



UNIVERSIDADE FEDERAL DE SANTA CATARINA
CAMPUS FLORIANÓPOLIS
PROGRAMA DE PÓS-GRADUAÇÃO EM OCEANOGRAFIA

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Avaliação dos algoritmos de sensoriamento remoto para a clorofila-a do oceano através de dados de fluorescência in situ nas águas costeiras do sul do Brasil

FLORIANÓPOLIS

2020

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Dissertação submetido(a) ao Programa de Pós-Graduação em Oceanografia da Universidade Federal de Santa Catarina para a obtenção do título de Mestre em Oceanografia

Orientador: Prof. Dr. Carlos Alberto Eiras Garcia

Florianópolis

2020

Ficha de identificação da obra elaborada pelo autor,
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Silva, Gabriel Serrato de Mendonça
Avaliação dos algoritmos de sensoriamento remoto para a
clorofila-a do oceano através de dados de fluorescência in
situ nas águas costeiras do sul do Brasil / Gabriel
Serrato de Mendonça Silva ; orientador, Carlos Alberto
Eiras Garcia, 2020.
69 p.

Dissertação (mestrado) - Universidade Federal de Santa
Catarina, Centro de Ciências Físicas e Matemáticas,
Programa de Pós-Graduação em Oceanografia, Florianópolis,
2020.

Inclui referências.

1. Oceanografia. 2. Cor do oceano. 3. Fluorescência da
clorofila-a. 4. Sensoriamento remoto. 5. SimCosta. I.
Alberto Eiras Garcia, Carlos . II. Universidade Federal de
Santa Catarina. Programa de Pós-Graduação em Oceanografia.
III. Título.

Gabriel Serrato de Mendonça Silva

Avaliação dos algoritmos de sensoriamento remoto para a clorofila-a do oceano através de dados de fluorescência in situ nas águas costeiras do sul do Brasil

O presente trabalho em nível de mestrado foi avaliado e aprovado por banca examinadora composta pelos seguintes membros:

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Florianópolis, 2020

AGRADECIMENTOS

Agradeço a todos aqueles que apoiaram o desenvolvimento desta pesquisa.

À toda minha família.

À Universidade Federal de Santa Catarina (UFSC), campus Reitor João David Ferreira Lima, pela oportunidade em cursar o Mestrado em Oceanografia.

Aos professores, funcionários e colegas do PPGOceano

Aos meu orientador Dr. Carlos Alberto Eiras Garcia pelo apoio, incentivo e orientações.

Ao Projeto SiMCosta e toda a sua equipe pelas assistências envolvidas nas atividades de campo para manutenção da boia SiMCosta-SC01. Um agradecimento especial à Ella S. Pereira, gerente nacional de operações do SiMCosta.

Ao Ministério do Meio de Ambiente e, ao Ministério de Ciências e Tecnologia pelo financiamento do Fundo Clima

RESUMO

O presente estudo compreende uma avaliação do desempenho de algoritmos de determinação da concentração de clorofila-a por meio do sensoriamento remoto através de séries temporais horárias de fluorescência da clorofila-a (F_{chl}) medida por um sensor acoplado à boia SC01 do Sistema de Monitoramento Costeiro Brasileiro (SiMCosta) em águas costeiras no Sul do Brasil. Os algoritmos operacionais da clorofila-a são amplamente usados no sensor *Moderate-Resolution Imaging Spectroradiometer* (MODIS) a bordo dos satélites Aqua e Terra e no sensor *Visible Infrared Radiometer Suite* (VIIRS) a bordo dos satélites Suomi-NPP e NASA-20. Antes de iniciar as análises, os dados de F_{chl} e clorofila derivada de satélite (C_{sat}) passaram por rígidos controles de qualidade definidos pelo SiMCosta e pela NASA, respectivamente. Os valores de F_{chl} qualificados foram corrigidos com sucesso para extinção do efeito não fotoquímico através da interpolação das medições diárias nos períodos de nascer e pôr do sol. Posteriormente, um coeficiente de calibração derivado em laboratório foi aplicado para converter os valores de F_{chl} qualificados e corrigidos em unidades de concentração de clorofila (C_{flu}). No geral, a análise de regressão linear entre C_{flu} e C_{sat} derivada dos sensores MODIS e VIIRS mostrou bons resultados com coeficiente de determinação (R^2) variando entre 0,88 e 0,96, inclinação entre 0,92 e 1,02 e interceptação entre -0,17 e 0,13. O algoritmo MODIS ($R^2 = 0,96$, inclinação = 1,02, RMSE = 0,16 mg m⁻³, BIAS = 0,16 mg m⁻³, para N = 222 e intervalo de tempo ± 1 h) apresentou desempenho ligeiramente melhor do que VIIRS ($R^2 = 0,92$, inclinação = 0,96, RMSE = 0,25 mg m⁻³, BIAS = -0,25 mg m⁻³, para N = 284 e intervalo de tempo ± 1 h). Os erros percentuais absolutos médios e percentuais relativos foram de 33,4% e 17,97% para o sensor MODIS, enquanto 30,95% e -5,29% para o VIIRS, que podem ser considerados erros relativamente baixos em oceanos costeiros. Esses resultados representam a análise de dados de satélite mais abrangente para esta região, sugerindo que a abordagem adotada neste trabalho pode ser aplicável em águas relativamente rasas e turvas ao longo da costa brasileira.

Palavras-chave: MODIS, VIIRS, Cor do oceano, fluorescência da clorofila-a, Sensoriamento remoto, SiMCosta.

ABSTRACT

This article comprises an evaluation of the performance of ocean color chlorophyll-a algorithms based on time series of hourly in situ fluorescence chlorophyll concentration (F_{chl}) measured by a sensor placed on buoy SC01 of the Brazilian Coastal Monitoring System (SiMCosta) in coastal waters of South Brazil. The operational chlorophyll-a algorithms are widely used in Moderate-Resolution Imaging Spectroradiometer (MODIS) aboard Aqua and Terra satellites, and Visible Infrared Radiometer Suite (VIIRS) aboard satellites Suomi-NPP and NASA-20. Before initiating the analysis, F_{chl} and satellite-derived chlorophyll (C_{sat}) data passed through a rigid control of quality defined by SiMCosta and NASA, respectively. The high-quality F_{chl} values were successfully corrected for nonphotochemical quenching (NPQ) by an interpolation of sunrise and sunset daily measurements. Subsequently, a laboratory-derived calibration coefficient was applied to convert the unquenching F_{chl} values into chlorophyll concentration (C_{flu}). Overall, linear regression analysis between C_{flu} and C_{sat} derived from MODIS and VIIRS sensors showed good results with coefficient of determination (R^2) varying between 0.88 and 0.96, slope between 0.92 and 1.02 and intercept between -0.17 and 0.13. The MODIS algorithm ($R^2 = 0.96$, slope = 1.02, RMSE = 0.16 mg m⁻³, BIAS = 0.16 mg m⁻³, for N = 222 and time interval ± 1 h) presented slightly better performance than VIIRS ($R^2 = 0.92$, slope = 0.96, RMSE = 0.25 mg m⁻³, BIAS = -0.25 mg m⁻³, for N = 284 and time interval ± 1 h). The mean absolute percentage and relative percentage errors were 33.4% and 17.97% for MODIS sensor while 30.95% and -5.29% for VIIRS, which can be considered relatively low errors in ocean coastal environments. These results represent the most comprehensive satellite data analysis for this region, suggesting that the approach adopted in this work may be applicable in relatively low turbid waters along the Brazilian coast.

