienced a significant decrease of the total Sargassum coverage, after which only small amounts of scattered Sargassum slicks were found off the Amazon River mouth.

One interesting result is that after September 2012 and for the entire year of 2013, very few Sargassum slicks were found until April 2014, after which Sargassum distribution patterns nearly repeated those found during the summers of 2011 and 2012 but with greater abundance. The difference between 2014 and these two previous years is that between September and December 2014, there were still considerable numbers of Sargassum slicks, which continued to appear through the early months of 2015.

The most striking result was found in the extremely anomalous year of 2015. Not only did the Sargassum slicks appear from the very beginning of the year - which were again, apparently, left over from the previous year's bloom, but the Sargassum coverage during the spring and summer months was much greater than in any previous year. As of October and November of 2015, there were still considerable amounts of Sargassum in the offshore waters. This is analogous to conditions found in the same months of 2014, thus posing the question of whether similar extreme Sargassum blooms may occur in 2016.

The same method was used to generate seasonal and annual mean distribution maps. From these maps, the total area coverage was calculated to integrate Sargassum mean area coverage from all grids. While Table 3 presents a summary of the integrated annual mean area coverage between 2009 and 2015, Fig. 9 shows the time series of the integrated monthly and seasonal mean coverage. These statistics provide a quantitative measure of the amount of Sargassum in the CWA region at monthly, seasonal, and annual scales. The distribution maps in Fig. 8 closely resemble the time series which clearly shows the anomalous years of 2011, 2012, 2014, and 2015. Most striking is that 2015 is an extreme year when both the annual mean coverage and summer mean coverage were 4 times of those found in 2011, and the summer mean coverage exceeded those in the pre-bloom years (2009 and 2010) by 20 times

6. Discussion

While this is the first time that long-term Sargassum distribution maps and coverage statistics are presented by applying a sophisticated but objective methodology to MODIS observations, two questions naturally arise from these results. The first is how much can they be trusted? The second is, if they are trusted, what caused these long-term patterns? Due to the lack of field measurements, neither is easy to address. However, from spectral analysis, sensitivity analysis, and the analysis of several environmental variables, the following discussion may provide some useful hints.

6.1. Sargassum or other floating materials?

From the perspective of spectroscopy, it is difficult to condude that the observed red-edge reflectance (i.e., elevated AFAI values) is due to Sargassum instead of other floating vegetation. Using multi-sensor data and simulations, Hu et al. (2015) suggested that unless hyperspectral data are used, it is very difficult to differentiate Sargassum from other floating vegetation, as the latter also show elevated AFAI values. This is particularly true when the sub-pixel coverage is very small (<25%). Therefore, currently there is no way to validate all observed slicks from the AFAI imagery. However, two facts can help confirm that the observed slicks are mostly, if not all, Sargassum.

The first is scarce validation using the Hyperspectral Imager for the Coastal Ocean (HICO) observations. Hu et al. (2015) showed that corresponding to some of the MODIS-observed slicks, HICO spectra of the same slicks showed diagnostic spectral curvature around 630 nm due to chlorophyll c absorption. This is a unique feature for Sargassum macroalgae, thus confirming that at least some of the slicks observed from the MODIS AFAI imagery are indeed Sargassum. Likewise, the spectral curvature between reflectance of blue and green bands (Hu et al., 2010b) from randomly selected dense slicks (high AFAI values) did not reveal spectral characteristics of Trichodesmium mats, confirming that at least these randomly selected dense slicks were not Trichodesmium but likely Sargassum.

Fig. 9. Mean Sargassum area coverage at seasonal (a) and monthly (b) scales between 2009 and 2015 for the CWA region. The statistics between 2000 and 2008 are similar to those in 2009 nd 2010, and thus omitted

Local news reports from the Lesser Antilles Islands provide another indirect source of evidence. In 2011, 2012, 2014, and 2015, there were numerous new reports of Sargassum beaching on these islands. supporting the findings here. In particular, the news exposure increased tremendously in 2015, also supporting the statistical results that show 2015 as an extreme year.

Given the direct and indirect evidences, it is believed that most of these observed slicks, if not all, are Sargassum macroalgae. However, this does not mean that a field survey is not needed to further validate the observations here, particularly when area coverage estimations are to be made.

6.2. Uncertainties in the estimation of mean Sargassum area coverage

6.2.1. Sensitivity analysis

Several thresholds were used throughout the entire process to derive the final mean area coverage maps, which included T_c in the LLR cloud shadow masking, the global scope segmentation threshold T_0 to determine Sargassum-containing pixels, and AFAI₁₀ and AFAI₁₀ to determine sub-pixel Sargassum coverage. To understand the sensitivity of the final results to changes in these threshold values, a total of 187 AFAI images from MODIS Aqua and Terra in January and June 2015 were selected to generate the monthly mean area coverage maps with different combinations of variable threshold values.

Fig. 10a shows the comparison between the three choices for cloud shadow determination: no masking, LLR masking (this study), and cloud-edge dilation (6 pixels) masking. The global scope AFAL₁₀ and AFAI₁₀ were set as the default $(4.41 \times 10^{-2}$ and -8.77×10^{-4}). Compared to a proper masking method, no masking led to overestimated total Sargassum area coverage because some of the cloud shadow pixels were misclassified as Sargassum. The dilation-based cloud-masking method overestimated total Sargassum coverage even more because

the total number of valid observations (N in Eq. (11)) was significantly reduced in June when large Sargassum coverage appeared. Indeed, a 6pixel dilation led to up to 60% of data loss of total number of valid obser-.
vations from individual images in this analysis.

To assess the effect of To on the estimation of mean Sargassum area coverage, T₀ was varied between 1.28×10^{-4} and 2.55×10^{-4} , with mean Sargassum area coverage estimated for each T_0 (Fig. 10b). As expected, the estimated mean area coverage decreased with increasing T_{0} For June 2015, the mean Sargassum area coverage decreased by ~10% when T₀ was changed from 1.53×10^{-4} to 1.79×10^{-4} , A ~19% percentage decrease was observed for January of 2015. However, while the absolute area coverage changed with $T₀$, the seasonal and long-term patterns remained stable

The estimates of monthly mean Sargassum area coverage were also sensitive to changes in AFAI₁₀ and AFAI₁₀. When AFAI₁₀ was varied, AFAI_{LD} was set to be the default value (4.41×10^{-2}) . When AFAI_{U0} was varied, AFAI_{LO} was set to be the default value (-8.77×10^{-4}) . Fig. 10c shows that when AFAI_{LO} is increased, the mean Sargassum area coverage for January and June 2015 both increased slightly. Increasing the low bound from -8.77×10^{-4} to 6.21×10^{-4} results in larger estimation of ~0.57% for June 2015. As expected, Fig. 10d shows that when AFAI_{U0} was increased, the mean area coverage for January and June 2015 also decreased. Similarly, an increase of the AFAI_{U0} bound from 4.414×10^{-2} to 4.440×10^{-2} leads to a 0.44% decrease in the mean area coverage in June 2015. Since the range between AFAI_{u0} and AFAI_{LD} is up to \sim 4.4 \times 10⁻², adjustment of the AFAI_{U0} and AFAI_{L0} at scale of 1×10^{-4} will both result in minimal changes.

Although the absolute value of the area coverage changes with these changing threshold values, the relative long-term patterns are insensitive to changes in the thresholds. For example (Fig. 11 shows To varying from 1.28×10^{-4} to 2.30×10^{-4}), while the monthly mean area

Fig. 10. Sensitivity of mean Sargassum area coverage (km²) in January and June 2015 to different cloud sha dow masking me thods (a), different segmentation thresholds (b), different lower and upper bounds (c and d). The red dashed lines indicate the threshold values selected in this study for time series analysis

Hg. 11. Monthly mean Sargassum area coverage during 2014 generated with different global scope threshold T₀. In this study, T₀ = 1.79 \times 10⁻⁴ was selected to generate time-series statistics.

coverage decreased in all months of 2014, the temporal patterns remained nearly identical. Furthermore, the absolute area coverage appeared less sensitive to T_0 when T_0 was 1.79×10^{-4} . Therefore, a T_0 of 1.79×10^{-4} was selected in this study. In the future, field-based measurements may be used to help determine this threshold. At present, the results presented here represent the best knowledge one can obtain from MODIS observations and, even in the worst-case scenario, the relative temporal patterns as well as the distribution maps still remain valid.

6.2.2. Detection limit

The MODIS pixels used in this study have a ground resolution of 1 km, making it difficult to observe small Sargassum rafts. Using simulations and assuming 200:1 SNR, Hu et al. (2015) suggested that the lower detection limit of the red-edge reflectance is about 1-2% of a pixel size. However, the MODIS band used in examining the red-edge reflectance, the 748-nm band, has a SNR of 995:1 (Hu et al., 2012) under typical conditions. This would certainly enable MODIS AFAI to detect Sargassum rafts smaller than 1% of a pixel size. Manual analysis of delineated AFAI slicks with weak signals indicated that the detectable limit would be \approx 0.2% of a MODIS 1-km pixel. This is 5 times more sensitive than the estimates from the 200:1 SNR assumption. Correspondingly, a Sargassum raft with an effective width of >2 m and effective length of >2 km long is observable in MODIS AFAI imagery. Smaller Sargassum rafts are simply not observable.

6.2.3. Uncertainties due to non-optimal observing conditions

Many factors can impact satellite observations of surface slicks of Sargassum, For near real-time observations, clouds, severe sun glint, cloud shadows, and other artifacts simply make many pixels unusable, presenting a major hurdle for near real-time Sargassum tracking. However, these pixels are not counted in long-term statistics, thus would have minimal impacts on the statistical results once sufficient number of images is used in the statistics. On the other hand, non-optimal observing conditions such as variable winds and currents may have significant impacts on the statistical results (Gower & King, 2011; Marmorino, Miller, Smith, & Bowles, 2011; Szekielda, Marmorino, Bowles, & Gillis, 2010; Woodcock, 1993). Under high winds, Sargassum may be dissipated and become undetectable to MODIS imagery while they may still be observed in high-resolution airborne imagery or field sampling through neuston net tows. Attempts were made to determine the optimal wind range from sequential images, however mixed results were obtained. When wind speed was >7 m s⁻¹, Sargassum tended to be undetectable in MODIS imagery. However, this threshold could not be generalized, and therefore was not applied to screen data. In this sense, because Sargassum aggregate or mat size is important to Sargassum coverage or biomass estimates (Dierssen et al., 2015), the results obtained here are likely underestimates and they represent only those Sargassum slicks observable by MODIS. In other words, the absolute area coverage values represent lower bound of Sargassum coverage. Regardless, the lack of significant inter-annual variability or wind speed trends suggests that wind should not impact the observed distribution patterns and temporal area coverage changes (Hu et al., 2015, 2016).

6.3. Causes of the Sargassum bloom since 2011

Before satellites were used to map and quantify Sargassum blooms (Gower et al., 2006), assessment of Sargassum biomass was based on shipboard observations only (Butler, Morris, Cadwallader, & Stoner, 1983; Butler & Stoner, 1983; Huffard, von Thun, Sherman, Sealey, & Smith, 2014; Parr, 1939; Schell, Goodwin, & Siuda, 2015; Siuda, Schell, & Goodwin, 2016; Stoner, 1983). Most of these shipboard observations were focused on the Sargasso Sea, where no significant Sargassum biomass changes were found between 1933 and 1981 (Butler & Stoner, 1984). Recently, Schell et al. (2015) found Sargassum morphological changes in the Caribbean, Yet these shipboard surveys relied on neuston net tows that may have missed large Sargassum rafts as captured by synoptic and frequent satellite measurements. Then, what could cause the sudden increase in these MODIS-observed Sargassum coverages after 20117

While it is extremely difficult to pinpoint the exact reason of a largescale oceanic phenomenon, a preliminary effort was attempted to explain the observed long-term changes. We fully recognize that a thorough understanding requires multi-disciplinary efforts to analyze both physical and biological forcing, yet analysis of several environmental variables may provide some hints to address the following questions: Where do the Sargassum slicks originate? And, what caused the recent increases in the area coverage?

Indeed, although the MODIS statistics started in 2000, there is no record in either local newspaper or in fishemen's memory of any major Sargassum beaching event for the past 50-60 years prior to 2011 (Dr. Jean-Philippe Maréchal, Caribbean Global Coral Reef Monitoring Network (GCRMN) advisor, personal comm.), suggesting that there might be a significant change in the local environment in the past half century.

Daily image sequences were examined to determine the potential origin of the Sargassum slicks, similar to the methodology used in Hu and He (2008), to determine the origin of the Ulva bloom off Qingdao (China) in the Yellow Sea, Although several sequences did reveal the first appearance of Sargassum slicks and their temporal movements, it is hard to conclude that they originated from the location where they first observed. This may be due to the fact that many small Sargassum slicks are unlikely to be captured by coarse pixels resolution (Hu et al., 2015). It is more likely that Sargassum originates in a certain location, moves, and is detectable in MODIS AFAI imagery only when surface aggregation results in large, observable slicks $(>2 \text{ m wide and} > 2 \text{ km long})$ see Section 6.2.2). Thus, this effort did not lead to any solid inference on the origin of Sargassum slicks. On the other hand, recent shipboard observations showed that Sargassum in the CWA region in 2015 had a different dominant form than in the Sargasso Sea, suggesting that the Sargasso Sea is unlikely to be the source region (Schell et al., 2015). This is supported by hindcast numerical models, which suggested that Sargassum may bloom in the north equatorial recirculation region (NERR) due to favorable environmental conditions (Johnson, Ko, Franks, Moreno, & Sanchez-rubio, 2013).

Excessive nutrient supply may be responsible for the increase in Sargassum biomass (Smetacek & Zingone, 2013). Could the temporal patterns be related to the Amazon River discharge and associated river plume? Fig. 12 shows that between May and August 2015 (the maximum Sargassum months in the maximum year), Sargassum slicks did appear in the vicinity of the Amazon plume (where the plume was inferred from elevated K_d490 values from the monthly mean K_d490 images. This is because Kd490 is highly correlated with colored dissolved organic matter rich in river plume, Hu,

Iπ Mav Iun ma Diffu e atter ation coefficient at 490 nm (m²) 0.01 0.03 0.12 0.42 1.44 5.00 May Jun Jul Aug

Fig. 12. MODISA monthly mean diffuse attenuation coefficient at 490 nm $(K_d$ 490, m⁻¹) from May to August 2015, overlaid with Sargassum coverage (red area in the top row and red outline in the bottom row). Here the Sargas

Montgomery, Schmitt, & Muller-Karger, 2004). This, however, could simply be a coincidence as both the plume and the Sargassum slicks were driven by the same ocean currents. Indeed, the Amazon River discharge (Fig. 13e) and the Sargassum area coverage does not appear to be correlative, suggesting that river discharge might not be the dominant reason for increased bloom activity.

Fig. 13. Monthly mean values of several environmental variables over the CWA region. (a) Se a Surface Temperature (SST); (b) Photosynthetic Available Radiation (PAR); (c) doud fraction; (d) precipitation rate; (e) Amazon River discharge anomaly; (e) aerosol optical depth (AOD).

Analysis of other environmental variables indicated that although PAR and cloud fraction did not show any apparent correlation with the Sargassum temporal patterns, a combination of SST, precipitation. and AOD might explain some of them. For example, precipitation was much higher in 2010 and 2011 than in other observable years. The higher than usual precipitation may have brought additional nutrients (iron) from aerosols (dust) to the surface ocean (Paerl et al., 1999), favoring Sargassum growth in the following years (2011 and 2012). The winter of 2014 showed lower SST (~0,4 °C lower than monthly mean climatology), possibly associated with stronger upwelling (or deeper mixing) than other years (Black et al., 1999; Peterson, Haug, Hughen, & Röhl, 2000; Weingartner & Weisberg, 1991) or with more African dust according to the correlation of North Atlantic SST with African dust proposed by Wang, Dong, Evan, Foltz, and Lee (2012) using a dataset back to 1950's (which may be excluded as no significant change in AOD is detected in Fig. 13f), providing more nutrients to Sargassum and resulting in blooms in 2014 and 2015. The same mechanism could also be used to explain the 2011 and 2012 blooms as SST in these two vears was also lower than in other years. Therefore, the following hypothesis may be generalized from these visual interpretations: while the origin of the Sargassum is still unclear, the 2011 and 2012 blooms appear to be a result of the combined effect of higher precipitation (more atmospheric nutrients) and lower SST (deeper mixing or stronger upwelling), and the 2014 and 2015 blooms appear to be the result of deeper mixing or strong upwelling. AOD shows a strong seasonal pattern with more dust input in summer and less in winter (corresponds well with the annual cycle of African dust transport to the Caribbean Basin as mentioned in Prospero, Collard, Molinié, & Jeannot, 2014). This is positively correlated with the Sargassum temporal patterns in Fig. 9, suggesting dust input may stimulate Sargassum growth. Regardless, the exact mechanisms leading to the annual fluctuations and the 2015 anomaly in Sargassum coverage will still require a significant amount of multi-disciplinary effort to resolve. In the meantime, the distribution maps in Fig. 8, the long-term temporal patterns in Fig. 9, and those obtained from historical and recent shipboard observations (Butler & Stoner, 1983; Butler et al., 1983; Parr, 1939; Schell et al., 2015; Siuda et al., 2016; Stoner & Greening, 1984), may serve as guides on how to perform such a multi-disciplinary investigation.

6.4. Continuity and other considerations

The distribution patterns and long-term trends of Sargassum coverage, as revealed in Figs. 8 and 9, suggest that it is likely that Sargassum blooms may occur in future years. Given aging MODIS instruments (they were both designed for 5-year mission life but have been operational for >13 years), the question is whether the observations can be continued if one or both MODIS instruments cease to function? In other words, is one instrument enough? And, if both fail, what other instruments can be used?

To address these questions, statistics were generated from individual MODIS instruments and compared with those from combined observation platforms. Between 2009 and 2015, 9013 AFAI images were used to generate the statistics, of which 4953 were from MODISA and 4060 were from MODIST. Fig. 14 shows that when MODIST and MODISA were used separately, the estimated annual mean Sargassum coverage was nearly identical between 2009 and 2013, but showed slight differences (<20%) from the coverage estimates in 2014 and 2015 when both satellite platforms were combined. Thus, if and when one of instruments stops functioning in the future, reliable statistics can still be generated from the other one, with potentially <20% uncertainty as referenced against the combined observations.

The Visible Infrared Imaging Radiometer Suite (VIIRS) instrument has provided daily data since 2012. VIIRS has all required spectral bands to calculate a VIIRS AFAI. In addition, a VIIRS swath width (3000 km) is greater than a MODIS swath (2330 km), providing

Fig. 14. Annual mean Sargassum coverage (km²) over the CWA region estimated from MODIST, MODISA, and MODIST/MODISA combined. The 2015 data contains data through 21 November 2015.

more data coverage than a single MODIS instrument. Therefore, even if both MODISA and MODIST stop functioning, VIIRS can be used to continue the Sargassum observations. Once proper crosssensor calibration is achieved. VIIRS is expected to provide a seamless data record for the foreseeable future. The Ocean Land Colour Instrument (OLCI) onboard the Sentinel-3 satellite was launched on 16 February 2016. As a MERIS-heritage sensor (300-m resolution, 1400km swath) but with more spectral bands (from 15 of MERIS to 21 of OLCI, Donlon et al., 2012), OLCI is also capable of providing AFAI and MCL products once data become available. We expect to perform the cross-sensor calibration on these sensors and generate VIIRS and OLCI AFAI data products soon.

The Pre-Aerosol, Cloud, and ocean Ecosystem (PACE) mission is currently planned at NASA (http://pace.gsfc.nasa.gov), with the aim of providing hyperspectral data at similar coverage and revisit frequency of MODIS. Such a hyperspectral mission is expected to not only provide continuity observations from MODIS and VIIRS but more importantly to provide diagnostic capacity to differentiate Sargassum from other floating materials (Dierssen et al., 2015; Hu et al., 2015). Likewise, NASA's Hyperspectral InfraRed Imager (HyspIRI) mission (Lee et al., 2015) and Geostationary Coastal and Air Pollution Events (GEO-CAPE) mission (Fishman et al., 2012) will both have hyperspectral capacity for spectral diagnostics. In particular, the GEO-CAPE mission on a geostationary platform will enable multiple images a day at the same location, making it easier to avoid cloud cover and to track Sargassum movement using sequential images. This feature has been demonstrated already for tracking blooms of the green macroalgae U. prolifera in the Yellow Sea using the Geostationary Ocean Color Imager (GOCI) (Son, Min, & Ryu, 2012). Furthermore, the future Geostationary Operational Environmental Satellites - R Series (GOES-R) series will have two spectral bands in the red (640 nm) and NIR (860 nm), respectively, with a ground resolution of 1 km (Schmit et al., 2005). Once proven with sufficient SNRs, the GOES-R series may provide more frequent data than any other sensors to monitor and track Sargassum blooms.

The daily MODIS images have a lready served as useful guides to local residents of the Lesser Antilles Islands as well as other regions in the Intra-Americas Sea, and helped management agencies to prepare for Sargassum beaching events. Compared to the Sargassum Early Advisory System (SEAS) to forecast Sargassum beaching events using LANDSAT imagery (30-m resolution) and other ancillary data (Webster & Linton, 2013), the daily MODIS images have coarser spatial resolution but higher revisit frequency and more spatial coverage, thus enabling the derivation of long-term and large-scale perspectives on the size and trend of Sargassum blooms. Although it is difficult to pinpoint the reason of the recent blooms, one may still conclude that the blooms were not due to local pollution but to large-scale atmospheric and oceanic forcing, possibly related to weather fluctuations and dimate change. The findings here may therefore provide unprecedented

information to help local residents to adapt and prepare for future Sargassum beaching events in a changing climate in order to sustain tourism and a healthy economy.

7. Conclusions

An objective method has been developed to quantify Sargassum distributions and area coverage from MODIS observations. The MODIS data were then used to generate distribution maps and area coverage between 2000 and 2015 over the Central West Atlantic region. While some of these results were reported previously using MERIS observations up to 2011 using a different method, this is the first time that a longer time series has been objectively developed which has revealed unprecedented Sargassum coverage patterns after 2011 ever since MODIS was put in orbit in 2000. In particular, Sargassum coverage in 2014 and 2015 was found to be significantly higher than in any previously observable year, with 2015 being the extremely anomalous year. Although it is currently difficult to pin point the reasons for these changes, the findings here may provide guidance on future multi-disciplinary studies to understand their origin, causes, and possible consequences to the ocean environment.

We want to emphasize that the data processing required to generate the statistics from low-level MODIS data is computationally expensive. Our initial effort was therefore dedicated to methodology development with the focus on the CWA region only. Our next step is to extend this methodology to the entire Intra-Americas Sea (including Caribbean Sea and Gulf of Mexico et al.), the Sargasso Sea, and the entire tropical Atlantic. Combined with ocean circulation and other data, a larger picture than presented here may provide more information to solve the puzzle of Sargassum origin, bloom transport, and future trends in a changing climate.

Notations

VIRS Visible Infrared Imaging Radiometer Suite

Adknowledgment

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Appendix B:

Remote estimation of *Sargassum* **biomass, nutrients, and pigments**

Wang, M., Hu, C., Cannizzaro, J., English, D., Han, X., Naar, D., Lapointe, B., Brewton, R., & Hernandez, F. (2018, accepted). Remote estimation of *Sargassum* biomass, nutrients, and pigments. *Geophysical Research Letters.*

Remote sensing of Sargassum biomass, nutrients, and pigments $\mathbf{1}$ Mengqiu Wang¹, Chuanmin Hu⁺¹, Jennifer Cannizzaro¹, David English¹, Xingxing Han¹, $\overline{2}$ David Naar¹, Brian Lapointe², Rachel Brewton², and Frank Hernandez³ $\overline{3}$

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$\overline{7}$ Abstract

8 Field and laboratory experiments are designed to measure Sargassum biomass per area (density), surface reflectance, nutrient contents, and pigment concentrations. An Alternative Floating Algae \mathbf{Q} 10 Index (AFAI)-biomass density model is established to link the spectral reflectance to Sargassum biomass density, with a relative uncertainty of \sim 12%. Monthly mean integrated Sargassum 11 12 biomass in the Caribbean Sea and Central West Atlantic reached at least 4.4 million tons in July 13 2015. The average % C, % N, and % P per dry-weight are 27.16, 1.06, and 0.10, respectively. The mean chlorophyll-a (Chl-a) concentration is \sim 0.05% of the dry-weight. With these 14 parameters, the amounts of nutrients and pigments can be estimated directly from remotely 15 sensed Sargassum biomass. During bloom seasons, Sargassum carbon can account for \sim 18% of 16 17 the total particulate organic carbon in the upper water column. This study provides the first 18 quantitative assessment of the overall Sargassum biomass, nutrients, and pigment abundance from remote-sensing observations, thus helping to quantify their ecological roles and facilitate 19 20 management decisions.

21 1. Introduction

Pelagic Sargassum is a unique type of brown macroalgae that is mainly found in the 22 23 Atlantic Ocean. It serves as a critical habitat and refuge to various marine organisms [Council, 24 2002; Doyle and Franks, 2015; Hu et al., 2016; Lapointe et al., 2014; Rooker et al., 2006; Witherington et al., 2012], and Sargassum sinking can potentially contribute to the carbon input 25 to the deep-sea communities [Baker et al., 2017; Johnson and Richardson, 1977; Krause-Jensen 26 and Duarte, 2016; Rowe and Staresinic, 1979]. On the other hand, massive Sargassum beaching 27 28 events can cause various environmental and economic problems in coastal areas of the Gulf of Mexico (GOM), Caribbean Sea (CS), and West Africa during bloom seasons [Franks et al., 29 30 2011; Hu et al., 2016; Schell et al., 2015; Webster and Linton, 2013]. While large Sargassum aggregations in the Atlantic Ocean have been noted for centuries, a robust quantitative 31 assessment of their total biomass is still lacking due to technical limitations. Early Sargassum 32 biomass estimations mainly come from ship-based samplings using neuston tows [Butler et al., 33 34 1983; Butler and Stoner, 1984; Parr, 1939; Stoner, 1983]. Parr measured the Sargassum biomass density in various locations in the Sargasso Sea and the tropical Atlantic, and estimated a total 35 biomass of 7-10 million tons in the Sargasso Sea [Parr, 1939]. Stoner conducted another 36 quantitative study and reported a major decrease of Sargassum biomass [Stoner, 1983], which 37 was later attributed to the geographic variations within the Sargasso Sea and the sampling 38 39 method [Butler and Stoner, 1984]. More recently, the Sea Education Association collected

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neuston measurements in both Sargasso Sea and tropical Atlantic over the last 50 years and 40 41 observed significant abundance changes especially in the tropical Atlantic [Schell et al., 2015; 42 Studa, 2011]. However, given the significant seasonal and inter-annual variabilities of 43 Sargassum abundance and distributions in the Intra-Americas Sea (IAS) and North Atlantic 44 [Wang and Hu, 2016; 2017], ship-based field measurements are likely biased for the basin-scale biomass estimation. 45

46 Because Sargassum has enhanced reflectance in the near-infrared (NIR) spectral bands 47 (this is often called "red-edge" reflectance), satellite and airborne instruments have been used to 48 detect and quantify Sargassum [Dierssen et al., 2015; Gower and King, 2011; Hu, 2009; Hu et 49 al., 2015; Hu et al., 2016]. However, due to a lack of field or laboratory measurements, nearly all 50 remote sensing studies have focused on the areal density or relative amount [Gower et al., 2013; 51 Gower and King, 2011; Wang and Hu, 2016; 2017]. On the other hand, knowledge of Sargassum 52 biomass and its pigment compositions and nutrient contents, especially their distributions and temporal changes, is critical in quantifying its roles in biogeochemical cycling and ocean ecology 53 54 [Baker et al., 2017; Lapointe, 1995; Lapointe et al., 2014; Rooker et al., 2006].

55 Therefore, the objective here is to fill this knowledge gap by (1) developing a model to 56 estimate Sargassum biomass density from reflectance, (2) determining Sargassum nutrient and 57 pigment compositions and concentrations through field and laboratory measurements, and (3) 58 mapping distributions of Sargassum biomass, nutrients, and pigments in the study region.

59 2. Materials and Methods

60 Sargassum samples were collected from the GOM and Florida Straits in June - July 2017 61 (Figure S1). One station from Belize was also included in the analysis. Five types of Sargassum data were collected: (1) wet-weight, (2) surface area, (3) surface reflectance, (4) pigment 62 concentrations, and (5) nutrients of C, N and P. Additional data of (1-3) collected in June 2018 63 in the GOM were also used. 64

65 2.1 Sargassum biomass-per-area

66 Sargassum biomass density was estimated by measuring the wet weight and areal coverage of an isolated patch (Figure 1) and repeating the measurements. A photo with both a 1-67 m² quadrat and the Sargassum patch was taken before collecting the Sargassum patch. The 68 69 former was used to estimate the patch's area, while the latter was used to estimate the patch's 70 weight. The sample was rinsed to remove vertebrates and invertebrates, drained for a few 71 minutes to reduce the loose water, and then the wet-weight was measured using a spring scale of 72 0.1 kg accuracy.

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Figure 1. Quantification of Sargassum patch areal coverage using a 1-m² quadrat. (a) Original 74 75 photo with the Sargassum patch inside the quadrat. The patch was collected immediately after 76 the photo collection in order to determine its biomass; (b) Rectified image based on the 8 control 77 points marked as red dots, as illustrated in (c) and (d).

78 Because the digital photos typically have strong distortions, they were first rectified using the 8 control points marked on the quadrat (Figure 1). Then the Sargassum areal density (D_s , kg/ 79 $m²$) was calculated as: 80

$$
A_s = \frac{c_S}{c_Q} A_Q, \quad D_s = W_s / A_s \tag{1}
$$

where A_5 is the area (m²) of the *Sargassum* patch, A_0 is the area of the quadrat (1 m²), C_5 is the 82 83 pixel count of the patch, C_0 is the pixel count of the quadrat, and W_5 is the wet-weight (kg) of 84 the patch.

85 2.2 Reflectance and AFAI versus to Sargassum biomass density

86 In separate bucket experiments, Sargassum reflectance was measured at different 87 biomass densities in order to develop a model to estimate biomass density. The 88 SpectralEvolution spectrometer covers the spectral range of 277 - 1908nm, with a field of view 89 of 25° (Figure S2a).

90 Sargassum samples collected from the ocean were weighed using a spring scale with 1 g 91 accuracy and put in a cooler. Twenty 25 g bags, six 70 g bags, and three 100g bags of samples 92 (29 total) were prepared. These samples were added one at a time to the black bucket filled with 93 seawater forming 29 different densities, six of which are shown in Figure S2b. Sargassum 94 biomass density was calculated as Sargassum weight divided by the bucket surface area (π × 95 $(0.47/2)^2$ m² = 0.17 m²). Surface reflectance was measured at each of the 29 biomass densities ~ 6 times to establish a relationship between biomass density and reflectance (Figure S2c). 96

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97 AFAI-biomass density model: Following Wang and Hu [2016], alternative floating 98 algae index (AFAI) was calculated using surface reflectance corresponding to MODIS bands, 99 after applying the MODIS relative spectral response (RSR) to the hyperspectral reflectance 100 measured above:

$$
AFAI = R_{748} - R_{667} - (R_{869} - R_{667}) \frac{748 - 667}{869 - 667},
$$
\n⁽²⁾

where the numbers denote the MODIS bands in nanometers. 102

103 Each measured $R(\lambda)$ had a corresponding AFAI and biomass density, which were used to create a 104 regression model. To apply the regression model to the satellite derived AFAI, the in situ AFAI 105 was converted to MODIS AFAI using simulations under different atmospheric conditions. Two 106 aerosol types were considered: maritime aerosol (90% humidity) and coastal aerosol (50% 107 humidity). The aerosol optical thickness at 869nm (τ_{869}) was tested from 0.04 – 0.44, where τ_{869} 108 $= 0.10$ represented the mean condition for the study region [Wang and Hu, 2016]. In situ AFAI 109 measurements were then converted to MODIS AFAI, with the new AFAI-biomass density model applied to MODIS AFAI. In practice, because Sargassum % coverage per pixel or per 0.5° grid 110 111 was already derived [Wang and Hu, 2016] and each % coverage corresponds to a MODIS AFAI value, such developed MODIS AFAI-biomass density model can be applied directly to the % 112 113 coverage maps.

114 Model validation and uncertainty estimations: Direct model validation from satellite 115 measurements is challenging due to the difficulty in linking the field-measured patch to the 116 satellite-measured patch [Hu et al., 2017]. There is further difficulty in conducting such 117 measurements precisely within a MODIS 1 km \times 1 km pixel area due to Sargassum patchiness. 118 Reflectance data of ten relatively dense and homogenous patches were collected while floating on the ocean surface, and their biomass densities were quantified with the method described in 119 section 2.1. Additional black bucket (section 2.2) experiments were conducted to measure 120 121 Sargassum reflectance to validate the model at various biomass density ranges.

122 2.3 Sargassum pigments and nutrient concentrations

123 Sargassum samples were collected for tissue nutrient and pigment analyses from both the neritic and oceanic locations. At each station, ~30g Sargassum samples of both Sargassum 124 fluitans (SF) and Sargassum natans (SN) were collected, rinsed, and stored at -20°C immediately 125 126 after weighing and packing.

127 Sample preparation: In the lab, frozen samples were freeze-dried with the "Labconco 128 freeze-dryer system" for 48-72 hours. The dried samples were ground into fine powders with a 129 clean mortar and pestle. The corresponding dry-weight for each Sargassum sample was 130 measured to quantify the dry-to-wet weight ratio with a digital scale of 0.1 mg accuracy. The 131 ground materials were transferred in plastic vials and stored at -20°C until analyzed.

132 The ground samples were divided into three parts (subsamples) and analyzed as follows: 133 two were used for pigment analyses (using spectrophotometry and High Performance Liquid 134 Chromatography (HPLC)) and one for nutrient content measurements. For the 1st subsample,

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135 pigment extraction was conducted via vortexing ~ 0.1 g of the dried sample dissolved in 10 ml of 136 90% acetone for 30 seconds. The sample was then sonicated in Branson 5510 ultrasonic cleaner 137 for 30 seconds. The mixture was stored in a -20°C freezer for 24 hours to allow for sufficient 138 pigment extraction. The absorption spectra of the pigment extracts were measured with a Perkin 139 Elmer Lambda 25 UV/Vis spectrophotometer. Concentrations of Chl-a and Chl-c were 140 calculated using Jeffery and Humphrey equations [Jeffrey and Humphrey, 1975]. Figure S3 summarizes the main measurement processes and Figure S4 shows the absorbance spectra collected. For the 2^{nd} subsample, pigment composition was analyzed by NASA-GSFC using 141 142 HPLC with similar pigment extraction protocols [Hooker et al., 2005; Van Heukelem and 143 Thomas, 2001]. For the 3rd subsample, the nutrient content analysis was conducted at the 144 145 University of Georgia Analytical Chemistry Lab to determine tissue %C, %N, and %P per unit 146 dried materials.

147 3. Results

148 3.1 Biomass density of pure Sargassum patch

149 A total of 43 measurements were conducted from isolated Sargassum patches, of which 150 38 were from the GOM and 5 from the Florida Straits. The estimated biomass density is 3.54 \pm 151 1.27 kg/m² in the GOM and 1.79 \pm 0.55 kg/m² in the Florida Straits. For all samples, the average 152 is 3.34 \pm 1.34 kg/m², with a maximum of 6.74 kg/m² and minimum of 1.26 kg/m².

153 3.2 Sargassum AFAI-biomass density model and its uncertainties

154 Fig. 2 shows the MODIS RSR-weighed in situ AFAI against biomass density between 155 0.14 and 7.03 kg/m².

156

Figure 2. Sargassum biomass density (kg/m^2) versus in situ AFAI, determined from the bucket 157

158 experiments (Figure S2) or measured in the ocean (Figure 1). The red line is the model fit (Eq 3)

159 using training data (red circles). The blue squares represent validation data from other bucket

160 experiments, while the gray triangles are from measurements in the ocean.

At low densities (< 0.93 kg/m², AFAI < 0.04), AFAI increases linearly with density (R^2 = 161 162 0.98). At higher densities, a two-degree polynomial relationship was established ($R^2 = 0.96$). 163 Thus, the AFAI-biomass density model was established as:

 $y = 23.34x$

$$
(0 < x \leq 0.04)
$$

164
$$
y = 104.88 (x - 0.04)^2 + 65.26 (x - 0.04) + 0.93
$$
 $(x > 0.04)$ (3)

165 where x is the AFAI value and y is the modeled Sargassum biomass density (kg/m^2).