Keywords: Ocean color, MODIS, VIIRS, Southern Brazilian Coastal Waters, in situ fluorescence chlorophyll-a

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LISTA DE ABREVIATURAS E SIGLAS

APD	<i>Absolute Percent Difference</i>
ATMFAIL	<i>Atmospheric correction failure</i>
CEBIMar	Centro de Biologia Marinha
C_{flu}	Concentração de clorofila-a após correção para quenching e calibrada em laboratório
Chl-a	Clorofila-a
CI	<i>Color Index</i>
CLDICE	<i>Probable cloud or ice contamination</i>
C_{sat}	Concentração de clorofila-a estimada por satélite
CV	Coeficiente de Variância
CZCS	<i>Coastal Zone Color Scanner</i>
F_{chl}	Fluorescência da clorofila-a após testes de qualidade
$F_{chl-raw}$	Fluorescência da clorofila-a medida pelo WQM
GFSC	<i>Goddard Space Flight Center</i>
HILT	<i>Observed radiance very high or saturated</i>
HPLC	<i>High-performance liquid chromatography</i>
ICMBio	Instituto Chico Mendes de Conservação da Biodiversidade
INMET	Instituto Nacional de Meteorologia
LAC	Local Area Covered
LAND	<i>Pixel is over land</i>
MAArE	Projeto de Monitoramento Ambiental da Reserva Biológica Marinha do Arvoredo e Entorno
MAE	<i>Mean Absolute Error</i>
MBR	<i>Maximum Band Ratio</i>
MODIS	<i>Moderate-Resolution Imaging Spectroradiometer</i>
NASA	<i>National Aeronautics and Space Administration</i>
NGP	Número de Pixeis Bons
NOAA	<i>National Ocean and Atmosphere Agency</i>
NTP	Número Total de Pixeis
OB.DAAC	<i>Ocean Biology Distributed Active Archive Center</i>
OCTS	<i>Ocean Color and Temperature Scanner</i>

PAR	<i>Photosynthetically Active Radiation</i>
PCSE	Plataforma Continental Sudeste Brasileira
POA	Propriedades Ópticas Aparentes
POI	Propriedades Ópticas Inerentes
PPW	<i>Plate River Plume Water</i>
QARTOD	<i>Quality Assurance / Quality Control of Real-Time Oceanographic Data</i>
Rebio Arvoredo	Reserva Biológica Marinha do Arvoredo
RMSE	<i>Root Mean Square Error</i>
RPD	<i>Relative Percent Difference</i>
R_{rs}	<i>Remote Sensing Reflectance</i>
SACW	<i>South Atlantic Central Water</i>
SIMCosta	Sistema de Monitoramento da Costa Brasileira
STRAYLIGHT	<i>Probable stray light contamination</i>
TW	<i>Tropical Water</i>
UFSC	Universidade Federal de Santa Catarina
USP	Universidade de São Paulo
VIIRS	Visible Infrared Imaging Radiometer Suite
WIM	<i>Windows Image Manager</i>
WQM	<i>Water Quality Monitor</i>
ZCIT	Zona de Convergência Inter Tropical

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1 INTRODUÇÃO

Desde a década de cinquenta até o presente a clorofila-a (Chl-a), principal pigmento fotossintetizante presente em organismos fitoplanctônicos é utilizada como indicativo de sua biomassa (STRICKLAND, 1960) e a produtividade primária nos oceanos, além de ser uma variável importante caracterizando o estado trófico de ecossistemas costeiros e oceânicos (e.g. FALKOWSKI e KIEFER, 1985; ANTONINE e MOREL, 1996; CLOERN et al., 2014). Algumas técnicas para a determinação em laboratório e in situ da clorofila-a utilizam sua capacidade de fluorescência, resultante da absorção de radiação luminosa emitida por uma fonte natural ou artificial (e.g.; YENTSH e MENZEL, 1963; HOLMS-HANSEN, 1965). As propriedades de absorção de luz por esse pigmento também permitem estimativas por medidas de cor do oceano obtidas por sensores de sensoriamento remoto (e.g. CLARKE et al., 1970; MOREL e PRIEUR, 1977; CULLEN et al., 1997).

A variedade de cores que o oceano pode apresentar é determinada pelas concentrações de propriedades ópticas aparentes (POA) são aquelas que dependem das características do meio e das suas condições de iluminação (e.g. presença de nuvens e aerossóis), e as propriedades ópticas inerentes (POI) que são aquelas caracterizadas pelos materiais (particulado ou dissolvido) presentes na água (PREISENDORFER, 1976). Vale ressaltar que tanto as POA quanto as POI exercem uma interferência direta na penetração da luz solar na água o que ocasiona alterações em diferentes processos e fatores relacionados à distribuição e concentração do fitoplâncton na água, tais como: a absorção da luz pelos organismos fitoplanctônicos; a temperatura da água; a disponibilidade de oxigênio; o estado fisiológico dos organismos; o grupo taxonômico, dentre outras que, segundo Cullen et al., (1982) podem alterar a relação entre as concentrações de Chl-a e a biomassa de fitoplâncton em até duas ordens de grandeza.

Nos ambientes costeiros as variações no tempo e no espaço dos constituintes ópticos presentes na água se tornam ainda mais complexas de compreender devido ao aporte de água provindo da drenagem continental e pela influência dos processos meteorológicos e oceanográficos atuantes nestas regiões resultando em falhas nas estimativas de Chl-a fornecidas pelos dados de cor do oceano. Para se obter melhores estimativas através das técnicas de sensoriamento remoto, diversos autores apontaram como imprescindível a calibração de algoritmos e modelos através da integração das concentrações de Chl-a adquiridas pelos sensores orbitais com as

medidas *in situ* feitas em superfície (WERDELL e BAILEY, 2005; CIOTTI et al., 2010; IOCCG, 2013; BLONDEAU-PATISSIER, 2014).

A exigência por maior precisão e acurácia na estimativa da concentração de Chl-*a* através de informações satelitais norteou diversas pesquisas no desenvolvimento de algoritmos e modelos nos últimos quarenta anos. Blondeau-Patissier et al. (2014) apresentaram a evolução das técnicas e métodos empregados para a detecção, mapeamento e análise das florações de fitoplâncton, para águas costeiras e oceânicas, desde o início do sensoriamento remoto dos oceanos até o presente. Dentre os algoritmos desenvolvidos destacam-se os semi-analíticos, desenvolvidos através de formulações matemáticas teóricas com ajustes estatísticos, e os algoritmos empíricos que são obtidos através da relação entre medições ópticas e as concentrações dos constituintes amostrados *in situ* (IOCCG, 2000).