166 The above model was based on in situ AFAI. Simulation results in Figure S5a showed 167 tight relationship between MODIS AFAI and in situ AFAI. Under mean aerosol conditions (T869 = 0.10), MODIS AFAI is ~75% of in situ AFAI (Figure S5b, R^2 = 1.00). Therefore, a multiplier 168 169 of 1.33 was applied to convert MODIS AFAI to in situ AFAI before applying Eq. 3 to MODIS 170 AFAI imagery (Figure S6).

The model's relative uncertainties were determined using independent measurements 171 172 collected both in the bucket (blue squares in Figure 2) and in the ocean (gray triangles in Figure 2). The mean uncertainty was determined to be \sim 11% and it appeared to be relatively consistent 173 174 for both low and higher densities. Additional uncertainty comes from the variable atmospheric conditions. Under different conditions, the mean relative uncertainty in the MODIS AFAI was 175 176 1.2% with a maximum of 2.0%. Considering all uncertainty sources, the overall uncertainties in 177 the modeled Sargassum biomass density should be \leq 12% for a local patch.

178 3.3 MODIS-derived Sargassum biomass density distributions

179 Of all the Sargassum-containing pixels extracted from available MODIS images in 2015 180 covering the Central West Atlantic (CWA) region, 99.5% have AFAI values lower than 0.0028 181 (i.e., within the linear range of $0 - 0.04$ in the AFAI-biomass density model), corresponding to \le 182 6.23% Sargassum coverage within a pixel. For the monthly aggregated 0.5° grids, mean 183 Sargassum % coverage is usually < 0.1% within a grid.

184 The monthly mean total biomass in the CS and CWA from 2011-2017, estimated from 185 the MODIS-derived % coverage (and its corresponding AFAI value) [Wang and Hu, 2016] and 186 the AFAI-biomass density model (Eq. 3), are summarized in Table S1 and Figure 3 for the 0.5° grids. Note that these biomass estimations did not consider the dense Sargassum aggregations in 187 188 the vertical direction, thus only representing lower-bound estimations. If the % coverage were first converted to area coverage $(m^2$ in each 0.5° grid) and then converted to biomass using the 189 190 field measured value of 3.34 kg/m^2 for pure Sargassum patches, the estimated biomass density 191 would be 1.91 times the values in Fig. 3b. According to the previous ship-based measurements [Butler and Stoner, 1984; Parr, 1939; Stoner, 1983], Sargassum biomass density in the GOM, 192 193 CS, and North Atlantic typically ranged from 0.0 to 0.84 (g/m²) [Schell et al., 2015; Siuda, 194 2011]. However, for the bloom conditions shown here, MODIS-derived biomass density could 195 reach ~ 100 g/m² for the 1-km pixels (Figure S6). Such dense patches at MODIS pixel scale 196 would be unrealistic to sample in the field, therefore justifying the use of remote sensing to 197 assess the large-scale Sargassum distributions.

198 The mean total Sargassum biomass in the CS and CWA for July 2015 is at least (i.e., 199 lower bound) 4.4 million tons. This is within the same magnitude of the biomass estimation 200 conducted by Parr [Parr, 1939] for the Sargasso Sea (7-10 million tons). However, because the 201 coarse MODIS pixels (1 km) cannot detect any Sargassum patch < 2000 m² (0.2% of a MODIS 202 pixel [Wang and Hu, 2016]) and because vertical aggregation of Sargassum cannot be remotely 203 sensed, the MODIS-based estimates can only be used as a lower bound. Also note that if the 204 central eastern Atlantic is included the total biomass would be much higher. On the other hand, 205 even this lower bound is \sim 2.5 times of the daily maximum Ulva prolifera biomass in the Yellow 206 Sea in 2015 [Hu et al., 2017], indicating the unprecedented scale and intensity of the Sargassum 207 bloom.

208 3.4 Major pigment and nutrient concentrations of Sargassum

209 The Sargassum nutrient contents are summarized in Table 1. Most stations here are from 210 neritic waters (see Figure S1). There are only 3 stations that are relatively offshore, but their 211 nutrient compositions did not show a large difference from neritic stations. Overall, nutrient 212 compositions are relatively stable for all samples. The mean %C, %N, and %P per dry-weight 213 $(d.w.)$ are 27.16, 1.06, and 0.10, respectively.

214 Table 1. Sargassum nutrients and compositions per unit dry-weight and major pigment concentrations measured by HPLC (Unit: ng mg d.w.⁻¹). SF: Sargassum fluitans; SN: Sargassum 215 216 natans; SW: Sargassum whole samples containing both SN and SF. NAN means not calculated.

217

218 Table 1 and Table S2 summarizes Chl-a and Chl-c pigment concentrations determined 219 from both spectrophotometric and HPLC measurements. The mean Chl-a concentration (HPLC) is 485.20 \pm 101.28 ng mg d.w.⁻¹, representing ~ 0.05% of the total dry biomass. The Chl-a: Chl-c 220 221 ratio is 0.08 ± 0.01 from all HPLC measurements. Overall, pigment compositions are stable for 222 both species. The two major light-harvesting pigments are Chl-a and fucoxanthin, accounting for 223 \sim 60% and 20% of the total major pigment contents (Table S3). All other pigments are an order 224 of magnitude lower. The results from the spectrophotometric measurements are close to those 225 from the HPLC measurements.

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226 The HPLC-measured mean concentrations from all samples were used to derive pigment 227 concentrations from biomass density and to compare with those values reported by Schofield et 228 al.[1998]. The concentrations from this study are consistently higher for all major pigments for 229 both SF and SN (Table S3). It is unclear whether this is due to seasonal variations, measurement 230 protocols, or real changes during the 20-year period. However, the relative fractions of the major 231 pigments are consistent from both studies (Figure S7).

232

233

234 Figure 3. Monthly mean Sargassum areal coverage (%), biomass density, Chl-a, C, N, and P in 235 each 0.5° grid in the CS and CWA in July 2015. Based on the mean concentrations measured in 236 this study, the biomass, nutrients, and pigments in (b-f) were derived from the Sargassum % 237 coverage (and the corresponding AFAI) in (a) using Eq. (3). The total integrated Sargassum areal 238 coverage, wet biomass, nutrients, and pigments over the bloom areas (density $> 0.0\%$) are 239 annotated in each panel.

240 4. Discussions

241 Sargassum pigments: Sargassum reflectance properties are determined primarily from 242 pigment composition: each pigment has its own absorption characteristics. For example, the 243 reflectance troughs at 630 nm and 670 nm are caused by the strong absorption by Chl-c and Chl-244 a, respectively [Bricaud et al., 2004]. The low Chl-c: Chl-a ratio (0.08) can explain the different 245 magnitudes of these reflectance troughs. Likewise, the low reflectance between 400 - 500 nm
246 (the reason why Sargassum does not have any blueish-greenish colors), is caused by Chl-a 247 absorption around 440 nm and fucoxanthin absorption around 500 nm [Bricaud et al., 2004]. The 248 low reflectance in the green wavelengths is expected, and helps discriminate Sargassum from 249 Trichodesmium. This cyanobacteria (also called blue-green algae) is also abundant in the Atlantic Ocean [Hu et al., 2015] and similar to Sargassum in that it also shows red-edge 250 251 reflectance when algae cells or colonies form surface scums. These reflectance characteristics, 252 associated with the major pigment absorptions, might eventually be used to develop algorithms 253 to assess Sargassum life stages and physiological states.

254 Sargassum Carbon: As shown in Figure 3d, the massive Sargassum bloom in the CS 255 and CWA contained large amounts of carbon that have not been considered in any carbon cycle 256 models. Is this a negligible component when compared to the traditional water-column 257 phytoplankton carbon (i.e., particulate organic carbon or POC)? Or, is it a vital component 258 required to improve carbon cycle models? As Sargassum lives mostly in nutrient-poor open-259 ocean waters with low water-column Chl-a concentrations, POC from a layer 50-m deep of 0.1 mg/m³ Chl-a concentration was used to compare with Sargassum carbon. The former is 260 equivalent to an integrated water column Chl-a density of 5.0 mg/m^2 . Assuming the mean C:Chl-261 262 a ratio of 74 (g:g) in the Atlantic Ocean [Wang et al., 2013], the water column POC is 0.37 g/m^2 . In comparison, for waters with Sargassum biomass density > 0.0 g/m² in July 2015 (an area of 263 7.23×10^6 km²), Sargassum Chl-a, wet biomass, and carbon were estimated to be 0.06 mg/m², 264 265 0.61 $g/m²$, and 0.03 $g/m²$, respectively. Although these numbers are lower than those of the water-column phytoplankton, the Sargassum contributions to total carbon $(-9%)$ should not be 266 neglected. On the other hand, for the entire study region $(1.16 \times 10^7 \text{ km}^2)$, because some waters 267 268 have 0.0 g/m^2 Sargassum, the mean Sargassum Chl-a, biomass, and carbon in July 2015 are reduced to 0.04 mg/m², 0.38 g/m², and 0.02 g/m², respectively. This still indicates that 269 270 Sargassum carbon can represent a significant component (\sim 6%).

271 In addition to MODIS observed Sargassum, there may also exist many small-scale 272 Sargassum features that are undetectable by MODIS. Given the detection limit of 0.2% coverage 273 within MODIS 1-km pixels [$Wang$ and Hu , 2016], the lowest biomass density measured from a 274 MODIS pixel is 2.80 g/m^2 , higher than most field-measured values. Given the fact that field 275 measurements are mostly through neuston nets for small Sargassum mats or clumps, field 276 collected Sargassum densities may represent the undetected proportion. Adding the field-277 measured biomass density of 0.84 g/m^2 (during November 2014 – May 2015) [Schell et al., 278 2015] to MODIS measurements (0.38 g/m^2) (note that this value appears lower than the pixel-279 level detection limit, but it is a result of monthly averaging), the mean Chl-a, biomass, and carbon are 0.12 mg/m², 1.22 g/m², and 0.07 g/m² in the entire study regions, respectively. Thus, 280 281 the total Sargassum carbon can account for ~18% of the phytoplankton carbon over the entire 282 study region during the peak months. By failing to account for this much carbon, it is clear that 283 current carbon cycle models could be improved by including total Sargassum carbon.

284 Sargassum nutrient limitations: Compared to the Redfield Ratio (106:16:1) [Redfield, 285 1934], the Sargassum C: N: P data suggest a strong nutrient limitation of both N and P. 286 According to the neritic baseline from Lapointe et al. [2014, 2015], %N, N: P, C: N, and C: P of 287 SF are about 1, 10, 27, and 268, respectively. Compared to historical baselines, the results from this study did not show a significant increase of %N for SF, which dominated the sample 288

289 collections. However, the mean N: P (23.11) and C: P (727.39) of SF are much higher than the 290 neritic baseline for all cases, suggesting a consistent stronger P-limitation than historical 291 samples. The %N and %P of SN are slightly lower than those of SF, but their %C is higher. Our 292 results indicate that the recent Sargassum blooms could benefit from the long-term nutrient 293 enrichment, especially the N-enrichment during the past decades [Galloway et al., 2008; 294 Rockstrom et al., 2009].

295 Sargassum sedimentation on the deep-sea floor: Carbon and nutrients in Sargassum 296 also impact the deep-sea ecosystems once the algae die and sink to the ocean bottom. In fact, 297 connection of Sargassum to the deep-sea communities has been confirmed in field surveys where 298 sinking Sargassum was observed on the ocean floor [Johnson and Richardson, 1977; Rowe and 299 Staresinic, 1979]. These observations suggest that macroalgae may play an important role in 300 carbon transport to the deep-sea fauna [Krause-Jensen and Duarte, 2016]. Considering the 301 enormous blooms in the CS and CWA in recent years, massive carbon sedimentation may have 302 already provided significant carbon input, thus potentially affecting the deep-sea fauna distribution patterns [Baker et al., 2017]. Additional support for carbon sedimentation comes 303 304 from sediment core studies near the Deepwater Horizon Wellhead MC252 following the April 305 2010 oil blowout in the Gulf of Mexico. The cores showed elevated accumulations of carbon-306 rich sediments likely resulting from a major marine snow event associated with hydrocarboninduced microbial blooms [Brooks et al., 2015; Paul et al., 2013] and sediment porewater 307 308 genotoxicity [*Paul et al.*, 2013]. Although the initiations of these sedimentation events are 309 different, the resulting major carbon sedimentary accumulation should be similar. In the end, 310 once field data are available to link Sargassum deposition and remotely sensed biomass, the 311 basin-scale biomass estimation from this study may help quantify the amount of carbon 312 deposition and infer its potential impact.

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Appendix C:

Modelling Sargassum transport in the Tropical Atlantic Ocean

Wang, M., Hu, C., & Mitchum, G. (in preparation). Modelling *Sargassum* transport in the Tropical Atlantic Ocean.

Modeling Sargassum transport in the Tropical Atlantic Ocean

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5 Abstract

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Since 2011, massive Sargassum blooms have occurred frequently in the Tropical Atlantic, causing 6 7 beaching events and other environmental and economic problems for the Caribbean islands. Several studies have investigated the potential bloom sources and the transport pathways through 8 9 physical modeling. However, most studies are limited by the lack of large-scale Sargassum distribution data for model initiation and validation. Here, the mean Sargassum distributions 10 derived from Moderate Resolution Imaging Spectroradiometer (MODIS) observations are used to 11 initiate and evaluate a Lagrangian particle tracking model that tracks Sargassum advection under 12 surface currents and winds. Among the 39 experiments, adding surface currents alone improves 13 14 model performance (i.e., by reducing difference between modeled and observed Sargassum distributions) in 82% of the cases after tracking Sargassum for one month. Adding 1% wind 15 forcing to the advection model also shows improved performance in 67% of the cases. Adding a 16 time- and location-dependent Sargassum growth/mortality rate (i.e., change rate), derived from 17 time-series of the MODIS-based Sargassum abundance and the corresponding environmental data 18 19 via a Random Forest regression, leads to further improvement in model performance (i.e., by 20 increasing the matchup percentage between modeled and observed Sargassum distributions) in 64% of the cases, although the modeled change rates only explain \sim 27% of the variance of the 21 validation dataset, possibly due to uncertainties in such-derived change rates. The Sargassum 22 transport model, with the mean currents, winds, and change rates acting as the forcing, is applied 23 to track the mean Sargassum distributions forward and backward. The results demonstrate the 24 25 model's capacity of simulating the Sargassum distribution patterns, with emphasis on the role of biological terms in determining the large-scale distributions. These tracking experiments also 26 suggest that Sargassum blooms in the Caribbean Sea are strongly connected to the Central Atlantic 27 28 regions, and blooms in the Tropical Atlantic show relatively weak connections to the Atlantic regions further north. 29

30 **Key points:**

- 31 ٠ Satellite-derived Sargassum distributions are used to initiate and evaluate a Lagrangian particle tracking model. 32
- Sargassum growth/mortality (i.e., change) rate is derived from satellite-based observations 33 and environmental variables. 34
- 35 The roles of physical advection, winds, and growth/mortality rate in determining the Sargassum distributions, transport, and regional connectivity are studied. 36

37 1. Introduction

38 Pelagic Sargassum, previously known to be abundant in the Sargasso Sea and Gulf of Mexico (GOM) [Butler et al., 1983; Butler and Stoner, 1984; Parr, 1939], has formed intensive 39

40 blooms in the Tropical Atlantic and the Caribbean Sea (CS) in recent years [J Gower et al., 2013; 41 JF Gower and King, 2011; Wang and Hu, 2016; 2017]. As a critical marine habitat, the changes 42 of Sargassum distributions could significantly influence various related marine fauna [Council, 43 2002; Doyle and Franks, 2015; Lapointe et al., 2014; Rooker et al., 2006]. Massive coastal 44 beaching events in the CS and West Africa (WA) also induced environmental, ecological, and 45 economic problems to the local areas [Hu et al., 2016; A Siuda et al., 2016; Smetacek and Zingone, 46 2013].

Understanding the origin and distribution of Sargassum blooms requires thorough 47 investigations of the Sargassum response to environmental forcing such as temperature, light, 48 nutrients, salinity, and ocean currents. Recent studies using both remote sensing and field sampling 49 50 have documented synoptic distribution patterns of Sargassum and their temporal changes [J Gower et al., 2013; JF Gower and King, 2011; Schell et al., 2015; Wang and Hu, 2016; 2017; 2018], yet 51 52 Sargassum transport over synoptic scales, for example in the Tropical Atlantic is still not well understood, mainly due to lack of field-based measurements to constrain the transport models. 53

Several studies have been dedicated to modeling Sargassum transport in the Atlantic Ocean 54 55 and analyzing the regional connectivity. Franks et al. [2011, 2016] proposed several regions to be 56 critical for Sargassum accumulation and consolidations in the tropics through backtracking from the reported beaching locations and studying drifting buoy pathways. Nathan et al. [2018] 57 58 conducted several tracking experiments to investigate the transport connections between the CS 59 and the Central Atlantic (CA) with both forward-tracking and backtracking. These studies 60 provided critical information on the Sargassum transport patterns and regional connections via 61 physical transport modeling. However, due to the lack of large-scale observations, most modeling 62 efforts are initiated either using limited field reported locations or through random assignment, 63 and there is also lack of validation of the simulation results for the same reason. Currently, the 64 Sargassum distributions in the Intra-Americas Seas (IAS) and Atlantic Ocean derived from Medium Resolution Imaging Spectrometer (MERIS) [J Gower et al., 2013; J F Gower and King, 65 2011] has already been used in the Sargassum transport models to understand the seasonal patterns 66 67 of the Sargassum in the Atlantic Ocean [Brooks et al., 2016]. However, the "Sargassum year" in the Caribbean did not start until 2011, but MERIS stopped functioning in 2012, therefore unable 68 to provide updated information for the recent bloom years in the Tropical Atlantic. In addition, the 69 MERIS-derived Sargassum distributions have relatively high level of noise contamination [Wang 70 and Hu, 2016]. With a recently developed procedure, the monthly Sargassum mean distributions 71 72 are generated from Moderate-resolution Imaging Spectroradiometer (MODIS) observations with improved data quality and coverage $(2000 - present)$ [Wang and Hu, 2016; 2017]. These 73 74 Sargassum distributions can be incorporated in physical models to help understand the Sargassum transport in the Tropical Atlantic especially for recent years. 75

76 Besides the physical transport caused by ocean currents and surface winds, Sargassum 77 distributions are also largely determined by the biological growth and mortality. In fact, the role of biological factors has already been emphasized by previous modeling efforts using the simulated 78 Sargassum growth/mortality rate, suggesting that the biological terms can greatly affect the 79 Sargassum seasonal distributions in the Atlantic Ocean [Ardron et al., 2011; Brooks et al., 2016]. 80 81 Although the general impacts of temperature, salinity, light, and nutrient conditions on the 82 Sargassum growth/mortality rate have been studied in previous experiments [Hanisak and Samuel, 1987], there is still a lack of sufficient measurements to establish a solid relationship to model the 83 Sargassum growth/mortality rate in response to variable environmental conditions. As such, most 84

85 Sargassum transport models did not consider their biological growth/mortality [J Franks et al., 86 2011; J S Franks et al., 2016; Putman et al., 2018 (in revision)].

In this study, MODIS-derived Sargassum distributions are adopted to: 1) investigate the 87 Sargassum distribution patterns in the tropical Atlantic; 2) initiate and validate a physical transport 88 model; 3) establish a model to estimate Sargassum change rate using environmental data. The 89 primary objectives of this paper are to establish and evaluate a Lagrangian particle tracking model 90 with ocean currents, surface winds, and MODIS-based Sargassum change rate. The model's 91 92 response to each individual forcing factor is examined. The model is then applied to MODIS 93 observations to improve our understanding of the Sargassum distribution patterns and cross-region connectivity in the Atlantic Ocean. 94

2. Data and methods 95

2.1 Data preparation 96

97 MODIS Level-0 data covering the IAS and Atlantic Ocean (10°S - 40°N, 89°W -15°E) 98 from 2000 - 2016 were downloaded from the U.S. National Aeronautics and Space Administration 99 (NASA) Goddard Space Flight center, and then processed to mapped Rayleigh-corrected reflectance (Rrc) to generate Alternative Floating Algae Index (AFAI) products at 1 km spatial 100 101 resolution. Sargassum areal coverages were derived from MODIS AFAI data and were then 102 averaged to get the monthly mean distributions using the approach described in Wang and Hu 103 [2016]. The monthly mean products were applied to represent the Sargassum distributions in the in the middle of each month. 104

105 The surface current velocities were downloaded from global Hybrid Coordinate Ocean Model (HYCOM) (GLBa0.08) with a 0.08° resolution [Chassignet et al., 2007]. The wind speed 106 data were obtained from National Centers for Environmental Prediction (NCEP) Reanalysis 107 [Kalnay et al., 1996] at 10 m above the sea level and were interpolated to the 0.08° HYCOM grid. 108 Both the current and wind data provide daily observations and were incorporated in the Lagrangian 109 110 particle tracking model to model the Sargassum transport. The source and resolution of the environmental data used to derive the Sargassum change rate model, including Sea Surface 111 Temperature (SST), chlorophyll a (Chl-a) concentrations, Photosynthetically Available Radiation 112 113 (PAR), Sea Surface Salinity (SSS), precipitation rate, nutrient concentrations (nitrate (N) and 114 phosphate (P), and dust deposition (both wet and dry deposition) rate, are summarized in Table 115 $\mathbf{1}$

116 Table 1. Summary of the environmental data used to model Sargassum local change rate (i.e., the net growth/mortality rate, which can be positive or negative). 117

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Precipitation rate	Tropical Rainfall Measuring Mission (TRMM, TRMM 3b43) v7	Monthly mean	0.25°
nutrient (N, P) concentrations	The biogeochemical model Pelagic Interaction Scheme for Carbon and Ecosystem Studies: PISCES http://marine.copernicus.eu/	Monthly mean	$1/4^{\circ}$
dust deposition rate	Spectral Radiation-Transport Model for Aerosol Species (SPRINTARS) model version 5.9.0 [Takemura et al., 2000]	daily	1125°

Note: The daily products were averaged to the monthly mean composite to investigate their 118 119 impacts on the monthly mean change rate. All the data were interpolated to the 0.08° HYCOM 120 grid to be incorporated in the transport model.

2.2 Lagrangian particle tracking with HYCOM surface current and NCEP wind 121

The Sargassum transport was simulated using the daily outputs from the Global HYCOM 122 123 surface current and the NCEP Reanalysis wind velocity (10m above sea level). A Runge-Kutta 4thorder method was used to approximate the successive positions of the Sargassum particles at a 124 time step of 30 minutes. As the diffusion term is much smaller than the advection term $[Brooks]$ et 125 126 al., 2016] and hard to properly quantify, it was not considered in our tracking model. In other 127 similar Sargassum transport studies, diffusion terms are also generally ignored [Brooks et al., 2016; J S Franks et al., 2016; Putman et al., 2018 (in revision)]. The monthly mean Sargassum 128 129 distributions were assigned to represent the Sargassum distributions in the middle of each month. 130 The particles were seeded based on the monthly mean Sargassum areal density $(i.e.,$ percent cover). 131 An initial weight was assigned to each particle based on the mean Sargassum areal density in that 132 grid.

Ideally, larger number of particles could better represent the smaller-scale Sargassum 133 134 movement. However, the computational stress and memory consumption will increase with the increasing number of particles initiated. Here, two methods were used to initialize the Sargassum 135 particles: 1) Put the particles based on the corresponding mean Sargassum density of the 0.5° grids. 136 137 Inside each 0.5° grid, multiple number of particles were assigned evenly based on the Sargassum 138 areal density to account for the small-scale Sargassum distributions. All the particles inside that 139 grid were assigned an equal weight which sum up to the total density. For example, for a grid with 140 0.2% coverage, 100 particles were assigned inside that grid and each particle will have an initial weight of 0.002%. The number of particles to initiate was proportional to the Sargassum areal 141 density in that grid. The selection of the number of particles is a compromise between the 142 143 computational stress and memory consumption, and the simulation performance. 2) Put the 144 particles based on the corresponding mean Sargassum areal density of the finer scale (0.05°) grids. 145 Inside each grid, one particle was seeded and assigned an initial weight of the total density. The 146 particles initiated based on higher resolution grids should be more representative of the actual Sargassum distributions. 147

Because Sargassum generally has variable proportions above the sea surface, Sargassum 148 149 transport will likely be affected by surface winds in addition to ocean currents. The influence may 150 come from direct wind forcing or residual transport due to waves. The impact could depend on the morphology of the Sargassum features and the relative percentage of submergence. When 151 modeling oil trajectories, a 3% wind factor is generally adopted to simulate the wind impact [Lehr 152 153 and Simecek-Beatty, 2000]. As the majority of the Sargassum plant is typically submerged, surface 154 winds are expected to have a weaker influence. Here, a factor of 1% was tested to evaluate the

- 155 significance of wind induced transport. The same parameter is also used in similar studies to model 156 the wind-induced Sargassum transport [Putman et al., 2018 (in revision)].
- 157 2.3 Modeling Sargassum growth/mortality (change) rate

Due to lack of field or laboratory measurements of Sargassum change rates, the satellite 158 159 derived monthly mean Sargassum coverage maps were applied to infer their change rates at 160 monthly scales. These change rates and the environmental variables were then analyzed to estimate Sargassum change rate under different environmental conditions. 161

162 To determine the regional Sargassum change rate from satellite observations, one obstacle 163 is to find the corresponding Sargassum features in adjacent months. This is because their 164 morphological characteristics could change drastically in a few days in response to variable oceanographic conditions, making it extremely difficult to locate the corresponding features from 165 166 monthly observations. Moreover, as pelagic Sargassum is free-floating on the ocean surface, it is also challenging to determine the environmental conditions the individual Sargassum feature lived 167 168 through (i.e., the trajectories) during that one month. Therefore, the critical problem is to determine 169 the corresponding Sargassum features and their transport pathways. Ideally, if the transport 170 model is accurate, this can be readily solved through tracking the Sargassum particles and 171 recording their trajectories. However, the current transport model is unable to perfectly match the 172 model outputs with observations, especially after tracking for one month. Here, two methods were 173 tested to approximate the areas where the corresponding features and the transport pathways were 174 located.

175 One method is to divide the region into uniform grids and assume that Sargassum stays inside the grid during the one-month period (referred as the grid method, shown in Figure 1a and 176 177 1c). As the area-averaged mean surface current speed in the Tropical Atlantic is ~ 0.2 - 0.3 m/s, the distance of Sargassum transport by surface current is \sim 500 - 800 km in 30 days. Thus, the grid 178 sizes varied from $5^{\circ} \times 5^{\circ}$ to $13^{\circ} \times 13^{\circ}$ were tested to derive the *Sargassum* change rate in adjacent 179 months. The other method is to identify the Sargassum features from adjacent months via semi-180 objectively selection of large features (referred as the patch method, shown in Figure 1b and 1d). 181 182 Any pixel within the selected region of interest (ROI, identified by visual inspection) which has a % cover > 5×10^{-3} % (the bloom threshold used in the CS in July [*Wang and Hu*, 2017]) was 183 184 considered as the bloom pixel. The bloom pixels were dilated 31 pixels outward to account for the 185 smaller scale features near the bloom regions. The assumption is that the Sargassum feature evenly 186 stayed inside the defined regions and that areas can reflect the environmental conditions the 187 Sargassum feature went.

188

189 Figure 1. The methods to determine the corresponding the Sargassum features in adjacent months. 190 (a) and (c) demonstrate the grid method, with the $11^{\circ} \times 11^{\circ}$ grids marked by the red lines. The 191 shaded squares are an example of the corresponding grid in adjacent months. (b) and (d) 192 demonstrate the patch method, with the boundary of the determined Sargassum patches delineated 193 by the white lines. The background images are the monthly mean Sargassum coverage 194 distributions. The colorbar of the Sargassum coverage maps is inserted in (d), with values indicating percent Sargassum cover (0.1 indicates 0.1%). 195

196 Sargassum change rate: Within that specified area (defined by the grid or patch method), 197 all the environmental data (summarized in Table 1) were averaged to get the mean environmental 198 conditions. Since the change rate was derived from two adjacent months, the environmental data 199 were averaged for that two months. To account for the natural growth cycles of Sargassum, an 200 independent variable representing the time of the year (the number of days since the beginning of 201 the year divided by 365) was also included as an explanatory variable. The non-linear transformation forms for each variable (x), including $ln(x)$, $log_{10}(x)$, $x^{0.25}$, $x^{0.5}$, and x^2 , were also 202 203 used in the regression. An Akaike Information Criterion (AIC)-based variable selection method 204 was conducted to choose the appropriate environmental variables to be included in the Random 205 Forest (RF) regression model [Breiman, 2001; Liaw and Wiener, 2002]. The selected variables were then used to build the change rate model through RF regression. The general process is 206 summarized in Figure 2. The regression model was trained with the Sargassum distributions and 207 208 environmental data from 2011-2015 and their performance was evaluated using an independent dataset from 2016 in the study region. 209

210

Figure 2. The process to model the Sargassum change rate. The definition of the corresponding 211 features is either based on the grid or patch method. A variable representing the time of the year is 212 213 also used to training the change rate model. The colorbars of the Sargassum coverage and change 214 rate maps are inserted, with values indicating the % cover (0.1 means 0.1%) and change rate (0.05 means 0.05 doublings day⁻¹). 215

216 The Sargassum particles were assigned an initial weight based on the MODIS-derived 217 Sargassum areal density (i.e., percent cover). The time- and location-dependent change rate was 218 then adopted in the tracking model to adjust that particle weight along the trajectories to account 219 for Sargassum growth/mortality during the transport.

220 2.4 Evaluating Sargassum transport modeling performance

The Sargassum transport model performance was evaluated by comparing the modeled 221 Sargassum particle distributions with the corresponding mean distributions derived from satellite 222 223 observations. The simulated Sargassum distributions was first resampled to 0.5° resolution (the 224 resolution of the MODIS-derived mean distributions) to make such a comparison. The abundance 225 difference (abundanceast) of each model outputs was quantified by the mean difference between 226 observations (the ground truth) and the modeled *Sargassum* distributions (equation (1)). The overall agreements between observations and the modeled Sargassum distributions were evaluated 227 using the matchup percentage of Sargassum abundance (abundance $_{\text{match}}$) after weighting the 228 particles with their areal densities (equation (2)). 229

$$
abundance_{diff} = \frac{\sum_{i=0}^{N_{obs}} |f_{track}(i) - f_{obs}(i)|}{\sum_{i=0}^{i=N_{obs}} f_i} \times 100\%
$$
 (1)

231
$$
abundance_{match} = \frac{\sum_{i=0}^{i=N_{match}} f_i}{\sum_{i=0}^{i=N_{obs}} f_i} \times 100\%
$$
 (2)

232 where the subscript obs, track, and match represent the pixels from valid MODIS observations, 233 the modeled Sargassum pixels, and the matchup pixels where both the observations and the model 234 outputs indicate Sargassum presence, respectively.

2.5 Model applications 235

236 Once the model performance was verified with the satellite observations, the model was 237 then applied to investigate Sargassum distribution pattern formations and regional connectivity in the Tropical Atlantic areas through tracking the MODIS-derived mean distributions forward and 238 239 backward. The mean currents, winds, and Sargassum change rates were averaged from 2011-2015 240 to represent the average environmental conditions. For backtracking with the change rates added, 241 a negative time step was applied to quantify the amount of areal density change. The Sargassum 242 distributions in January and July were selected to represent the typical winter blooms and summer 243 blooms in the Tropical Atlantic.

2.5.1 Reproducing the seasonal distribution patterns through forward-tracking 244

245 The monthly mean Sargassum distributions were first derived for the recent bloom years since 2011, when significant amount of Sargassum occurred in the tropics every year except 2013. 246 The mean ocean surface currents and winds were then used to simulate the Sargassum transport 747 248 over the IAS and Atlantic Ocean to see if these patterns can be reproduced. Particles were released based on the satellite derived mean Sargassum distributions with and without including the change 249 rate. The overall agreement of the model outputs with the mean Sargassum distributions were 250 evaluated the *abundancematch*. Forward-tracking was conducted in January when typical winter 251 252 blooms were observed in the CA to investigate how the Sargassum distribution patterns may 253 evolve from the previous locations, and to better understand the formation and dissipation of the 254 large Sargassum aggregations in the tropics.

255 2.5.2 Assessing the cross-region connectivity

256 The transport model was also applied to assess the cross-region connectivity of Sargassum 257 in the Atlantic Ocean. Sargassum blooms typically occurred in the eastern Tropical Atlantic in the

258 winter and transported to other regions in the following months. Here, four important regions were 259 defined to analyze the regional connectivity: the CA (10° S - 23° N, 58° W - 15° W), the North 260 Atlantic (NA, 23°N - 40°N, 80°W - 15°W), the WA (10°S - 15°N, 15°W - 15°E), and the CS (8°N 261 - 23°N, 89°W -58°W). The NA was considered to be linked to the Sargasso Sea.

262 Forward-tracking and backtracking experiments initiated in January and July were 263 conducted to see how large Sargassum patches are connected between these regions and to search 264 for the potential linkage of the Sargassum in the winter bloom locations in the CA and the summer 265 blooms in the CS, CA, and WA. The percentage of particles transported in/out of each region from 266 another during the tracking experiments were used to evaluate the transport connectivity between regions. The percent of self-retention was also calculated for the same region as the percent of 267 268 particles remained in the previous region after running the simulation for the given period. The transport pathways were analyzed with the particle trajectories. 269

270 3. Results

271

3.1. Sargassum accumulations in the Tropical Atlantic and the "new Sargasso Sea"

Since 2011, large amount of Sargassum has occurred in the Tropical Atlantic regions. This 272 273 is revealed by MODIS-derived mean distribution maps (Figure 3), field observations, and coastal beaching reports [J Gower et al., 2013; Schell et al., 2015; Wang and Hu, 2017]. On the other 274 275 hand, both field and satellite observations indicate much lower Sargassum abundance in the 276 Sargasso Sea, where massive Sargassum used to be found. It seems that the "new Sargasso Sea" 277 has been formed in the Tropical Atlantic in recent years.

278 The Sargassum seasonal distributions are very different from the patterns before the 279 "Sargassum year" of 2011. As shown in Figure 3, large Sargassum aggregations first appeared in 280 the CA during the winter months. The bloom extent increased in the spring and moved towards 281 the CWA (near the Amazon River mouth) around April. In summer, the Sargassum accumulations 282 were further transported and developed across the Tropical Atlantic, forming large Sargassum accumulations in the Tropical Atlantic. The bloom started to decrease from August to September 283 284 and most Sargassum biomass were carried to the eastern Tropical Atlantic Ocean. Depending on 285 the environmental conditions, the bloom can further diminish or retain high abundance and initiate 286 the bloom events in the coming year.

287

288 Figure 3. The monthly mean Sargassum distributions in January (a), April (b), July (c), and 289 October (d) derived from recent bloom years (averaged from 2011-2012 and 2014-2015). The 290 dashed circles mark the typical bloom locations in January. The colorbar of the Sargassum 291 coverage is inserted, with values indicating percent Sargassum cover (0.1 indicates 0.1%). Note 292 that although the general patterns were consistent, there could be large inter-annual variabilities of 293 the Sargassum distributions in the tropical Atlantic region.

3.2. Sargassum local change rate under different environmental conditions 294

295 Seventy-five (75) groups of training data were generated from the patch method. With that, 296 the AIC-based RF regression selected the SST, N concentration anomaly, and the time of the year 297 to be the most significant factors in determining the Sargassum change rate. 55% variability of the 298 training data was explained by the RF regression model (Figure S1a). The validation results of the 299 RF model were less satisfactory, with a R^2 of \sim 27% on the validation dataset (Figure S1b). The 300 relatively low variance explained could be partly ascribed to errors in the nutrient data and other 301 environmental variables, satellite derived Sargassum abundances, and such-selected Sargassum 302 transport areas.

303 For the RF model derived from the grid method, the regression model performance was 304 not as good, with a R^2 of ~ 5% obtained on the validation dataset (Figure S1c & S1d). This could 305 be due to the confused signals of the Sargassum transport in/out of the grid. Also, the Sargassum 306 decrease rate was generally less represented in the training data obtained from the grid method. 307 That may be related to the invalid decrease rates derived when most Sargassum particles were 308 transported out to adjacent grids during decreasing phases. As a result, the modeled Sargassum 309 change rates were mostly positive values and can't well capture the Sargassum decrease in the CS 310 and CWA, making it unsuitable for simulating the overall Sargassum abundance changes. 311 Therefore, the change rate model derived from the patch method was adopted in this study.