Devido a diferentes condições de iluminação, da presença de materiais particulados em suspensão e matéria orgânica dissolvida, as estimativas de concentração de Chl-*a* em águas costeiras fornecidas pelos algoritmos necessitam de processos de validação para a determinação de erros ocasionados pelas propriedades óticas existentes. O processo de validação em si inclui o desenvolvimento de comparações com conjuntos de dados obtidos através de observação em campo e das estimativas de satélite coincidentes no tempo e espaço. A qualidade das validações também depender de diferentes fontes de incerteza como, por exemplo, a qualidade dos dados *in situ* e do desempenho dos esquemas de correção atmosférica e dos algoritmos em si.

A importância de avaliar a qualidade dos produtos da cor do oceano também é enfatizada pela necessidade de mesclar observações de satélite para melhorar a consistência das séries temporais da cor do oceano, bem como a cobertura espacial e temporal dos mapas de produtos aplicáveis como Variável Climática Essencial (ECV) para estudos de mudanças climáticas. Diferentes projetos focaram na fusão de dados para fornecer produtos globais contínuos, incluindo o projeto GlobColour (<http://www.globcolour.info>), o Programa SIMBIOS da NASA (Fargion et al., 2003; Maritorena & Siegel, 2005), projetos MEASURE (por exemplo, Maritorena, d'Andon, Mangin, & Siegel, 2010) e o recente projeto ESA OC-CCI (<http://www.esa-oceancolour-cci.org/>)

Especificamente para a região costeira do estado de Santa Catarina, poucos estudos relacionaram as concentrações de Chl-*a* *in situ* e estimativas de satélite. O

Projeto de Monitoramento Ambiental da Reserva Biológica Marinha do Arvoredo e Entorno (MAArE) contemplou durante os anos de 2015 a 2016 campanhas oceanográficas com intuito de compreender a variabilidade espaço-temporal dos processos oceanográficos e ecológicos da Reserva Biológica Marinha do Arvoredo (Rebio Arvoredo). Parte do projeto MAArE foi direcionado à avaliação do algoritmo de cor do oceano através de dados in situ e estimativas por satélites. Foi identificada a necessidade de análises mais refinadas, com maior número de amostras, e do desenvolvimento de um algoritmo regional obtido através da relação entre as bandas de reflectância e as concentrações de Chl-a in situ para a região (MAARE, 2017).

Nos últimos anos, uma rede integrada de monitoramento da zona costeira está sendo implementada no Brasil, possibilitando suprir a demanda dessas medidas in situ. O Sistema de Monitoramento da Costa Brasileira (SiMCosta) utiliza-se de plataformas flutuantes ou fixas, dotadas de instrumentos e sensores, com funcionamento autônomo e capacidade de coletar regularmente variáveis oceanográficas e meteorológicas (<http://simcosta.furg.br/artigos/projeto>) Devido à relevante importância ambiental e socioeconômica da Rebio Arvoredo, em fevereiro de 2017, o projeto SiMCosta instalou uma boia meteo-oceanográfica na região, que abre uma oportunidade para a validação das estimativas de satélite para a zona costeira de Santa Catarina apresentados pelo Projeto MAArE

2 OBJETIVOS

2.1 OBJETIVO GERAL

Avaliar a performance das estimativas da concentração de clorofila-a fornecidas por sensores satelitais na região central da costa do estado de Santa Catarina através de séries temporais de fluorescência da clorofila-a in situ.

2.2 OBJETIVOS ESPECÍFICOS

- Implementar um controle de qualidade nos dados in situ;
- Estimar a precisão e a acurácia associadas as estimativas da concentração de clorofila-a fornecidas pelos sensores MODIS e VIIRS utilizando os dados in situ fornecidos pela boia SiMCosta-SC01;

2.3 CONTRIBUIÇÕES

Esta proposta visa dar continuidade aos esforços dispendidos pelo projeto MAArE, adicionando conhecimento científico para estimar as concentrações de Chl-a através do sensoriamento remoto na região costeira do estado de Santa Catarina – Brasil e, mais especificamente, para a área da Rebio do Arvoredo. Os procedimentos adotados neste estudo visam implementar uma metodologia que possa ser adotada em outras boias do Projeto SiMCosta.

Gabriel Serrato de Mendonça Silva

Evaluation of ocean chlorophyll-a remote sensing algorithms using in situ fluorescence data in Southern Brazilian Coastal Waters

Esta seção é destinada à apresentação do artigo científico desenvolvido e submetido à revista *Ocean and Coastal Research*, como parte dos requisitos para a obtenção do Grau de Mestre em Oceanografia pela Universidade Federal de Santa Catarina.

Florianópolis

2020



Evaluation of ocean chlorophyll-a remote sensing algorithms using in situ fluorescence data in the Southern Brazilian Coastal Waters

Journal:	<i>Ocean and Coastal Research</i>
Manuscript ID	OCR-2020-0014
Manuscript Type:	Original Article
Date Submitted by the Author:	05-Oct-2020
Complete List of Authors:	Silva, Gabriel; UFSC, Centro de Ciências Físicas e Matemáticas - CFM Garcia, Carlos; UFSC, Centro de Ciências Físicas e Matemáticas - CFM
Keyword:	Ocean color, MODIS, VIIRS, Southern Brazilian Coastal Waters, in situ fluorescence chlorophyll-a

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1 INTRODUCTION

The variety of colors that the ocean can display is determined by the lighting conditions and the different optically active biological, chemical and geological components that are present in the water (Morel, 1974). Observation of the spectral behavior of light at sea made it possible to obtain relevant geophysical parameters such as turbidity, suspended particulate matter, organic and inorganic carbon particulates and Chl-a concentration (Gordon, 2010). In order to identify the relationship between the different concentrations of organic and inorganic particulates and dissolved materials, and also the presence of phytoplankton in the spectral composition of light reflected and absorbed by seawater, Morel and Prieur (1977) classified marine waters in two cases. Case 1 waters, commonly found in open ocean, have a predominance of phytoplankton and low concentrations of colored dissolved organic matter and suspended particulate matter. The waters of Case 2, normally found in coastal and estuarine regions, have a predominance of colored dissolved organic matter and suspended particulate matter while light absorption by photosynthetic pigments is comparatively lower

With technological advances in space missions in past decades, sensors such as the Coastal Zone Color Scanner (CZCS), Moderate Resolution Imaging Spectroradiometer (MODIS) (Salomonson et al., 1989), Ocean Color and Temperature Scanner (OCTS) (Iwasaki et al., 1992), Sea-viewing Wide Field-of-view Sensor (SeaWiFS) (Hooker et al., 1992), Medium Resolution Imaging Spectrometer (MERIS) (Rast and Bezy, 1999) and, more recently, Visible Infrared Imager / Radiometer Suite (VIIRS) (Welsch et al., 2001), allowed researchers to evaluate the sea color through remote sensing with high spatial and temporal resolutions and to perform oceanic studies synoptically.

The knowledge of Chl-a concentrations and distribution is necessary to understand fundamental ecological processes such as primary productivity rates, as well as detect some effects of anthropogenic impacts and global climate change on coastal and oceanic environments ([Cloern et al., 2014](#)).

Different research fields of oceanography use ocean color satellite imagery, and including evaluation of eutrophication processes (e.g. [Peñaflor et al., 2007](#); [Klemas, 2011](#); [Banks et al., 2012](#)), spatiotemporal distribution of Chl-a (e.g. [Gower and King, 2007](#); [Garcia and Garcia, 2008](#); [Henson et al., 2009](#); [Park et al., 2010](#); [Song et al., 2010](#)), biogeochemical cycles (e.g. [Focardi, et al., 2009](#); [Chang and Xuan, 2011](#)) and marine ecosystem responses to climate change and to anthropogenic impacts ([Shi and Wang, 2007](#); [Zhao et al., 2008](#); [Kahru et al., 2010](#); [Henson et al., 2010](#)).

Thus, a demand for decreasing uncertainty in estimating Chl-a concentration using satellite information exists and guided the development of algorithms and models in the last forty years. [Blondeau-Patissier et al. \(2014\)](#) reviewed and presented the evolution of techniques and methods employed for the detection, mapping, and analysis of phytoplankton blooms for coastal and ocean waters from the beginning of the satellite era to the present. Among the developed algorithms, we can highlight the empirical algorithms that are obtained through the relationship between optical measurements and the concentrations of constituents sampled *in situ*, and the semi-analytical algorithms developed through theoretical mathematical formulations with statistical adjustments ([IOCCG, 2000](#)).

In order to evaluate the performance of different empirical and semi-analytical algorithms used to estimate Chl-a concentration in the southwestern Atlantic continental shelf region, [Garcia et al. \(2006\)](#) used radiometric data sampled on two cruises carried out in 2003 and 2004. The results demonstrated that the appropriate

calibration of the semi-analytical algorithms from measurements of the inherent optical properties measured *in situ* can provide significant improvements in the estimation of Chl-a concentration in the coastal region. [Giannini et al. \(2013\)](#) presented an update of the regional empirical algorithm OC2-LP ([Garcia et al., 2006](#)) for the region influenced by the La Plata river discharge based on the relationship between low salinity and high turbidity in the area. From this update, the operational empirical algorithms should be applied within the limits of salinity and turbidity defined by the OC2-LP algorithm.

By comparing the Chl-a concentration estimates provided by the CZCS, OCTS, SeaWiFS and MODIS sensors, [Ciotti et al. \(2010\)](#) evaluated the seasonal and meridional variability of surface Chl-a concentration for the entire Brazilian continental shelf. High variations in Chl-a concentration were found due to the river discharge of the Amazon River (in the north) and due to the plume of La Plata River (in the south). In the eastern and north eastern part of the Brazilian continental shelf, a direct influence of wind patterns has been identified due to the seasonal and southern migration of the Inter-Tropical Convergence Zone (ZCIT). The authors concluded that the use of remote sensing for time series construction makes it possible to estimate phytoplankton biomass and to identify long-term trends in primary productivity off the Brazilian coast. Such systematic studies that use several platforms, multiple instruments and for several years have been recommended because they allow understanding the interdecadal climatic variations in phytoplankton blooms in the Brazilian continental shelf.

Specifically, for the coastal region of Santa Catarina state, few studies have related Chl-a concentrations from *in situ* data and satellite estimates. The Environmental Monitoring Project of the Arvoredo and Surrounding Marine Biological

Reserve (MAARE) contemplated oceanographic campaigns during the years 2015-2016 in order to understand the spatio-temporal variability of oceanographic and ecological processes of the Arvoredo Marine Biological Reserve (Rebio Arvoredo). It is noteworthy that Rebio Arvoredo is one of two fully protected marine conservation units in Brazil and the only Marine Biological Reserve present in the South and Southeast regions of Brazil. Part of the MAARE project was directed to the evaluation of the ocean color algorithm through *in situ* data and satellite estimates. For this, the authors used time windows (time difference between data collection and satellite passage) of approximately 24 hours to validate estimates with *in situ* data. Due to the complexity to identify matchup values for bio-optical constituents the authors found a relatively low number of 53 paired samples. The relationship between the Chl-a concentration measured *in situ* and that which was estimated by the MODIS sensor was found to have low consistency ($r^2 = 0.36$). The need for more refined analyses with larger number of data under different oceanographic conditions in the region have been identified (MAARE, 2017).

In recent years, the Brazilian Coast Monitoring System (SiMCosta) has been implemented along the Brazilian coast. SiMCosta uses floating and/or fixed platforms, equipped with instruments and sensors, with autonomous operation and the ability to regularly collect oceanographic and meteorological variables (<http://simcosta.furg.br/artigos/project>). In February 2017, a SiMCosta meteocean buoy, named SiMCosta-SC01, was deployed in the Rebio Arvoredo. Among the oceanographic variables sampled by sensors placed on SiMCosta-SC01 buoy, we highlight the sea surface temperature, salinity, dissolved oxygen, turbidity and Chl-a stimulated fluorescence (calibrated in Chl-a concentration units). This set of information acquired simultaneously allows for an integrated analysis through

statistical methods to understand which factors are responsible for Chl-a variability in the region.

It is important to highlight the social and economic significance of studies related to the distribution patterns of phytoplankton biomass and its associated processes in the Santa Catarina coastal region, as presented by Rörig et al. (2018). The authors identified that the structure of the phytoplankton communities and their distribution are modulated by river discharges, the phenomenon of coastal resurgence and seasonal variation in the distribution of water mass in the region. The authors also pointed out that the economic activities of fishing and mariculture, traditional in the region, are directly influenced by phytoplankton blooms, producing positive and negative effects (toxic algae). Hence, this study may also contribute with data to support wider socio-economic research in the region.

Several authors pointed out the relevance of acquiring sea-truth data simultaneously to the passage of the orbital sensors (e.g., [Werdell and Bailey, 2005](#); [Ciotti et al., 2010](#); [IOCCG, 2013](#); [Blondeau-Patissier, 2014](#)). Therefore, due to the availability of *in situ* fluorescence data collected by buoy SiMCosta-SC01, this study evaluates the existing operational Chl-a concentration algorithm for MODIS-Aqua, MODIS-Terra, VIIRS-NOAA20 and VIIRS-SNPP by comparing satellite Chl-a estimates with *in situ* chlorophyll concentration. The metrics used for those comparisons followed the most recent recommendations published on [Seegers et al. \(2018\)](#) and [Pereira et al. \(2018\)](#). An effort was made to infer the consequences of using pixels contaminated and not contaminated by straylight.

2 DATA AND PROCEDURES

2.1 STUDY SITE

The central coast of Santa Catarina has unique characteristics that demonstrate the need for research and technical-scientific development that foster sustainable management and development in its coastal and marine environments. Located in the internal and extreme south portion of the Southeast Brazilian Continental Platform (PCSE) - limited to the north at latitude 23 °S close to the city of Cabo Frio in Rio de Janeiro, and to the south at latitude 28.5 °S close to Cabo de Santa Marta Grande in the state of Santa Catarina ([Castro Filho and Miranda, 1998](#)) - the central coast of the state of Santa Catarina has attributes of economic relevance such as the largest production of oysters, scallops and mussels in Brazil. Due to its environmental relevance, the Arvoredo Marine Biological Reserve (Rebio Arvoredo) was created in 1990 for the integral protection and conservation of coastal ecosystems, their islands and islets, as well as their waters, the continental shelf and its associated resources ([BRAZIL, 1990](#)). Rebio Arvoredo covers an area of 17,104.60 hectares, approximately 11 km north of the Island of Santa Catarina, and delimited between the coordinates 27.15° S, 48.31° W and 27.30° S, 48.42° W.