The seasonal and spatial patterns of the modelled Sargassum change rate in the Tropical 312 313 Atlantic are summarized in Figure 4. The area-averaged mean Sargassum change rate in the CWA (0°S - 22°N, 63°W - 38°W) from the bloom years during 2011 to 2016 were generated and 314 compared with the observed change rate in Figure 4a. Overall, the seasonal trends are similar to 315 the observations. Although some of the high growth/mortality rates in the CWA are not well 316 317 captured, the change rates in the spring to summer months are consistently higher than those from 318 winter months. For the spatial patterns, mean Sargassum change rates within the high Chl-a water are lower than those in the nearby low Chl-a areas in most $($ > 80%) cases. This is consistent with 319 320 the previous conclusion that Sargassum prefers to grow in the open water [Hanisak and Samuel, 321 1987].

To summarize, although the change rate model did not achieve high agreements with the 322 323 observations, the dominant spatial and seasonal patterns are well reflected. Therefore, the change 324 rate model could be applied to simulate the general response of the Sargassum biological growth 325 and mortality under variable environmental conditions along the transport trajectories.

326

327 Figure 4. Summary of the spatial and temporal patterns of the modeled Sargassum change rate. 328 (a) Comparison of the area-averaged modeled mean change rates (from 2011 - 2016) in the CWA 329 with MODIS observations. (b) Comparison of the mean change rate in the high Chl-a region (Chl-330 a concentrations > 1.0 mg/m³) and the nearby low Chl-a region (dilated 500 km outward). The black solid line is the 1:1 line. 331

332 3.3. Sargassum transport model performance

333 The transport experiments were conducted for adjacent months when sufficient Sargassum 334 patches were found. Sargassum distribution data from 2011-2015 were tested using the initial 335 conditions in the earlier month, tracked for one month with the transport model, and then compared the modeled distributions with the MODIS observations in the later month. 336

337 Here, the transport model performance is evaluated from the following three perspectives to investigate the roles of surface current advection, wind forcing, and Sargassum change rates: 1) 338 Has adding the surface current advection (referred as the advection model) improved the model 339

340 performance compared to the one takes the initial Sargassum distributions from previous month 341 to be the Sargassum distribution in the following month (referred as the initial model)? 2) Has 342 adding the wind forcing to the advection model (referred as the advection $+1\%$ wind model) 343 improved the model performance? 3) Has adding the Sargassum change rate to the advection 344 model (referred as the advection + change rate model) improved the model performance?

Figure 5 shows an example of the Sargassum distributions during a forward-tracking 345 experiment from August 2012 to September 2012. Figure 6 summarizes the comparison of 346 347 abundancediff of the modelled Sargassum distributions using different methods. Among the thirtynine (39) forward-tracking experiments, 82% of the cases showed lower *abundance* after adding 348 the advection of the currents alone (Figure 6a), suggesting Sargassum distributions are strongly 349 affected by the surface current. However, more variable results were obtained after including 1% 350 wind forcing: 64% of the cases showed lower *abundance* aff compared to the results from the 351 advection model, although the general impact is relatively small (Figure 6b). As Sargassum 352 patches are likely affected by wind forcing, the 1% wind factor was still considered in the 353 354 Sargassum transport model. Adding the Sargassum change rate to the advection model showed less improvement in terms of abundancediff, with 36% of the cases obtained smaller abundancediff 355 than the results from the advection model. Larger improvements (64% of the cases) were found 356 for matchup percentage of the modeled Sargassum abundance (abundancematch). Besides the 357 358 uncertainties from the change rate model itself, the transport model performance can also be 359 affected by the errors of the particle trajectories, where Sargassum "feel" the local environmental 360 conditions and adjust their growth/mortality rate. Although adding the change rate doesn't always 361 improve the Sargassum distributions simulation, it helps to explain the variations of the total 362 Sargassum abundance changes at monthly scales.

Considering the coarse resolution of the 0.5° mean distribution data, higher resolution 363 (0.05°) monthly mean composite data were also tested to initiate the transport model. In Figure 6d, 364 365 the *abundance* af the tracked distributions from the advection model using 0.05° grids were 366 compared with the *abundance* diff of the advection model outputs using 0.5° grids. In 56% of the 367 cases, the tracked results were improved by using the higher resolution initial conditions. This 368 suggests that the transport model uncertainties could be partly associated with the imperfect initial 369 conditions.

370 Overall, these tracking experiment results prove that the Sargassum transport model, driven 371 by surface currents, winds, and change rates, indeed helps to interpret Sargassum distribution 372 patterns in the tropical Atlantic Ocean, although unsatisfactory model performance can occur especially for the wind and change rate contributions. 373

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Figure 5. Sargassum distributions from the forward-tracking experiments from August 2012 to 376 September 2012. (a) is the initial Sargassum particles distributions; (b) and (d) are the simulated 377 Sargassum distributions in September 2012 using the advection model and advection $+$ change 378 379 rate model, respectively; (c) is the MODIS derived mean distributions in September.

381 Figure 6. Comparison of the *abundance* af modelled results using difference methods. The 382 black solid lines are the 1:1 lines. The points corresponding to model improvement are marked by 383 the dash boxes. "advection (0.05° initial)" represents the advection model initiated with the 0.05° 384 resolution mean Sargassum distributions. Lower abundance if values would suggest better model 385 performance. For example, in (a), adding surface current advection showed improved results in most cases compared to the initial model, with lower *abundance* af from the advection model 386 387 outputs.

3.4. Bloom pattern formation, regional connectivity, and bloom source investigations 388

389 3.4.1. Sargassum seasonal distribution pattern formation

390 Forward-tracking with the initial Sargassum distributions in January showed good 391 agreement with the satellite observations in terms of spatial patterns, although large difference is found in their total matched abundance. In fact, the *abundance*_{match} were consistently lower than 392 10% - 20% after tracking for two months when no growth/mortality terms were considered (Figure 393 7a). After including the modeled change rate, the match up percentage increased significantly and 394 most values were higher than 100%. This is understandable because the Sargassum abundance 395 396 could increase or decrease drastically during a year. Based on MODIS observations, the highest Sargassum change rate can be > 0.12 doublings day⁻¹ while the lowest value is \sim - 0.10 doublings 397 day⁻¹. The lower matchup percentage before adding the Sargassum change rate further revealed 398 399 the important role of the biological growth/mortality term in determining the distribution patterns. 400 Since the change rates applied here are the averaged values from 2011-2015, the unmatched 401 abundance after adding the modeled change rate could be related to the inter-annual variability of 402 the Sargassum growth/mortality rate. In months when Sargassum growth rate are highly variable 403 (such as April to May), the unmatched abundance are comparatively higher as shown in Figure 7a.

 404 The majority of the tracked Sargassum particles were found inside the regions where large 405 amounts of Sargassum were observed, indicating that the Sargassum initiated in January in the 406 CA indeed contributed to the pattern formation in July. Similar to satellite observations, large 407 Sargassum accumulation in the tropics typically occurred in summer months during the forward-408 tracking (Figure 7d). The Sargassum accumulations in the tropics and CS started to dissipate 409 around September and decreased drastically in the following winter months. Considerable amount 410 of the Sargassum were transported eastward in the later months and end up within the CA during 411 the winter months.

412

Figure 7. Simulation of mean Sargassum distributions using forward-tracking from the mean 413 414 distributions in January. (a) Comparison of the matchup rate of the model result before and after 415 adding the change rate to the advection $+1\%$ wind model. (b) The simulated Sargassum distributions in July using the advection + 1% wind model. (c) The MODIS-derived mean 416 Sargassum distributions in July. (d) Similar to (b) but the Sargassum change rate was accounted 417 418 for during tracking. The higher Sargassum densities in the tracked results could be due to the limited number of particles initiated in January and smaller-scale motions were not well 419 represented. 420

421 3.4.2. Cross-region connectivity assessment

422 Both forward-tracking and backtracking were tested to investigate the regional 423 connectivity of the Sargassum across the Atlantic Ocean, with the major results summarized in 424 Figure 8.

425 For the summer blooms in July, forward tracking with the initial conditions in January 426 suggests that the majority (\sim 98%) of the *Sargassum* particles that end up in the CS in July are 427 from the CA. This is also supported by the backtracking results from July to January. Most particles 428 \sim 51%) located in the CS in July are from the CA in January. The reason that \sim 47% of the 429 Sargassum particles are from CS in July is because those particles were blocked by the Caribbean 430 islands and were unable to track back to the CA. The summer blooms in the CA can be mostly 431 traced back to the CA, indicating a strong retention in the CA region. Backtracking from July to 432 January indicated that some $(-15%)$ of the particles in CA could be originated from WA in 433 January. For the Sargassum presented in the WA in July, most of the particles did come from the 434 WA, but ~ 44% of them are from the CA area in January. The forward tracking also indicate that 435 Sargassum in the CA can lead to blooms in the WA.

The winter blooms in January are mostly located in the CA and very few Sargassum were 436 437 detected elsewhere. Backtracking from January to July indicates that most Sargassum (~77%) in 438 the CA are traced back to the CA in summer months. Small amount $(-19%)$ are linked to the WA, 439 while very weak connection is found with the NA. This is also supported by the forward tracking 440 initiated with Sargassum distributions in July.

441 All this tracking results show almost no connection of the Sargassum blooms in the tropics 442 coming from Northern regions, but the blooms can be transported from the CA or CS into the NA. 443 However, one caveat is that error accumulation could be large during such long-term tracking experiments. Still these simulations help to understand the connections of the blooms in different 444 445 regions.

(a) Forward-tracking from January to July

	CS	CA	WA	NA
CS	2.2	0.0	0.0	7.7
CA	97.8	95.9	97.8	4.7
WA	0.0	4.0	2.2	0.0
NA	0.0	0.1	0.0	86.0

(b) Backtracking from July to January

	CS	СA	WA	NA
CS	47.1	0.0	0.0	17.2
CA	51.2	84.5	44.0	10.1
WA	1.1	15.2	20.1	0.0
NA	0.6	0.1	0.0	62.7

(c) Forward-tracking from July to January

	CS	CA	WA	NA
CS	66.6	0.0	0.0	43.5
CA	34.3	99.3	94.7	8.3
WA	0.0	0.5	5.5	0.0
NA	0.0	0.2	0.0	31.0

(d) Backtracking from January to July

	CS	CA	WA	NA
CS	58.1	0,0	0.0	4.6
CA	35.5	77.4	7.5	1.0
WA	5.6	19.2	26.8	0.0
NA	0.2	0.1	0,0	87.8

446

447 Figure 8. The cross-region connectivity analyzed with forward and backward tracking from the 448 mean Sargassum distributions in January and July. (a) and (c) are the forward-tracking results 449 initiated with the Sargassum distributions in January and July. (b) and (d) are the backtracking 450 results initiated with Sargassum distributions in July and January. These percentages are relative 451 to the total Sargassum in the corresponding column region in July ((a) and (b)) or January ((c) and (d)). For example, 97.8% in (a) means that 97.8% of Sargassum located in the CS in July are from 452 the CA back in January. The percentages of Sargassum belong to the CA in January ((a) and (b)) 453 or July ((c) and (d)) are highlighted by bold borders. 454

As discussed in the connectivity analyses, the CA serves as an important region for bloom 455 456 initiation. Most of the summer blooms that occurred near the CS are originated from the CA. Here, 457 the trajectories of the Sargassum particles tracking from the CA in January are plotted in Figure 9 458 and Figure S2 to show their transport pathways. Two regions with relatively high Sargassum 459 abundance were defined (Figure S2). In April, Sargassum particles in region B (0°N - 12°N, 35°W - 15°W) haven't reached the CS while many particles from region A (9°N - 19°N, 58°W - 33°W) 460 already entered the CS area. This suggests that region A should be more related to the spring 461 blooms in the CS. In Wang and Hu [2017], a hotspot region in the CWA is identified to be 462 463 indicative of the bloom conditions in the Caribbean in the summer. Our simulations suggest that 464 the particles seeded in this region in February do not account for a significant proportion of 465 particles entering the CS (4.8% Sargassum particles in the CS in July were traced back to the hotspot region). However, as the Sargassum abundance in the hotspot is highly correlated to the 466

total Sargassum abundance in the CA in February ($R^2 = 0.88$), thus justified the good prediction 467 468 performance.

469

Figure 9. Forward tracking trajectories of the Sargassum particles initiated in January and tracked 470 forward for 6 months to July using the mean currents and winds. The trajectories are indicated by 471 the colored lines. Note that particles were initiated in most locations, with the weights determined 472 473 by the Sargassum areal density. In places with higher Sargassum densities, more particles were 474 initiated.

4. Discussions and conclusions 475

A Lagrangian particle tracking model was built in this study to investigate the Sargassum 476 distributions and their transport in the Tropical Atlantic Ocean. The analyses reveal that the 477 478 Sargassum distributions are strongly determined by the advection of the ocean currents while the surface wind impact on the Sargassum transport is more variable. The Sargassum change rate 479 480 model derived from MODIS observations emphasizes the importance of SST, nutrient concentrations, and the natural growth cycles on influencing the Sargassum biological 481 482 growth/mortality rate. In most cases, including the biological change rate increased the matchup 483 percentage of the Sargassum abundance between model outputs and satellite observations.

484 Simulation results using the mean Sargassum distributions lead to the several important 485 conclusions: 1) The majority of the *Sargassum* blooms in the CS could be linked to blooms in the 486 CA in winter months; 2) The Sargassum blooms in the CA in winter would contribute to the large 487 Sargassum accumulations in the tropics in summer; 3) The CA has shown strong retention. Most 488 Sargassum particles will stay inside the CA and initiate the blooms in the coming year depending 489 on environmental conditions; 4) Although Sargassum can be transported into the North Atlantic 490 from the CA, there is very week linkage of the Sargassum transported back to the CA from the northern areas. 491

492 The current model still suffers from several potential error sources. Firstly, the Sargassum 493 distributions used are limited by the temporal and spatial resolutions of the satellite data. As the MODIS observations are often impacted by cloud, cloud shadow, and sun glint, it is very difficult 494

495 to have a complete picture of the Sargassum distributions covering the entire tropical regions at 496 short time scales. Even the weekly products have many data gaps (http://optics.marine.usf.edu/cgi-497 bin/optics_data?roi=C_ATLANTIC¤t=1). This is understandable because the typical Daily Percentage of Valid Observations (DPVOs) in the CWA is only \sim 20% [*Wang and Hu*, 2018]. The 498 499 uncertainties of the density values may be high due to limited valid observations. On the other hand, Sargassum features can change drastically in a few days: either dissipate or sink under highly 500 turbulent environment, or aggregate near the frontal zone. Using the monthly mean composite to 501 represent the daily snapshot in the middle of that month induces uncertainties. For example, a 502 503 dense Sargassum feature may be transported in the grid at the end of the month and resulted in a strong signal in the monthly mean distributions, while there was no Sargassum until the last day 504 505 of the month. In that case, the feature would be tracked for extra half a month, inducing large errors 506 in the tracked locations. Moreover, MODIS-derived Sargassum observations are also limited by spatial scale of the features. As reported in field measurements [Butler et al., 1983; Schell et al., 507 508 2015; A N Siuda, 2011], large amounts of Sargassum are below the MODIS detection limit, which needs to be considered in the modeling. 509

Secondly, the Sargassum growth/mortality rate is not well described. To date, there is still 510 511 a lack of measurement on the Sargassum change rate under different environmental conditions. 512 As Sargassum is free-floating on the ocean surface, change rate modeling based on satellite data is hindered by the difficulty of tracking the local Sargassum change rate, let alone errors from the 513 514 satellite observations. This study utilized the satellite derived mean distributions along with the 515 environmental data from satellite or model derived results to establish a mean Sargassum change 516 rate model through identifying consistent large-scale Sargassum features. However, the environmental conditions in that large area may be highly patchy and area-averaging would 517 inevitably smooth out signals. Also, the area where the Sargassum lived (i.e., transport trajectories) 518 519 may not be constrained inside the area determined by the observed distributions. Besides that, the 520 physical transport model also need further improvement in the following aspects: 1) simulation of 521 the wind contributions; 2) initialization of *Sargassum* particles to account for the small-scale 522 movements.

523 Despite all these limitations, this study still provides a preliminary attempt to understand the Sargassum distributions and transports patterns using a Lagrangian particle model with 524 updated MODIS-derived large-scale Sargassum observations. The conclusions regarding the 525 526 pattern formation, bloom source, and regional connectivity are expected to be further investigated 527 in future studies with better satellite or field observations, better understanding of the Sargassum 528 growth/mortality rate, and improved modeling techniques.

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Appendix D:

Predicting *Sargassum* **blooms in the Caribbean Sea from MODIS observations**

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Key Points:

- · Saraassum blooms in the Caribbean Sea lag those in the Central West Atlantic as determined from MODIS 2000-2016 observations
- A forecast system is established to predict blooms and nonblooms in .
May-August in the CS by the end of February
- Higher prediction accuracy is found in the eastern CS than in the western CS

Supporting Information:

- Supporting Information S1

- · Supporting Information S2 $-$ Text S1
- Movie S1

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Predicting Sargassum blooms in the Caribbean Sea from MODIS observations

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Abstract Recurrent and significant Sargassum beaching events in the Caribbean Sea (CS) have caused serious environmental and economic problems, calling for a long-term prediction capacity of Sargassum blooms. Here we present predictions based on a hindcast of 2000-2016 observations from Moderate Resolution Imaging Spectroradiometer (MODIS), which showed Sargassum abundance in the CS and the Central West Atlantic (CWA), as well as connectivity between the two regions with time lags. This information was used to derive bloom and nonbloom probability matrices for each 1° square in the CS for the months of May-August, predicted from bloom conditions in a hotspot region in the CWA in February. A suite of standard statistical measures were used to gauge the prediction accuracy, among which the user's accuracy and kappa statistics showed high fidelity of the probability maps in predicting both blooms and nonblooms in the eastern CS with several months of lead time, with overall accuracy often exceeding 80%. The bloom probability maps from this hindcast analysis will provide early wamings to better study Sargassum blooms and prepare for beaching events near the study region. This approach may also be extendable to many other regions around the world that face similar challenges and opportunities of macroalgal blooms and beaching events.