The central coast of the state of Santa Catarina is directly influenced by oceanic water and continental outflows. Through the thermohaline indices of the oceanic water masses present in the PCSE, Möller et al., (2008) identified the Tropical Water (TW) as hot and saline water ($T \geq 18.5$ ° C, $S \geq 36$), the South Atlantic Central Water (SACW), cold and less saline ($T \leq 18.5$ ° C, $S \geq 35.3$), the Subtropical Shelf Water (STSW), and the Plate River Plume Water (PPW), with low temperature and low salinity ($T > 10$ ° C, $S \leq 33.5$). Seasonally, due to the different wind patterns in the region, these water

bodies undergo mixtures and acquire peculiar characteristics. Especially during the summer and spring months (e.g., [Bordin et al. 2019](#)), TW undergoes periodic mixtures with SACW, forming the summer STSW ($T > 18.5\text{ }^{\circ}\text{C}$, $35.3 < S < 36$) The oceanographic phenomenon of coastal resurgence in the region occurs due to the action of the predominant N-NE winds causing the SACW intrusion on the platform ([Campos et al., 2013](#)). During the winter months, with the predominance of S-SE winds associated with the passage of cold fronts, the displacement of the PPW to the north occurs, and its mixture with the TW result in the winter STSW ($T > 14\text{ }^{\circ}\text{C}$, $33, 5 \leq S < 35.3$) (e.g. [Bordin et al., 2019](#)).

the supply of continental water is caused by the discharge of the Tijucas River, through the channel of the North Bay of Santa Catarina Island ([Schettini et al., 1996](#)) and the Itajaí-Açu River - the largest river in the region, to be highlighted - whose plume generally moves in the N-NE direction ([Carvalho et al., 2010](#)). [Campos et al. \(2013\)](#) point out that the influence of the Itajaí-Açu River over Rebio Arvoredo may occur in sporadic situations in the Rebio region.

The materials from these river systems are extremely important in the distribution of physical, chemical and biological properties in the waters of Rebio Arvoredo ([Paquette et al., 2016](#)). As it contains nutrients associated with urban effluents and local agriculture, the supply of continental material can sporadically cause significant changes in temperature, salinity, turbidity, concentrations of Chl-a, particulate and dissolved organic and inorganic material and, consequently, in the overall properties of the coastal waters.

Following the standard climatological classification of [Köppen and Geiger \(1954\)](#), the coast of Santa Catarina has humid subtropical mesothermal climate with hot summer (Cfa). The region has annual average temperatures between $19\text{ }^{\circ}\text{C}$ and

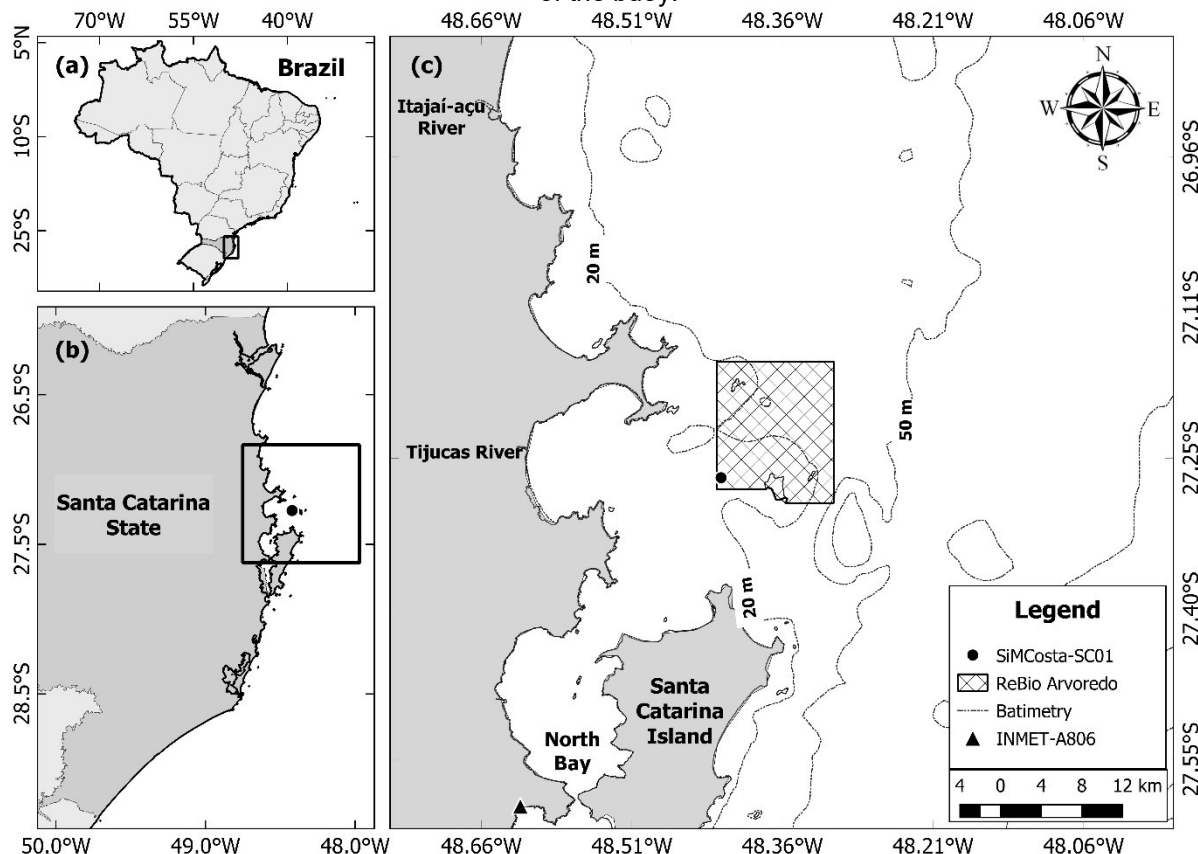
20 °C, with average annual minimums between 15 °C and 16 °C and average annual maximum between 25 °C and 26 °C. The annual relative humidity varies between 82% and 86%, and the total annual precipitation between 30 and 40 mm. The climatological information described was published in the Climatological Atlas of the State of Santa Catarina (Pandolfo et al., 2002). It should be noted that the region may have significant interannual variations influenced by climatic fluctuations, such as, for example, El Niño and La Niña (Grimm, 2009b).

2.2 IN SITU DATA COLLECTION

A moored monitoring buoy system SiMCosta-SC01 was deployed on 2017 February 22 inside Rebio Arvoredo, over the central coast of Santa Catarina state, at 27° 16.46' S and 48° 25.26' W (Figure 1). The buoy SC01 has an optical WET Labs WQM (Water Quality Monitor) sensor fixed approximately at 1-meter depth. The above WQM is part of four optical devices that was acquired by SiMCosta to be deployed along the Brazilian coast. All four WQM were calibrated at factory prior to deployment, and the first package, deployed in the São Sebastião channel (SP, Brazil) in 2014, was used for in situ calibration for the remaining instruments. The WQM sensor has an integrated copper anti-fouling bio-wiper system to clean the optical lens before any measurement can be taken to prevent fouling caused by natural algal biofilm. Full maintenance of the sensor occurs every three months by the SiMCosta team. During the maintenance stage, the WQM data was downloaded directly from the sensor to ensure that all information automatically sent by the buoy's telemetry system was equal to the sensors' backup. *In situ* dataset was composed by means of 20 seconds acquisitions every hour of chlorophyll-a fluorescence ($F_{chl-raw}$), temperature and

salinity, between 2017 February 22 and 2019 November 17 and obtained from <http://simcosta.furg.br/>.

Figure 1 – The study area. Brazil's reference map (a), subset area over the central coast of Santa Catarina State (b). The study area covered by satellite sensors (c). The limits of the Rebio Arvoredo are shown in the hatched area. The location of buoy SiMCosta SC01 (black dot) is shown at the bottom left corner of the Rebio Arvoredo. Tijucas river is the closest freshwater outflow in the vicinities of the buoy.



Complementary hourly data of solar radiation (in KJ/m^2) from a meteorological automated station located in Florianópolis city (see figure 1), at $27^\circ 36' \text{ S}$ and $48^\circ 36' \text{ W}$, was obtained through a request form at National Meteorology Institute (INMET). These data were firstly converted to photosynthetically active radiation (PAR) by a factor of 0.47 (Yunhua et al, 1984) and then used for correcting non-photochemical quenching effect on in situ Chl-a fluorescence data.

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2.3 SATELLITE-DERIVED CHLOROPHYLL-A CONCENTRATION

The satellite dataset was obtained for the same period of *in situ* dataset through request form at NASA Goddard Space Flight Center (GSFC) (<http://oceancolor.gsfc.nasa.gov/>) for Moderate Resolution Imaging spectroradiometer (MODIS), onboard Aqua and Terra satellites, and Visible Infrared Imaging Radiometer Suite (VIIRS) aboard satellites SNPP and NOAA-20. We used MODIS and VIIRS data with 1 km and 750 meters of spatial resolution, respectively. The satellite dataset was composed by daily Local Area Covered (LAC) Level 2 product suite images of near-surface chlorophyll-a concentration data (hereinafter called C_{sat}). The C_{sat} data was estimated by a default algorithm that merge Color Index (CI) algorithm of [Hu et al. \(2012\)](#) and OCx (OC3/OC4) band ratio algorithm of [O'Reilly \(2000\)](#). An empirical relationship derived from *in situ* measurements of Chl-a concentration and remote sensing reflectances (R_{rs}), obtained by radiometers in the region of the blue (λ_{blue}) and green (λ_{green}) bands of the visible spectrum, returns C_{sat} (in mg/m^3) in the surface layer of the sea. The algorithm is applicable to all current “sea color” sensors (https://oceancolor.gsfc.nasa.gov/atbd/chlor_a/).

The OCx algorithm (eq. 1) is a fourth order polynomial relationship between a ratio of R_{rs} and concentration of Chl-a, where the ratio $R_{rs}(\lambda_{blue})/R_{rs}(\lambda_{green})$ must be the maximum band ratio (MBR) value, for the wavelengths existing in these bands (eq. 2). The coefficients a_0 to a_4 to estimate C_{sat} for each sensor are specified in Table 1.

$$\log_{10}(C_{sat}) = a_0 + \sum_{n=1}^4 a_n = \text{MBR}^i \quad (\text{eq.1})$$

$$\text{MBR} = \log_{10} \left(\frac{Rrs(\lambda_{blue})}{Rrs(\lambda_{green})} \right) \quad (\text{eq. 2})$$

The reflectance wavelengths used for current implementation of the standard C_{sat} algorithm for MODIS (OC3M) were 443nm, 488nm, 547nm, and for VIIRS (OC3V) were 443nm, 486nm, and 550nm.

Table 1 – Specification of spectral band and coefficients used in the OCx algorithm for MODIS and VIIRS sensors.

Sensor	Algorithm	Blue	Green	a0	a1	a2	a3	a4
MODIS	OC3M	443, 488	547	0.2424	-2.7423	1.8017	0.0015	-1.2280
VIIRS	OC3V	443, 486	550	0.2228	-2.4683	1.5867	-0.4275	-0.7768

Source: https://oceancolor.gsfc.nasa.gov/atbd/chlor_a/

2.4 QUALITY CONTROL OF CHL-A FLUORESCENCE DATA

Prior to any analysis, the quality of $F_{chl-raw}$ was assessed based on the recommendations of the US Integrated Ocean Observing System (US IOOS) Quality Assurance / Quality Control of Real-Time Oceanographic Data (QARTOD) project. Several sequential tests were performed to filter spurious $F_{chl-raw}$ data that are commonly obtained by autonomous sensors. Those tests are fully described on the Ocean Optical Data Handbook (U.S. IOOS, 2017) to guide real-time data quality control testing. The quality control tests recommended by U.S. IOOS (2017) follow a hierarchical sequence of 13 tests divided into 3 groups. Group I require five tests for real-time data monitoring and telemetry, other five strongly recommended tests at group II for quality control, and group III contains three suggested tests (Table 2).

Table 2 – Description of tests used in QUARTOD for time series data quality control.

Group	Test number	Test name	Description
I	1	Timing/Gap	Check time of data received by telemetry
	2	Syntax	Checks the structure of the message received by telemetry
	3	Location	Checks the geographical location of data.
	4	Gross Range	Checks if data exceeds equipment limits
	5	Decreasing Radiance, Irradiance, and PAR	Checks if parameters decrease with depth
II	6	Photic Zone limit for Radiance Irradiance, and PAR	Checks if the parameters are below the photic zone
	7	Climatology	Checks if parameter is within seasonal expectations
	8	Spike	Checks if the parameter exceeds a limit on adjacent data
	9	Rate of Change	Checks whether the parameter has increased too much or too low for a given time
	10	Flat Line	Checks whether data value does not vary over time
III	11	Multi-Variate	Comparison with other variables
	12	Attenuated Signal	Checks for inappropriate time series variation
	13	Neighbor	Check data similarity compared to nearby sensors

Source: <https://doi.org/10.7289/V5XW4H05>

Among the five tests presented in Group I, only test number 4 was applied, as the remaining tests were made by SiMCosta team previously to data distribution, or not necessary (i., 3 and 5) similarly to test 6 of group II as samples were acquired at a fixed place and depth. Test 7 was not performed because climatological chlorophyll-a data for the region is non-existent, but the upper and lower limit values for $F_{chl-raw}$ were defined at 0.02 and 50 mg.m⁻³ respectively following the sensors range, meaning that values below 0.02 and above 50 mg.m⁻³ were excluded.