Plain Language Summary Blooms of Sargassum seaweed appear to have increased in the tropical Atlantic and Caribbean since 2011. These blooms provide important habitats for many marine animals (fish, turtles, shrimps, crabs, etc.) to maintain a healthy marine ecosystem, but large amounts of Sargassum deposition on the beaches have caused numerous problems to the local environment, tourism industry, and economy. There is currently little information on Sargassum distribution and bloom timing, not to mention a forecast system. In this work, based on satellite measurements and statistics, a forecast system has been developed for the Caribbean Sea. From this system, Sargassum blooms in May-August in the Caribbean can be predicted by the end of February, with overall accuracy often exceeding 80% in the eastern Caribbean. The system thus provides at least several months of lead time for the local residents and management agencies to better prepare for potential beaching events. The approach has significant implications for many other regions experiencing macroalgal blooms of either Sargassum or Ulva prolifera.

1. Introduction

Since 2011, massive Sargassum beaching events have occurred in the Caribbean Islands, causing significant environmental and economic problems [Gower et al., 2013; Maurer et al., 2015]. Similar beaching events have also been reported in western Africa and northern Brazil [Oyesiku and Egunyomi, 2014; Széchy et al., 2012]. Although pelagic Sargassum provides an important ecological function in the open ocean [Council, 2002; Rooker et al., 2006; Witherington et al., 2012; Lapointe et al., 2014; Doyle and Franks, 2015], large amount of Sargassum deposition on beaches can negatively impact the local economy, ecology, and environment [Siuda et al., 2016; Hu et al., 2016]. Usually, massive Sargassum deposition on beaches has to be physically removed [Webster and Linton, 2013; Partlow and Martinez, 2015], which represents a management burden as there is often no advanced warning on the amount of Sargassum or the timing of beaching events.

These technical obstacles may be overcome through mapping Sargassum abundance in the Caribbean Sea (CS) and the Atlantic Ocean and through numerical modeling to predict Sargassum growth and transport. While recent advances in satellite remote sensing have made the former possible [Gower et al., 2006; Gower and King, 2011; Gower et al., 2013; Hu, 2009; Wang and Hu, 2016], predicting Sargassum blooms in certain locations of the CS requires a thorough understanding of Sargassum biology (e.g., growth rate), which may then be coupled with physical forcing (wind- and current-driven transport and dissipation) to model Sargassum transport and abundance. Unfortunately, this capacity is currently unavailable due to lack of

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sufficient measurement and modeling efforts. Herein, based on remotely sensed Sargassum abundance maps, we propose a practical way to predict the likelihood of blooms and nonblooms in the CS. The objective is to provide bloom probability matrices for the CS in May-August based on conditions in the Atlantic in February through hindcast of historical observations; these probability matrices will then provide early waming information by the end of February of every year in the future to assist scientific understanding and management planning (e.g., field surveys, physical removal, and tourism).

2. Data and Methods

2.1. Prediction Concept

The prediction is based on the Sargassum distribution maps covering the Central West Atlantic (CWA) and CS derived from Moderate Resolution Imaging Spectroradiometer (MODIS) observations using a recently developed method [Wang and Hu, 2016]. Briefly, MODIS data collected from 2000 to 2016 were processed to Rayleigh-corrected reflectance (Rrc), which was used to derive an Alternative Floating Algae Index (AFAI) for each 1 km pixel [Hu, 2009] that detects the red-edge reflectance of floating vegetation. An automatic feature extraction algorithm was developed to extract Sargassum features after masking clouds, cloud shadows, and other artifacts. A linear unmixing scheme was used to determine the subpixel coverage, which was then aggregated to 0.5° × 0.5° grids in each calendar month, resulting in monthly mean Sargassum area density (% cover) maps. While Figure 1 shows two sample maps for March 2014 and August 2014, respectively, more maps are presented in an animation in the supporting information, in Figure 2 for bloom years, and in Figure S2 for nonbloom years.

Sargassum blooms appear to develop first in a CWA hotspot region in February-March. Then, following the dominant currents and winds, Sargassum in the CWA is transported to the CS in later months where it can develop into a massive bloom. Based on the connectivity and time lag between blooms in the two regions, we hypothesize that blooms and nonblooms in the CS can be predicted from the CWA hotspot region.

2.2. Selection of the Hotspot Region and Bloom Threshold

A hotspot was determined from the multimonth mean using a threshold (Figure S1), where a rectangular region (0°-8°N, 45°-29°W) was selected to cover the objectively selected area. For the CS (8°-23°N, 88°-59°W), the region was divided into 1° × 1° grids to evaluate the bloom conditions in each grid.

To determine the bloom threshold for each location, mean conditions between 2000 and 2010 (i.e., "non-Sargassum years") were used as the reference. For the CWA hotspot, mean and standard deviation of Sargassum density of all February months between 2000 and 2010 were first calculated. Then, for any February in the later years of 2011-2016, if the mean Sargassum density was greater than the previously calculated mean plus 2 standard deviations, that February was considered to be a bloom (B) month, otherwise it is a nonbloom (N) month (Figure 1d). Likewise, mean and standard deviation of Sargassum density for the CS for each month of May-August were calculated separately from the 2000-2010 MODIS data. Then, for each 1° grid, if Sargassum density during a certain month in 2011-2016 was greater than its corresponding mean plus 2 standard deviations, the grid was considered to be a bloom for that month, otherwise a nonbloom (Figure 1c).

2.3. Bloom and Nonbloom Statistics and Prediction Accuracy

First, bloom and nonbloom statistics for the CS and the CWA hotspot region were established. Then, the prediction of bloom or nonbloom in the CS was carried out in a hindcast mode as follows: if there was a bloom (or nonbloom) in the CWA hotspot region in February, it was predicted that there would be a bloom (or nonbloom) in each grid of the CS in each month of May-August of the same year. Finally, the accuracy of the prediction was evaluated using the above bloom and nonbloom statistics with a suite of statistical measures.

Specifically, for each 1° grid in the CS, time series of blooms and nonblooms for each month of May-August between 2007 and 2016 were first generated using the bloom threshold of that month. An example for the month of August is shown in each row of the top left table in Figure 3 part II. Similarly, time series of blooms and nonblooms in the CWA hotspot region in the month of February were also generated using the bloom

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Figure 1. Sargassum area density (% cover) maps in (a) March 2014 and (b) August 2014 derived from MODIS observations [Wang and Hu, 2016], suggesting Sargassum transport from the CWA to the CS following dominant winds and currents (white arrow). The green box and orange box delineate the CS and CWA hotspot regions, respectively. (cand d) Sargassum density thresholds used to determine blooms and nonblooms in the 1° x 1° grids of the CS and in the CWA hotspot region, respectively. Vertical bars represent standard deviations of each month of 2000-2010 (nonbloom years). The bloom threshold was determined as the mean plus 2 standard deviations. For example, in July, if the density in any grid in the CS is $>5.2 \times 10^{-3}$ %, it is considered as a bloom in that grid; in March, if Sargassum density in the CWA hotspot is $>1.3 \times 10^{-4}$

threshold of February for the CWA hotspot region (top left table in Figure 3 part II). The month of February was selected to be the "predicting" month.

The accuracy of these predictions was evaluated using several statistical measures including the user's accuracy, producer's accuracy, overall accuracy, and kappa coefficients [Story and Congalton, 1986; Congalton, 1991]. The equations of the accuracy assessment, as well as examples for four locations in the CS, are listed in the tables of Figure 3. The overall accuracy tells the overall agreement between prediction and ground truth (i.e., observation), and it is defined as the sum of all correct predictions (diagonal elements in the tables) divided by the total number of observations. For a specific grid, X_{NB} (pink color in all tables) is the number of observations when the CWA hotspot shows nonbloom and therefore predicts nonbloom in the CS but the CS grid shows a bloom. X_{NN} (blue), X_{BN} (yellow), and X_{BB} (green) are defined in the same way. The user's accuracy of bloom prediction is defined as the number of correct bloom prediction (XBB) divided by the total number of bloom prediction ($X_{BN} + X_{RR}$). The user's accuracy of nonbloom prediction is defined as the number of correct nonbloom prediction (X_{NN}) divided by the total number of nonbloom prediction $(X_{NN} + X_{NB})$. The producer's accuracy of bloom or nonbloom prediction is defined similarly, but with the total number of observations (in the CS) instead of total number of predictions used in the denominator (Figure 3).

Kappa analysis was also preformed to all 1° grids to calculate the kappa coefficient [Cohen, 1960; Congalton, 1991], which measures the difference between the actual agreement (i.e., the overall accuracy) and the chance agreement (i.e., expected agreement). In this study, kappa coefficient measures the overall difference between the proposed prediction and a random guess. A kappa coefficient of 0 means that there is no difference between prediction and random guess. Larger kappa indicates better prediction performance. Conditional kappa, which can test the individual category agreement [Coleman, 1966; Light, 1971], was also calculated to help interpret the prediction accuracy. Conditional kappa measures the difference between prediction for a certain category (i.e., bloom or nonbloom) and random guess for that category.

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Figure 2. Monthly mean Sargassum density maps for bloom years between 2007 and 2016 (2007-2010 and 2013 are nonbloom years). Land and coastlines are masked in black and white, respectively. A value of 0.05 indicates 0.05%. The red dashed box marks the February maps used for the prediction.

3. Results

From 2007 to 2016, 5 years were classified as bloom years (2011-2016 except 2013), and 5 years were classified as nonbloom years (2007-2010, 2013) (Figure S3). Figure 4 shows the summary results of hindcast prediction accuracies for each month of May-August.

Generally, the conditional kappa and user's accuracy show consistent results in terms of overall trend and spatial patterns, but kappa-like measures are less interpretable than user's accuracy. For example, in the top left image of Figure 4 (prediction of bloom in the CS in May), the bottom right comer (near Trinidad) shows a value of 0.60 (orange color). This means that if a May bloom is predicted for this location at the end of February, the odds of a bloom developing there are 60%. Likewise, if a May bloom is not predicted, the odds of a correct prediction are >90% (second image set in Figure 4). Because the interpretation of user's accuracy for both bloom and nonbloom predictions is straightforward, the user's accuracy is recommended for future predictions.

The user's accuracy for nonbloom prediction (mostly >90%) is much higher than for bloom prediction (mostly <50%). This is because most 1° grids in the CS did not have blooms between May and August (Figure 2) regardless of the February conditions in the CWA hotspot. For this reason, for bloom predictions the producer's accuracy and overall accuracy are much higher than the user's accuracy, but for nonbloom predictions the user's accuracy is much higher than the producer's accuracy. These observations may vary between regions and months. For example, for the month of August and near the Lesser Antilles Islands, the user's accuracy of bloom prediction can reach >80%. The producer's accuracy for bloom prediction in this region is also high, suggesting that when a bloom occurs in August near the Lesser Antilles Islands, there is likely a bloom in the CWA hotspot region back in February of the same year. In general, prediction accuracy decreased in the westem CS regardless of the accuracy measures, due to a longer distance between the western CS and the bloom source (i.e., the CWA hotspot region).

From these hindcast evaluations, the following findings may be summarized for the prediction of blooms and nonblooms in the CS between May and August using conditions in the CWA hotspot region in February of the same year:

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Figure 3. Part I: Illustration of statistical measures to assess prediction accuracy. *B* represents bloom, and "N* represents nonbloom. Part II: Demonstration of the process to generate the estimated accuracy maps. Top left: bloom and nonbloom statistics in the CWA hotspot in February (top rows) and in four locations in the CS in August (bottom rows). Right: accuracy assessment when conditions in February in the CWA hotspot are used to predict conditions in each of the four 1° grids in the CS. The overall prediction accuracy in August for the entire CS is shown in the color coded map, with the four sample locations (P1-P4) annotated.

- 1. Predicting a nonbloom is much more reliable than predicting a bloom when measured with the user's accuracy.
- 2. There is a large spatial gradient in the user's accuracy map in bloom predictions, where accuracy in the eastem CS is significantly higher than in the westem CS.
- 3. A similar spatial gradient exists in the overall accuracy map for both bloom and nonbloom predictions, but overall accuracy for the entire CS is much higher than user's accuracy for just bloom prediction.
- 4. In all predictions, most 1° grids showed kappa coefficient and conditional kappa significantly higher than 0.0, indicating that these predictions have significantly higher success rates than random guesses.

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Figure 4. Estimated hindcast prediction accuracy of blooms and nonblooms in the CS between May and August of 2007-2016, based on the bloom conditions in the CWA hotspot region (Figure 1a) in February. Further interpretations of these maps can be found in the text.

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5. The accuracy maps shown in Figure 4 may be used as guides for future predictions of bloom and nonbloom conditions in the CS between May and August, where the predictions can be made at the end of February of the same year.

4. Discussion

4.1. Coincidence or Physics Driven

In nature, many phenomena can be highly correlated without a causal effect. The prediction above is based on the fact that if a bloom occurs in one place (CWA), it occurs at a later date in another place (CS), and the same is true for nonbloom. Then, is it simply a coincidence?

The MODIS observations, as shown in the GIF animation in the supporting information, suggest that this correlation is beyond coincidence but driven by physics. Specifically, Sargassum in the CS did not initiate locally but from the CWA following the prevailing winds and currents. This observation is supported by the back-tracking results through ocean modeling [Doyle and Franks, 2015; Franks et al., 2011, 2014, 2016; Johnson et al., 2012]. Therefore, the prediction is supported by physics, even though the method is based on statistics.

Because of this, the method provides a simple yet effective way to predict Sargassum bloom occurrence in the CS with relatively high accuracy, especially in the windward Lesser Antilles Islands. For a nonbloom prediction, the prediction accuracy is nearly 100% for most locations in the CS. This is because even during bloom years most waters still have low Sargassum density. Overall, a nonbloom prediction is more reliable than a bloom prediction in the CS, while the accuracy of a bloom prediction for most windward Lesser Antilles islands can reach >80% in August.

4.2. Prediction Sensitivity

In this work data between 2007 and 2016 were used to estimate prediction accuracy because the numbers of bloom and nonbloom years are balanced during this period. If this period was extended to all MODIS years before 2007, the user's accuracy for bloom prediction would not be affected (Figure S4) because there was no bloom year before 2007. However, because of the extra nonbloom years included, the producer's accuracy for a nonbloom prediction increased significantly, while the user's accuracy for a nonbloom prediction only increased slightly (it is already near 100%). For the same reason, the overall accuracy and kappa coefficient both increased due to the increased number of successful nonbloom predictions. A test was conducted to see whether the month of January-April could be used as the prediction months. Table S1 shows that except for January, all months showed identical bloom conditions in the CWA hotspot, leading to identical prediction accuracy. Therefore, the month of February was determined to be the best prediction month, since it can provide at least 2 months of lead time for local management agencies in the Caribbean.

The work presented here used a binary classification of a bloom or a nonbloom scenario. In reality, blooms will vary in size and intensity. When blooms were further divided into small, medium, and severe blooms according to their intensity, the overall prediction accuracy was lower (Figure S5). However, for a local researcher or manager, knowledge of the bloom/nonbloom probability may be more important than knowledge of the bloom intensity. Therefore, the focus of this study is on the binary classification.

4.3. Applications and Potential Limitations

Although the statistics-based prediction is supported by physics, because the forcing terms (winds, currents, and Sargassum growth rate [Webster and Linton, 2013; Carpenter and Cox, 1974; Lapointe, 1996; Lapointe et al., 2014; Ardron et al., 2011; Brooks, 2016; Maréchal et al., 2017]) are not explicitly included in the prediction, the prediction may only be applicable to future years when these forcing terms are similar to the hindcast years used here. The fundamental question is as follows: are the years in this study "normal" years so the prediction can be applied to future normal years?

Time series of the area-averaged surface winds and currents from Windsat and current data from Ocean Surface Current Analyses Real-time (OSCAR), respectively, are plotted in supporting information Figure S6. No significant changes have been observed since 2011 when the first massive Sargassum bloom event occurred in the CS. Thus, if future years show winds and currents encompassed by those shown here, the prediction should be applicable.

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However, the prediction is not on beaching events but on bloom conditions in the CS. It is unknown whether the predictions correlate well with spatial-temporal distributions of beaching events in the CS because this information is not readily available. An online search using the keywords "Sargassum," "Caribbean," and "Inundation" resulted in 5 news reports in 2011, 2 in 2012, 0 in 2013, 10 in 2014, 28 in 2015, and 2 in 2016, which qualitatively agree with the interannual changes in the observed bloom conditions in the CS. In reality, whether or not a bloom will end up on beaches depends on local winds and currents, which can only be studied through high-resolution modeling or a combination of nearshore daily observations and currents/winds. For example, the Sargassum Early Advisory System [Webster and Linton, 2013] used periodic Landsat observations for short-term predictions of potential beaching events, while Maréchal et al. [2017] used MODIS daily imagery for the same predictions. Nevertheless, as Sargassum blooms are unlikely to diminish in the coming years, the simple forecast system developed here will provide timely information to the Caribbean residents and management agencies on the potentials of Sargassum blooms with several months of lead time. Decision makers can benefit from this prediction in several aspects, including improved planning for cleanup, commercial use, and tourism [Hu et al., 2016]. For example, at the time of this writing, a Sargassum bloom was found in the CWA hotspot region in February 2017; thus, we predict blooms in the eastern CS in summer 2017. The accuracy of this prediction will be assessed during summer 2017, while the prediction will be sent to interested parties (e.g., NOAA CoastWatch Caribbean and Gulf of Mexico node, Caribbean Coastal Ocean Observing System) through e-mails to provide early alerts.

4.4. Broad Impacts

The study region included the CS and CWA, yet both Ulva (a type of green macroalgae) and Sargassum macroalgae blooms appear to have increased in recent years all around the world [Smetacek and Zingone, 2013; Oi et al., 2016; Wana and Hu, 2016]. These include those in the Yellow Sea and East China Sea as well as waters off West Africa and north Brazil. Once time series of bloom characteristics and cross-region connectivity are established, the approach developed here could be extended to those regions. The forecasting capacity not only provides early warning to management agencies but also has significant implications for studies of ocean biogeochemistry and ocean ecology as researchers now have at least several months of lead time to prepare for coordinated cruise surveys. Furthermore, Sargassum can also be used to extract various products from animal food, biofuel, to plastics, and the U.S. Department of Energy is interested in improved use of Sargassum to make these products (https://vimeo.com/193881420). One of the potential challenges of such endeavors is to find the Sargassum "hotspots" for harvesting at the right time and right location, and the work presented here can help to address this challenge. Indeed, Sargassum blooms in recent years have provided both challenges and opportunities to many research and environmental groups [Hu et al., 2016]. and a forecasting system represents one significant step toward addressing these challenges.