Optical data may show peaks of variation due to the presence of particulate aggregates in water (e.g. Briggs et al. 2011) and test 8 was applied to identify and remove this spurious data. For each N value in time series, this test determines if there is a N-1 data peak by subtracting the midpoint from N-2 and N assuming the absolute value of that amount to check whether it exceeds a low or high limit. The lower and

upper limits for $F_{chl-raw}$ values were determined from the mean value and standard deviation for the entire time series, that is mean of 1.74 mg.m^3 and standard deviation of 0.93 mg.m^3 . The values of 3.67 and 4.56 mg.m^3 represent respectively the mean value plus two and three times the standard deviation of fluorescence data. Values that did not reach any limit were considered good. Values above the two limits were considered bad and excluded.

To verify the rates of change in the time series, test 9 was applied. This test inspects a time series to identify a time change index that exceeds a threshold value. The limit value determined for this test was 4 mg.m^3 per hour and represents a variation of 3 standard deviations of the complete series over a one-hour interval. Values below the stipulated limit were considered good data. Values above the stipulated limit were considered suspect and excluded.

Test 10 has been applied to check for data records that do not vary with time. This attempts to inspect a time series to identify values that are not within a scalar limit for a period used by the operator. For this test, it was stipulated a period threshold of 3 and 6 hours without variation over than 0.01 mg.m^3 . If the data did not vary by more than 0.01 mg.m^3 over a 3 hours period, the data was suspect. If this inheritance exceeded 6 hours, the data were considered bad and excluded from the time series. Finally, a hierarchical sequence of QARTOD tests performed in this study followed the order: 4, 8, 9 and 10 presented at Table 2. The approved chlorophyll-a fluorescence data will be denominated hereafter as F_{chl} .

2.5 NONPHOTOCHEMICAL QUENCHING CORRECTING OF CHLOROPHYLL-A FLUORESCENCE

The measurement of chlorophyll-a concentration using *in situ* fluorescence is affected by nonphotochemical quenching (NPQ) processes, which suppress fluorescence emission under high light intensity. The NPQ mechanisms help phytoplankton cells to protect themselves when light energy exceeds their capacity of light utilization (Behrenfeld et al., 2009). During this photo-protection period, photosynthesis is inhibited and fluorescence yield drops (Müller et al., 2001), therefore, F_{chl} do not reflect the content of chlorophyll-a concentration in the phytoplankton cells. Several methods have been proposed to correct the NPQ effect and retrieve the actual Chl-a concentration. Most of them follow two steps: (i) compare the fluorometric reading (in $\text{mg}\cdot\text{m}^{-3}$) with Chl-a concentration determined by either high performance liquid chromatography (HPLC) analysis or fluorometric measurement in laboratory, which ensure that F_{chl} is appropriated calibrated; (ii) correction for quenching based on measurements made by the *in situ* fluorometer at night or at the some depth where the NPQ effect could be neglected.

The WQM sensors, factory calibrated, acquired simultaneously by SiMCosta were distributed in three different places: Rio Grande (RS), São Sebastião (SP) and Florianópolis (SC) The relationship between extracted chlorophyll-a and *in situ* WQM measurements were processed by the Center for Marine Biology from S'ao Paulo University (CEBIMar/USP) da Universidade de São Paulo (USP), using fluorescence methods (Welschmeyer,1994). The relationship between unquenched F_{chl} and extracted chlorophyll-a was robust ($r=0.90$, $N=23$, $p<0.05$) and followed (Bellini and Ciotti, unpublished data):

$$C_{flu} = 1.55 F_{chl}(unquenched) \quad (\text{eq. 3})$$

Roesler et al (2017) presented a global validation data set for the WQM WET Labs series of chlorophyll-a fluorometers. Their results were based on a comparison between High-performance liquid chromatography (HPLC) data and *in situ* fluorescence match ups after removing the NPQ in fluorescence readings, and suggested a calibration factor of 2. Thus, the slope of 1.55 was used to convert the F_{chl} corrected for quenching to chlorophyll-a concentration and the result parameter was denominated as C_{flu} .

2.6 QUALITY CONTROL OF SATELLITE-DERIVED CHLOROPHYLL-A CONCENTRATION

The quality of the C_{sat} estimates were assessed using the flags contained as metadata in the products made available by the Ocean Biology Distributed Active Archive Center (OB. DAAC) of NASA. The following flags (Table 3) were used to exclude doubtful pixels in each of the images analyzed: atmospheric correction failure (ATMFAIL), pixel over land (LAND), observed radiance very high or saturated (HILT) and probable cloud or ice contamination (CLDICE). The usage of probable stray light contamination (STRAYLIGHT) flag over a 3x3 pixel window matchup was also evaluated due to highly occurrence of good pixels masked by it. This quality control processing was implemented for all C_{sat} data before any matchup analysis.

Table 3 – Description of flags used in the satellite data quality control procedure.

Flags	Description
ATMFAIL	Atmospheric correction failure
LAND	Pixel is over land
HILT	Observed radiance very high or saturated
CLDICE	Probable cloud or ice contamination
STRAYLIGHT	Probable stray light contamination

Source: <https://oceancolor.gsfc.nasa.gov/atbd/ocl2flags/>

2.7 *IN SITU* AND SATELLITE CHLOROPHYLL-A MATCHUPS

Satellite chlorophyll-a estimates between 2017, February 22 and 2019, November 17 were used in this work due to the availability of *in situ* data. To avoid the use of doubtful data through validation procedures highlighted by [Bailey and Werdell \(2006\)](#), this study adopted the subsequent criteria in the matchups. First, the quality flags were used to check all C_{sat} data prior to the analyses. The following flags were applied for L2 level data: ATMFAIL, LAND, HILT, CLDICE. In addition, the flag STRAYLIGHT was tested from its non-application until all pixels were verified. This last flag was considered to evaluate if the exclusion of unreliable data was not overestimated. A window of 3 x 3 pixels was fixed centered at SiMCosta-SC01 moored buoy position. We present here, the results with non- application of STRAYLIGHT flag and with application of it for more than 5 valid pixels in the 3x3 pixels window. The coefficient of variance (CV) was computed for each window as the spatial uniformity criterion for matchups. High CV indicates high variability within selected pixels and this effect could probably be caused by frontal zones or cloud edges. Those 3x3 pixel windows that presented CV value larger than 0.15 were excluded and, for the remaining ones, the median value was calculated. Finally, the absolute time interval