5. Conclusion

A preliminary forecast system has been developed to predict Sargassum blooms in the Caribbean Sea in May-August from bloom conditions in a hotspot region in the Central West Atlantic in February. This is through hindcast analysis of the Sargassum distributions derived from MODIS observations between 2000 and 2016 using a recently developed algorithm. Although the prediction is from statistics of bloom and nonbloom occurrence, it is supported by the physical mechanism to drive Sargassum transport and by biological factors to drive Sargassum growth. Accuracy assessment using historical MODIS observations showed that bloom occurrence in July and August near most of the Lesser Antilles islands can be accurately predicted (up to 80%) at the end of February. Prediction of nonbloom occurrence in most of the CS can be up to 100%. While the data record used to test the prediction is rather short (2000-2016, with only five bloom years in between) and the prediction requires similar environmental forcing factors in future years as in the past years, the forecast system provides a decision support tool to help prepare and make research and management plans with several months of lead time.

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Appendix E:

On the continuity of quantifying floating algae of the Central West Atlantic between MODIS and VIIRS

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On the continuity of quantifying floating algae of the Central West Atlantic between MODIS and VIIRS

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ARSTRACT

Studying abundance and distributions of floating macroalgae such as pelagic Sargassum calls for long-term continuous and consistent observations from multiple satellite sensors. Previous studies mainly relied on observations from the Moderate Resolution Imaging Spectroradiometer (MODIS) and the Medium Resolution Imaging Spectrometer (MERIS). As a follow-on sensor, the Visible Infrared Imager Radiometer Suite (VIIRS) also has the appropriate spectral bands to detect and quantify floating macroalgae. Based on previous works on MODIS, this study presents an improved procedure to extract floating algae pixels from VIIRS Alternative Floating Algae Index (AFAI) imagery, with image filtering used to suppress noise and adjusted thresholds used to mask sun glint, douds, and cloud shadows. The overall extraction accuracy is about 85%. Simultaneous daily observations from MODIS and VIIRS over the Central West Atlantic (CWA) show consistent spatial patterns, but VIIRS estimations of the algae coverage (in km^2) are consistently lower than MODIS (around $-$ 19% mean relative difference or MRD), possibly due to lower sensitivity of the VIIRS near-infrared (NIR) bands than the corresponding MODIS bands. Similarly, at monthly scale VIIRS also shows lower coverage than MODIS, and their difference (around - 29% MRD) is larger than the difference between MODIS-Aqua and MODIS-Terra estimates (around - 14% MRD). Despite these differences, the spatial and temporal patterns between VIIRS and MODIS observed algae distributions match very well at all spatial and temporal scales. These results suggest that VIIRS can provide continuous and consistent observations of floating algae distributions and abundance from MODIS as long as their differences are accounted for, thus assuring continuity in the future. Furthermore, once Sargassum biomass per unit Sargassum area is determined from field measurements, conversion of these area estimates to Sargassum biomass is straightforward.

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1. Introduction

Floating macroalgae of pelagic Sargassum in the Central West Atlantic (CWA) have shown an increasing trend and drastic inter-annual variability in recent years (Gower and King 2011; Gower, Young, and King 2013; Wang and Hu 2016; Wang and Hu 2017).

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Supplemental data for this article can be accessed here.

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During bloom seasons (spring and summer), massive Sargassum beaching events in the Caribbean countries have been frequently reported, which caused significant problems to local tourism, fishery, ecology, and environment (Hu et al. 2016; Webster and Linton 2013; Maurer, De Neef, and Stapleton 2015). Similarly, in other oceans, an increasing trend of other types of floating macroalgae has also been reported (Smetacek and Zingone 2013), such as *Ulva prolifera* (a type of green macroalgae) in the Yellow Sea (Qi et al. 2016; Hu, Hu, and He 2017). Synoptic and frequent observations from satellite ocean color sensors provide effective means to monitor, assess, and understand changes of floating macroalgae at large spatial and temporal scales.

Currently, remote detection of floating macroalgae mainly relies on the enhanced reflectance in the near-infrared (NIR) spectral bands (the vegetation 'red-edge') (Gower et al. 2006). The red-edge reflectance allows for the development and application of several indexes, including the Maximum Chlorophyll Index (MCI) for the Medium Resolution Imaging Spectrometer (MERIS; 2002-2012) and the Floating Algae Index (FAI) and Alternative FAI (AFAI) for the Moderate Resolution Imaging Spectroradiometer (MODIS; Terra: 2000-present, Aqua: 2002-present) (Gower et al. 2006; Hu 2009; Wang and Hu 2016). However, MERIS stopped functioning in 2012, and both MODIS sensors are aging with their designed 5 year mission life, calling for continuous observations from other similar sensors. The Visible Infrared Imager Radiometer Suite (VIIRS; 2011-present) on the Suomi National Polar-orbiting Partnership satellite is also equipped with spectral bands similar to those of MODIS, thus could be used to generate VIIRS AFAI images. Such images have been developed and used in the Sargassum Watch System (SaWS) for near real-time monitoring of floating macroalgae (Hu et al. 2016). With proper masking of clouds, cloud shadows, and sun glint, floating macroalgae appear as elongated slicks in the AFAI imagery, thus can be easily visualized even by a layperson (Wang and Hu 2016).

However, beyond near real-time monitoring, assessment of long-term trends requires accurate feature extraction and data-binning strategies as well as consistent data products from multiple sensors, including the most recent VIIRS. Gower and King (2011) made the first attempt to map and quantify Sargassum abundance using statistical analyses of MERIS images (Gower and King 2011; Gower, Young, and King 2013), followed by a new mapping scheme developed for MODIS AFAI imagery (Wang and Hu 2016; 2017). However, to date although VIIRS AFAI imagery has already been used for visual inspection in the near real-time SaWS (Hu et al. 2016), automatic algae detection is still hindered by noise contamination (see Figure 1, Figure S1, and Figure S2) and false positive detection near clouds and cloud shadows. Furthermore, it is unclear whether VIIRS could provide consistent observations of algae distributions and abundance to continue the MODIS time series in case both MODIS instruments stop functioning, although such a continuity has been demonstrated for other ocean color data products such as water clarity (Barnes and Hu 2015). Therefore, the objectives of this study are:

- . To develop an automatic algae extraction procedure to apply to VIIRS AFAI imagery;
- To compare VIIRS and MODIS performance on their ability to detect and quantify floating macroalgae using concurrent and collocated imagery;

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Figure 1. (a) A VIIRS AFAI image showing floating algae slicks outlined in the red box. The yellow boxes highlight the region with striping and other noise due to low SNRs (the brighter noise pixels are marked in red). (b) $-$ (c): Quasi-simultaneous (within 30 minutes) VIIRS AFAI and MODIS AFAI images from the same locations outlined by the red box in (a). (d) – (e): Extracted algae pixels (marked in red) on VIIRS and MODIS AFAI images. Note that MODIS images also contain some level of striping artifacts although it is not obvious in this example. The dashed ellipses highlight that more algae pixels are detected in MODIS image than in VIIRS image. In regions where both sensors have valid observations, the number of algae pixels extracted from VIIRS is 2536, and 4568 from MODIS. Such a large difference is largely removed after a pixel unmixing scheme is applied to estimate algae coverage (in km²).

. To quantify differences between VIIRS- and MODIS-derived long-term statistics in algae abundance and observing capacity.

2. Data and methods

MODIS and VIIRS Level-0 data for the entire year of 2016 with sufficient coverage (> 25%) over the CWA (0-22°N, 63-38°W) were obtained from the U.S. National Aeronautics and Space Administration (NASA) Goddard Space Flight Center (Ocean Color 2017), and processed to generate Rayleigh-corrected reflectance (R_{rc}) for each spectral band using the software package SeaWiFS Data Analysis System (SeaDAS) (version 7.2). Level-0 data instead of Level-1 data were used here because for a large region such as the CWA, multiple data granules may need to be merged together, and it is straightforward to merge Level-0 granules before processing. The R_{rc} data were then mapped at 1 km spatial resolution in the equidistant rectangular projection. A total of 1148 MODIS 5 minute granules (581 from MODIS-Aqua (MODISA) and 567 from MODIS-Terra (MODIST)) and 782 VIIRS 6 minute granules were downloaded and processed to R_{rc} data, which were then used to calculate AFAI for each pixel:

 \mathbf{r}

$$
AFAI = R_{rc,NIR} - R'_{rc,NIR}
$$

$$
R'_{rc,NIR} = R_{rc,RED} + (R_{rc,LNIR} - R_{rc,RED})(\lambda_{NIR} - \lambda_{RED})/(\lambda_{LNIR} - \lambda_{RED})
$$
(1)

The subscripts RED, NIR, and LNIR (long NIR wavelength) represent the corresponding spectral bands. For MODIS AFAI, $\lambda_{\text{RED}} = 667$ nm, $\lambda_{\text{NIR}} = 748$ nm, and $\lambda_{\text{LNIR}} = 869$ nm. For VIIRS AFAI, three similar bands were used ($\lambda_{\text{RED}} = 671$ nm, $\lambda_{\text{NIR}} = 745$ nm, and $\lambda_{\text{LNR}} =$ 862nm). AFAI was chosen over the original FAI for better cloud masking performance (Wang and Hu 2016).

Figure 1 illustrates an example of VIIRS AFAI imagery showing floating algae pixels as bright features outlined in the red box. Compared to the quasi-simultaneous MODIS AFAI image, the VIIRS AFAI image shows more noise contamination due to lower signalto-noise ratios (SNRs) of VIIRS. Such noise represent a major hurdle in automatic algae extraction. Therefore, noise reduction should be a critical preprocessing step to reduce false positive detection. After noise reduction, algae extraction from VIIRS AFAI imagery can follow the same workflow as that applied to MODIS AFAI imagery, including cloud and cloud shadow masking and removal of background variations (Wang and Hu 2016). Similar to MODIS processing, such a workflow was realized through a two-step procedure based on 4th order polynomial surface fitting and median filtering (Wang and Hu 2016). The thresholds for cloud and cloud shadow masking, however, were adjusted specifically for VIIRS (see Section 2.2).

2.1. Noise reduction

There are two types of noise in the VIIRS AFAI imagery. One is the striping artifacts due to imperfect detector calibration and different radiometric responses of the detectors of the whiskbroom scanner (Cao et al. 2014). To facilitate algae extraction, a recently developed destriping algorithm (Mikelsons et al. 2014) was tested on the VIIRS AFAI imagery (before map projection), with performance demonstrated in Figure S1. In most regions, the destriping algorithm effectively reduced the striping artifacts. However, some algae slicks aligned in parallel to the striping artifacts were also attenuated because they were treated as noise. On the other hand, although these stripes are noticeable in the VIIRS AFAI imagery, algae signals are often stronger and therefore can be well discriminated in both visual interpretation and threshold-based segmentation. Based on these considerations, destriping was not applied to VIIRS AFAI imagery.

The other type of noise often shows up near the scan edge (see Figure 1(a) and Figure S2). Unlike striping artifacts, these noise pixels are brighter than the nearby water pixels, thus must be removed to minimize false positive detection. Here, an 11×11 Gaussian filter was applied to the AFAI imagery to reduce such noise contamination. Several commonly used noise reduction methods were tested and compared in Figure S2. Among those, Gaussian filtering shows satisfactory performance as it can preserve most real features while reducing noise. However, because image filtering inevitably attenuates signals, algae extraction results from the filtered imagery were only used to determine a location buffer where real features (i.e., algae pixels) were extracted from the original image within the buffer, thus avoiding the noise-induced false positive detection outside the buffer. The buffer was determined from an 11 \times 11 pixel dilation over the extracted algae pixels from the Gaussian filtered imagery. The workflow of the extraction process is summarized in Figure S3. The window size of 11 \times 11 pixels used in the filtering was a compromise between reducing false positive detection and stabilizing false negative detection (Figure S4). Although signal

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attenuation can still occur, the final estimates of algae coverages are not strongly affected because most algae features are still detectable and feature extraction is conducted over the original images. This procedure proves to be effective in preserving true algae pixels while reducing false positives (Figure S2).

2.2. Selection of thresholds to mask sun glint, clouds, and cloud shadows and to extract algae pixels

In the presence of sun glint, clouds, or cloud shadows, no information can be retrieved from the contaminated pixels, and these pixels were masked and treated as no observations. Because both sun glint and clouds have higher reflectance than nearby water in all spectra bands, these pixels were masked using a set of criteria as defined in Equation (2). This threshold-based masking method is the same as that used for MODIS AFAI imagery (Wang and Hu 2016), but with updated thresholds determined through trials and errors.

$$
R_{\rm rc}(671) \geq 0.05, \text{ or } R_{\rm rc}(745) \geq 0.05, \text{ or } R_{\rm rc}(862) \geq 0.05 \tag{2}
$$

Although cloud shadow pixels show lower R_{rc} values than nearby water pixels in all spectral bands (Wang and 2016), the decreases in reflectance in different bands are not proportional, resulting in higher AFAI values than nearby water pixels, thus causing false positive detection. To mask these pixels, a local total R_{rc} (LTR), defined as the total R_{rc} in the 410 nm and 443 nm bands, was used:

$$
LTR = R_{rc}(410) + R_{rc}(443)
$$
 (3)

Pixels with LTR lower than the reference values (REF_{LTR}) by a threshold T_c (see Equation (4)) were masked and treated as no observations. REFLTR was calculated as the mean LTR of the surrounding 31×31 pixels.

$$
LTR - REF_{LTR} < T_c \tag{4}
$$

To better preserve the algae features while masking cloud shadow pixels, histograms of manually selected cloud shadow pixels and floating algae pixels were used to determine the cloud shadow threshold T_c (Figure 2(a,c)). T_c was determined to be $-8.0 10^{-3}$.

After correcting the large-scale gradient across the image, algae pixels were extracted using a global threshold T_0 . Following the same steps as those applied to MODIS images (Wang and Hu 2016), T_0 was determined to be 2.0 10⁻⁴. As demonstrated in Figure 2(b, d), over 96.0% of the adjacent water pixels are excluded while about 88.0% of the algae pixels are preserved after the global extraction threshold was applied.

2.3. Algae pixel unmixing

In nature, floating algae can rarely occupy the entire 1 km pixel (i.e., 100.0% coverage). A linear unmixing scheme was used to quantify the fractional coverage within each pixel through a global upper bound (representing 100.0% algae coverage) and a global lower bound (representing 0.0% algae coverage).

The lower bound was inferred from the nearby water pixels adjacent to the floating algae features, estimated to be $-$ 4.4 10⁻⁴. The upper bound was determined from field-

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Figure 2. Cumulative and normalized frequency distributions of algae pixels, cloud shadow pixels, and adjacent ocean pixels in several regions of interest. (a) and (c) show the distributions of the $(LTR - REF_{LTR})$ values of algae pixels and cloud shadow pixels. (b) and (d) show the distributions of the (AFAI - REF_{AFAI}) values of algae pixels and adjacent ocean pixels. The adjacent pixels were selected by dilating 5 pixels into the nearest algae-free pixels.

measured Sargassum reflectance after propagating to top-of-atmosphere using radiative transfer simulations (Wang and Hu 2016). The simulations applied the relative spectral response (RSR) of VIIRS to field hyperspectral data, with the upper bound determined to be 4.6 10^{-2} (see Table S1 for details).

After linear unmixing of the extracted algae pixels with the selected upper and lower bounds, algae coverage maps were obtained, where pixels were assigned a value of 0.0% for algae-free water pixels and between 0.0% and 100.0% for algae-containing pixels. Pixels with no observations due to clouds, cloud shadows, land, land adjacent area, sun glint, or no satellite coverage were all masked as invalid values.

2.4. Cross-sensor comparisons

VIIRS and MODIS data products were compared at different time scales, from snapshot imagery to composite imagery. Following Wang and Hu (2016), the entire study region was divided into $0.5^{\circ} \times 0.5^{\circ}$ grids, where fractional algae coverage from the original high-resolution images was aggregated into each grid to obtain mean algae density (% cover) for a given time interval (month, season, or year). The seasons were defined as boreal meteorological seasons. In the comparisons, unless Aqua or Terra is explicitly stated, the term 'MODIS' represents the combined observations from both Aqua and Terra.

The cross-sensor difference was assessed using the mean relative difference (MRD) (Barnes and Hu 2015) between the two measurements:

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$$
MRD = \frac{1}{N} \sum_{i=1}^{N} \frac{y_i - x_i}{x_i} 100\% \tag{5}
$$

where y_i and x_i stand for the measurement of algae coverage or number of valid observations. The comparison was conducted between MODIS (individual sensors or combined) and VIIRS where x_i represents the measurements from MODIS, and also between the individual MODIS sensors (MODIST and MODISA) where x_i represents the measurements from MODISA.

To evaluate whether differences in algae coverage statistics might be due to differences in the number of valid observations, the daily percentage valid observations (DPVOs) (Feng and Hu 2016) at any 1 km location from a given 0.5° grid was calculated as:

$$
DPVO = \frac{N_v}{3025 \ d} 100\% \tag{6}
$$

where N_v is the number of valid 1 km observations in each grid during a time interval and d is the number of days during the time interval, while $55 \times 55 = 3025$ is maximum possible valid observations in the same grid from a given day (0.5°Corresponds to about 55 1 km pixels). For example, a DPVO of 15.0% indicates that the probability of having a valid observation at any 1 km location within the grid in a given day in that time interval is 15.0%.

3. Results

3.1. Algae extraction accuracy

Accurate extraction of algae-containing pixels is a prerequisite for long-term statistical analyses. To evaluate the extraction performance, 12 representative VIIRS AFAI images (6 from February and 6 from August 2016) were selected. The 'ground-truth' data of true algae pixels were selected using an the Interactive Data Language (IDL) graphical user interface (GUI) designed to extract image features with morphological constraints guided by visual interpretations (Wang and Hu 2015). Results from the accuracy assessments are summarized in Table 1. For the area coverage estimated using unweighted algae pixels, false positive and false negative rates (Chinchor and Sundheim 1993) are 28.9% and 19.6%, respectively. After weighting each pixel using the fractional (percentage) coverage, both rates are reduced significantly, with an overall extraction accuracy of 85.5%, comparable to the algae extraction accuracy from MODIS (Wang and Hu 2016). The reason why a better extraction accuracy was obtained after weighting each algae-

Table 1. Accuracy assessment of delineation of algae-containing pixels from 12 VIIRS AFAI images in February and August 2016.

		False positive (%) False negative (%) Precision (%) Recall (%) F score (%)			
Area coverage using unweighted algae pixels (AUP)	28.9	19.6	73.6	80.4	76.8
Area coverage using weighted algae pixels (AWP)	13.4	10.6	86.3	84.6	85.5

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containing pixel (for its fractional coverage) is because the false-detection (both false positive and false negative) pixels generally have lower weights (fractional coverages) than those of the correctly extracted ones. For example, a pixel with 10.0% algae coverage is counted for 1.0 if weighting is not applied, but counted for 0.1 if weighting is applied. This suggests that the proposed algae extraction procedure for VIIRS is at least as accurate as that for MODIS, thus allowing for the comparison of VIIRS and MODIS on their capacity for quantifying algae coverage at both image level and long-term scales.

3.2. Comparison of quasi-simultaneous observations between MODIS and VIIRS

Before comparing algae coverage statistics derived from MODIS and VIIRS, it is important to understand whether they lead to the same algae coverages for simultaneous observations. To address this question, 98 image pairs of quasi-simultaneous measurements (within 30 minutes) in 2016 were selected. It is assumed that within 30 minutes algae features do not move or change significantly, thus allowing for a direct comparison. For the same reason, the comparison was performed from the common pixels where both MODIS and VIIRS showed valid observations.

Although there is a relatively large discrepancy between MODIS- and VIIRS-derived number of algae pixels (Figure 3(a)), after pixel weighting they show consistent algae coverages (Figure 3(b)). This is because that many of the undetected pixels in the VIIRS imagery have low weights (i.e., low sub-pixel fractional coverages), thus having relatively small effects on the area estimates. Linear regression between MODIS- and VIIRS-derived algae area coverages in Figure 3(b) shows a significant positive relationship (the coefficient of determination (R^2) = 0.95; F = 1211.1; p \ll 0.001). The slope of the linear regression is 0.94, suggesting that their coverage estimates only differ by a few percent for most images. The negative intercept (-2.27 km^2) (i.e., VIIRS is generally lower than MODIS) may be a result of undetected weak algae slicks in VIIRS AFAI imagery (Figure 1).

Two outlier clusters that depart from the main trend are worth mentioning here. One is for pixels that are marked as algae on VIIRS but not on MODIS AFAI imagery (blue

Figure 3. Quasi-simultaneous MODIS and VIIRS measurements over the same observed pixels in the CWA showing numbers of derived algae pixels in (a) and algae area coverages in (b) . The dashed lines are the 1:1 reference lines and the red solid lines are the linear regression lines. The outliers marked in the blue and red circles are explained in the text.

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dashed circle in Figure 3(b)). Visual inspection shows that this is due to false positive detection from residual cloud shadow pixels in the VIIRS imagery. The other is for pixels showing higher algae coverage from VIIRS than from MODIS (red dashed circle in Figure 3(b)). Visual inspection shows that this is due to the low detectability on the scan edge, where many algae features visible in the VIIRS imagery are located on the MODIS scan edge, thus too weak to be detected in the MODIS AFAI imagery. Nevertheless, the comparison shows a MRD of $-18.7%$ in the algae area estimates between MODIS and VIIRS, indicating relative consistency and compatibility between the two datasets. The lower algae detectability from VIIRS imagery is possibly due to its lower SNRs than MODIS, but it would not significantly impact the long-term statistics of algae coverage.

3.3. Comparison of long-term statistics

Because pixels near scan edge may be missed in algae extraction, they were masked before statistical calculations. Pixels with satellite view zenith angle (VZA) $> 60^{\circ}$ were regarded as having no observations and excluded from the calculations. The VZA of 60° is the standard threshold used in the Level-2 processing to flag data with large viewing angles, and pixels with VZA above this threshold are not used in the global composites of data products (Patt et al. 2003). The fraction of the observations meeting this masking criterion is 10.6% for MODIS and 29.3% for VIIRS in 2016.

Overall, statistics of mean area coverages from MODIS and VIIRS long-term measurements show larger differences than from quasi-simultaneous images, with lower coverages derived from VIIRS. The difference was quantified with the MRD between the total area coverage (in km^2) for each time interval. The MRD was determined to be -28.7%, - 30.4%, and - 24.9% for monthly, seasonal, and annual mean coverages between the two measurements. While detailed comparison results for monthly and seasonal mean algae coverages are summarized in Figure S5, Table S2, and Table S3, Figure 4 compares monthly mean algae coverage from MODISA, MODIST, MODIS (i.e., MODISA and MODIST combined), and VIIRS measurements, all showing significant positive correlations. MODIST shows lower estimations than MODISA but higher estimations than VIIRS. The MRD between MODIST and VIIRS measurements (-23.4%) is lower than that between the two MODIS measurements (-14.1%).

The difference between VIIRS and MODIS estimates appears to come from an offset of 30-50 km². Therefore, in summer months where algae coverage is much higher than in winter months, the relative difference can be much smaller. For example: in December 2016, VIIRS-derived algae coverage is only 33.0% of the MODIS estimate, but in July 2016 VIIRS shows 89.0% of the MODIS estimate (Figure 4(a), Table S2). Likewise, annual mean coverage in 2016 derived from VIIRS is 132 km² or about 75.0% of the MODIS estimate (176 km^2) .

The monthly and seasonal mean algae distribution maps are provided in Figure S6 and Figure 5, respectively. Although the algae abundance (in area intensity) derived from VIIRS is consistently lower than that from MODIS, the spatial patterns and their temporal variations are similar. Blooms first appear in the tropical Atlantic in spring, and are then transported to the Caribbean Sea in summer following the prevailing winds and currents (Wang and Hu 2017).

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Figure 4. (a) - (d): Monthly mean algae coverage over the CWA during 2016 determined from MODIST, MODISA, MODIS (i.e., MODIST and MODISA combined), and VIIRS. The MRD marked on (d) is between MODISA and MODIST. (e) - (h): Linear fit of the monthly mean algae coverages from different measurements. The dashed lines are the 1:1 reference lines and the red solid lines are the linear regression lines.

Figure 5. Seasonal mean algae area coverages in 2016 derived from MODIS (a), VIIRS (b), MODISA (c), and MODIST (d). Land and coastlines are masked in black and white, respectively. The color indicates % algae coverage in each $0.5^{\circ} \times 0.5^{\circ}$ grid.

These results from monthly, seasonal, and annual statistics suggest that VIIRS can provide estimates consistent to those from MODIS in both the spatial patterns and temporal variations. Furthermore, after applying the corresponding scaling and offset factors based on the relationships derived in Figure 4 and Figure S5, VIIRS observations may provide a consistent time series in the future to continue the MODIS observations, assuring cross-sensor continuity.

4. Discussions

In this study as well as in Wang and Hu (2016), Sargassum abundance is estimated as area density (% cover) in each grid cell and area coverage $(km²)$ for the study region. Once biomass per Sargassum area is determined from field measurements, conversion of these estimates to biomass per grid cell or total biomass for the area is straightforward. For example, assuming 2 kg Sargassum wet biomass per m² (Mizuno et al. 2014), a 0.1% area density corresponds to 2 g m⁻² wet biomass or 2000 kg km⁻² biomass. Such

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determined biomass per area or total biomass in a specific region will provide critical information to understand the potential environmental and ecological impacts and to guide management efforts. The question is what are the uncertainties in these estimates.

In addition to the algae extraction procedure itself, several inherent factors of the satellite sensors may lead to various uncertainties in the extraction results and in the area estimates. These factors include sensor SNRs, pixel spatial resolutions, and data availability.

4.1. Sensor SNRs

Using simulations and Sargassum spectra measured in the field, Hu et al. (2015) estimated that for a 200:1 SNR in the NIR wavelengths, the lower detection limit of sub-pixel algae coverage is about 1.0% of the pixel size (Hu et al. 2015). This simulation result is indirectly confirmed by MODIS statistics in Wang and Hu (2016), where the lower detection limit is about 0.2% of the MODIS pixel size because MODIS SNRs in the NIR wavelengths are about 1000:1 (Hu et al. 2012), 5 times of the SNRs used in the simulation. SNRs of VIIRS NIR bands under typical radiance inputs of ocean environments have not been reported, but our unpublished data using the same SNR estimation procedure indicate that VIIRS SNRs in the NIR bands are about 500:1 regardless of the aggregation zone along the scan direction. The lower SNRs of VIIRS thus may explain, at least partially, why VIIRS-based algae area estimates are generally lower than those from MODIS (Figures 3 and 4).

4.2. Pixel resolution

Once SNRs are fixed, the lower detection limit of sub-pixel algae coverage in terms of % pixel size is also fixed. Then, the lower detection limit in terms of algae area (in km²) is proportional to pixel size, which always increases from scan center to scan edge for a polar-orbiting scanner such as MODIS and VIIRS.

For MODIS, Figure S7 (a) suggests that pixel size increases rapidly after VZA $>$ 45 $^{\circ}$ (basically a cosine effect, about 6 times on scan edge over scan center). For VIIRS, the pixel growth rate is much constrained by aggregating sequential detector read-outs and the pixel size is approximately 2 times on scan edge over scan center (Schueler, Lee, and Miller 2013). To determine the impact of pixel size (or the spatial sampling size) on algae area estimates, we compared the percent of undetected Sargassum coverage using VIIRS-detected Sargassum in 2016, with results summarized in Table S4.

With a SNR of 1000:1 for MODIS, the detection limit is 0.2% of pixel size according to image statistics (Wang and Hu 2016). Then, for pixels near scan center, the detection limit is about 0.002 km². For pixels near scan edge (VZA $>$ 55°), the detection limit is 0.012 km².

For this change of pixel size from scan center to scan edge, if all detected Sargassum in 2016 were put in pixels near scan edge, 44.4% of detected Sargassum would be undetected. However, only 11.0% of satellite data are located near scan edge (VZA > 55°), so in reality only 11.0% \times 44.4% = 4.9% of all Sargassum will be undetected (last row of Table S4). Likewise, only 32.7% \times 0.9% = 0.3% of all Sargassum will be undetected from

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pixels between scan center and scan edge. For VIIRS, these numbers will be even smaller because near scan edge VIIRS pixel size is much smaller than MODIS.

Clearly, although pixel size impacts the detectability (i.e., larger pixel size leads to higher detection limit in terms of km²) of Sargassum within a pixel, the impacts on the overall area estimates are rather small (about 5.0%), lower than the uncertainties from the algae extraction procedure itself (around 14.5%, see Table 1). The impacts on VIIRS (from scan center to scan edge) are smaller than on MODIS, and they are both within the 5.0% uncertainty bounds, thus making negligible differences when cross-sensor consistency is the goal for observing continuity.

4.3. Data availability and valid observations

In addition to sensor sensitivity and pixel size, statistics of algae coverage can also be affected by data availability or number of valid observations. Insufficient number of valid observations could lead to statistical biases. For an extreme example, if during a month there is only one valid observation in the study region, if this observation is an algae pixel then the algae coverage is assumed to be 100.0% for the entire region in that month. Likewise, if this observation is an algae-free water pixel, then the algae coverage is assumed to be 0.0% for the entire region in that month. Obviously, neither is realistic due to lack of valid observations. To assess whether some of the differences in the algae statistics could be due to differences in their data availability, seasonal maps of DPVOs for MODIS and VIIRS are compared in Figure 6, and the area-averaged DPVOs are summarized in Figure 7.

During all seasons of 2016, a combination of MODISA and MODIST (i.e., MODIS) shows more valid observations than VIIRS or individual MODIS sensors, especially in the north of the CWA region. At lower latitudes, both MODIS and VIIRS show fewer valid observations due to frequent and persistent cloud cover near the Inter-tropical Convergence Zone (ITCZ) (Wylie et al. 2005). As shown in Figure 6, more valid observations are found in the summer and autumn for both MODIS and VIIRS. The mean area-averaged DPVOs is 20.8% for MODIS and 11.5% for VIIRS. Such a data availability (around 10.0%) from any single sensor (either MODIST, MODISA, or VIIRS) doubles that for global ocean chlorophyll observations from MODISA or MODIST (about 5.0%, Feng and Hu 2016) despite the fact that the study region is in the ITCZ. This is obviously due to the different requirements on data quality, as MODIS global composites have more stringent requirements on data quality. MODIST shows more valid observations than MODISA in all months (Feng and Hu 2016), but fewer valid observations than VIIRS. While the former is possibly due to more sun glint in MODISA than in MODIST images, the latter is a result of larger swath width of VIIRS (3050 km) than MODIS (2330 km). When all three sensors are combined, the maximum observing capacity is obtained. In any case, a combination of two or more sensors leads to significantly more valid observations than any single sensor, arguing for more instruments from polar-orbiting satellites or more measurements from, for example, a geostationary platform. This is not only important for reducing potential aliasing in statistics, but also critical for near real-time applications that require data availability every day (Hu et al. 2016).

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Figure 6. Comparison of DPVOs between MODIS and VIIRS in each season of 2016. (b), (c), (d), and (e) show the DPVOs from MODIS, VIIRS, MODISA, and MODIST, respectively. (a) lists the DPVOs from both MODIS and VIIRS. The regions near land (dilated 20 km outward from shoreline) are masked to avoid perturbations of the shallow-water bottom. A number of 25 in the color legend means that there is a 25% chance of obtaining valid observations at a given 1 km location in a given day.

4.4. Validation

Direct validation of the estimated Sargassum area coverage is extremely difficult or even impossible for several reasons. One, the coarse satellite pixels (about 1 km) will always miss small Sargassum mats, as shown in Hu et al. (2015) using satellite and airborne images with different resolutions (1 km, 30 m, 8 m, and centimetres). This has also been shown by the contrasting results from Gower and King (2011) and from Hardy (2014) where the former did not report any Sargassum in the eastern Gulf of Mexico through

Figure 7. Comparison of area-averaged DPVOs in each month of 2016 between different sensors. The mean DPVOs of MODIS, VIIRS, MODISA, and MODIST are 20.82%, 11.49%, 10.01%, and 10.81%, respectively. The MRDs between different sensors are annotated in the figures.

analyzing 1 km MERIS data but the latter showed large amounts through analyzing 30 m Landsat data (Hardy 2014). The contrasting results are mainly due to their resolution difference. Two, Sargassum mats in the ocean move with currents and winds, making it difficult to correlate field and satellite observations in the same locations at the same time. However, as stated in Wang and Hu (2016) when using MODIS to map Sargassum, the results represent Sargassum observable by the specific satellite sensor under realistic ocean conditions. Therefore, considering that the focus of this paper is on the continuity of Sargassum observing, the emphasis is not the absolute amount but rather the consistency between MODIS and VIIRS. For this purpose, the validation is on the unmixing approach using finer-resolution images to provide the 'truth'.

For this type of validation, two pairs of MODISA and Landsat-8 (L8) images were analyzed with results provided in Figure S8. As expected, Sargassum slicks extracted from MODISA and L8 images show similar patterns, with L8 capturing more small features. On the other hand, the area estimates derived from MODISA and L8 for the same slicks are very close, suggesting the accuracy of the unmixing approach.

4.5. Implications for different applications

Overall, with reduced SNRs but slightly improved spatial resolution, VIIRS shows Sargassum detection accuracy of 85.5%, comparable to MODIS performance. The area estimates as well as spatial/temporal patterns are also consistent with those obtained from MODIS, although in general VIIRS shows lower area estimates primarily due to its lower SNRs in the NIR bands as opposed to different data availability (DPVOs) from individual observations. The validity of the pixel unmixing results, as verified by comparisons of measurements from MODIS and Landsat, suggests that both SNRs and spatial resolution are key requirements for accurate detection and quantification of Sargassum mats.

There are several implications from these findings. First, operation of the near realtime SaWS requires as much data as possible from multiple sensors. This is because that the same locations that are not observable from one sensor (due to sun glint, clouds, cloud shadows, or large VZAs) may be observable from another. The validated performance of VIIRS makes such an addition in data quantity not only feasible, but with data quality comparable to that of MODIS. This is particularly useful when considering the wider swath width of VIIRS (3050 km) than MODIS (2330 km). Two, for science applications, VIIRS can serve as a continuity mission in case both MODIS sensors stop functioning, especially after adjusting their differences using regression equations derived from concurrent observations from all sensors. Likewise, because the recent Sentinel-3 Ocean and Land Color Instrument (OLCI) is also equipped with similar red and NIR bands as on MODIS and VIIRS, a similar continuity study may lead to consistent observations to those of MODIS and VIIRS as well. Finally, at the time of this writing, VIIRS-II on the Joint Polar Satellite System (JPSS) follow-on mission is planned to be in space by 2018, which is expected to provide consistent observations of floating algae from the MODIS and VIIRS time series, thus extending the current observations to the foreseeable future.

5. Conclusion

VIIRS is equipped with similar red and NIR bands as MODIS, and VIIRS AFAI imagery have been created and used routinely in the near real-time SaWS for detecting and tracking floating macroalgae such as Sargassum. However, VIIRS has different SNRs, spatial resolutions, and swath width from MODIS. This study presents the first evaluation results of VIIRS capacity for detecting and quantifying Sargassum macroalgae, in reference against MODIS observations. Results suggest that the inclusion of VIIRS data can not only increase data quantity with similar data quality of MODIS, but also provide continuous and consistent observations of spatial/temporal patterns of Sargassum macroalgae should MODIS sensors stop functioning.

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Disclosure statement

No potential conflict of interest was reported by the authors.

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Appendix F:

1. Publication list

- **Wang, M.**, & Hu, C. (2018). On the continuity of quantifying floating algae of the Central West Atlantic between MODIS and VIIRS. *International Journal of Remote Sensing*, *39*(12), 3852-3869.
- **Wang, M.**, & Hu, C. (2017). Predicting *Sargassum* blooms in the Caribbean Sea from MODIS observations. *Geophysical Research Letters*, *44*(7), 3265-3273.
- **Wang, M.**, & Hu, C. (2016). Mapping and quantifying *Sargassum* distribution and coverage in the Central West Atlantic using MODIS observations. *Remote sensing of environment*, *183*, 350-367.
- **Wang, M.**, & Hu, C. (2015). Extracting Oil Slick Features From VIIRS Nighttime Imagery Using a Gaussian Filter and Morphological Constraints. *IEEE Geoscience And Remote Sensing Letters, 12*(10), 2051- 2055.
- **Wang, M.**, Hu, C., Cannizzaro, J., English, D., Han, X., Naar, D., Lapointe, B., Brewton, R., & Hernandez, F. (2018, accepted). Remote estimation of *Sargassum* biomass, nutrients, and pigments. *Geophysical Research Letters.*
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