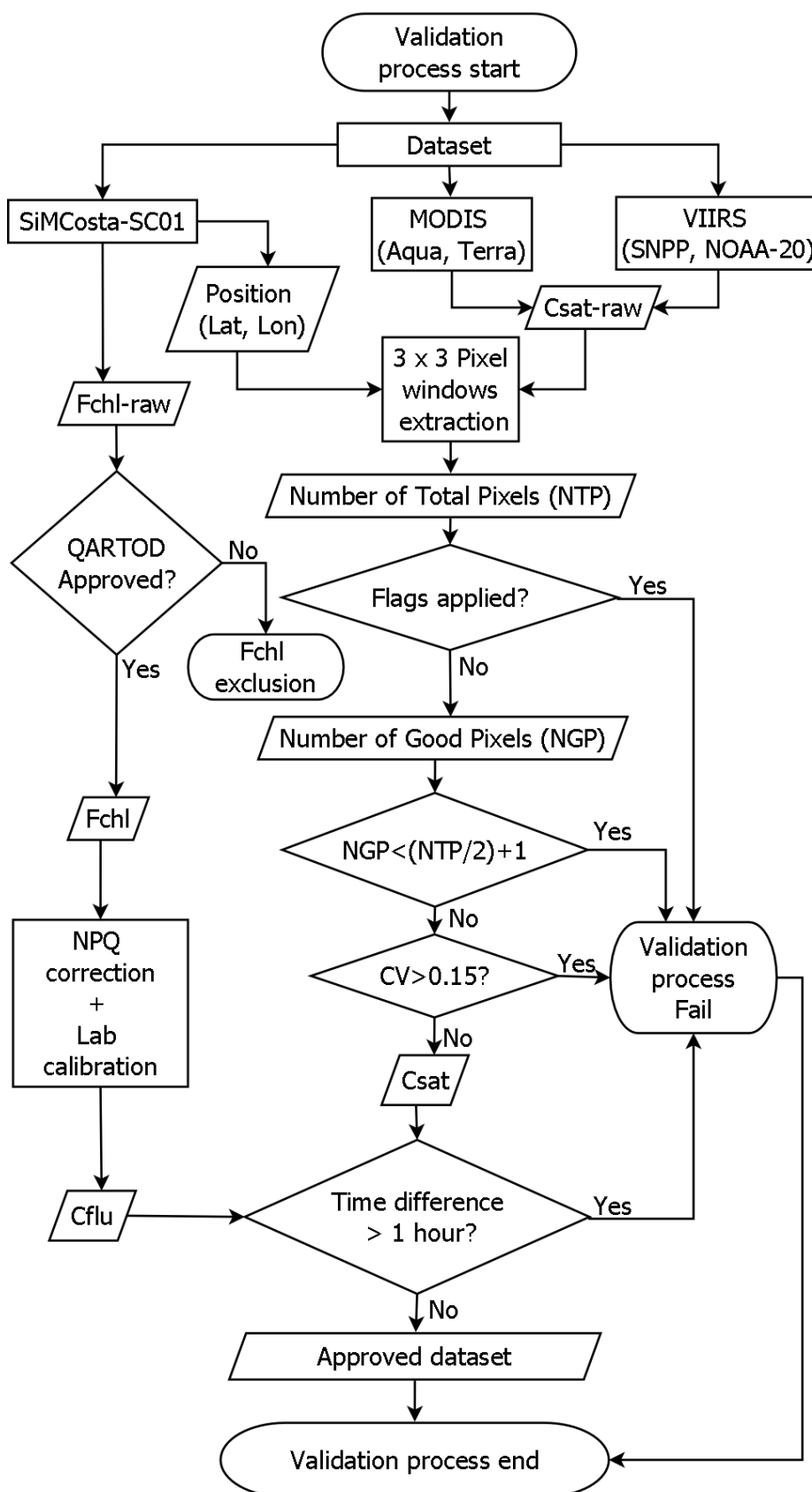
between satellite overpass and *in situ* fluorescence measurements should be less than 1 hour, which is more restrict than the criteria described in Bailey and Werdell (2006), but it is in agreement with the premisses presented by Carberry et al (2019), due to the availability of in situ data. In case of two C_{flu} measurements within the fixed +/- 1 hour interval, their mean value was used in the matchup procedure.

In this work, we have processed 5,074 L2 images (Table 4), which were downloaded from <http://oceancolor.gsfc.nasa.gov>. The software Windows Image Manager (WIM) and Python programming language were used to execute all matchups processing steps presented above and summarized in the flowchart shown in Figure 2.

Table 4 – Number of MODIS-Aqua, MODIS-Terra, VIIRS-SNPP and VIIRS-JPSS1 ocean color images investigated in this study. The Level 2 images contain calibrated and geolocated radiances, chlorophyll, and quality flags.

Year	MODIS-Aqua	MODIS-Terra	VIIRS-SNPP	VIIRS-JPSS1	Total
2017	376	395	372	25	1168
2018	460	487	573	543	2063
2019	412	443	495	494	1844
Total	1248	1325	1440	1062	5074

Figure 2 – Flowchart adopted in this work to evaluate satellite chlorophyll-a concentration algorithms. Adapted from Bailey and Werdell (2006).



2.8 ALGORITHMS PERFORMANCE EVALUATION

A variety of statistical and graphical criteria were used to evaluate the performance of satellite Chl-a algorithms. This study followed some recommendations by [Seegers et al. \(2018\)](#) and [Pereira et al \(2018\)](#). The performance of each algorithm was evaluated through statistical comparisons based on linear and log-transformed data. The following metrics were used to assess the performance of each Chl-a algorithm: slope and intercept of the reduced major axis linear regression analysis, coefficient of determination (R^2), root mean square error (RMSE, equation 4), BIAS (equation 5), mean absolute error (MAE, equation 6), relative percent difference (RPD, equation 7) and absolute percent difference (APD, equation 8).

$$\text{RMSE} = \sqrt{\frac{\sum_{n=1}^N (e_n - o_n)^2}{N}}, \sqrt{\frac{\sum_{n=1}^N (\log_{10} e_n - \log_{10} o_n)^2}{N}} \quad (\text{eq. 4a, 4b})$$

$$\text{BIAS} = \frac{\sum_{n=1}^N (e_n - o_n)}{N}, 10^{\wedge} \left(\frac{\sum_{n=1}^N \log_{10}(e_n) - \log_{10}(o_n)}{N} \right) \quad (\text{eq. 5a, 5b})$$

$$\text{MAE} = \frac{\sum_{n=1}^N |e_n - o_n|}{N}, 10^{\wedge} \left(\frac{\sum_{n=1}^N |\log_{10}(e_n) - \log_{10}(o_n)|}{N} \right) \quad (\text{eq. 6a, 6b})$$

$$\text{RPD} = \frac{\sum_{n=1}^N \frac{(e_n - o_n)}{o_n}}{N} \times 100, \frac{\sum_{n=1}^N \frac{(\log_{10}(e_n) - \log_{10}(o_n))}{\log_{10}(o_n)}}{N} \times 100 \quad (\text{eq. 7a, 7b})$$

$$\text{APD} = \frac{\sum_{n=1}^N \left| \frac{e_n - o_n}{o_n} \right|}{N} \times 100, \frac{\sum_{n=1}^N \left| \frac{\log_{10}(e_n) - \log_{10}(o_n)}{\log_{10}(o_n)} \right|}{N} \times 100 \quad (\text{eq. 8a, 8b})$$

In the above equations, o_n and e_n are respectively C_{flu} (observed) and C_{sat} (estimated) data, and \bar{e} and \bar{o} are their respective means. Equations 4a, 5a, 6a and 7a are used for chlorophyll-a data and 4b, 5b, 6b, 7b and 8b for log-transformed chlorophyll-a data.

3 RESULTS

3.1 IN SITU CHLOROPHYLL-A FLUORESCENCE

The hourly F_{chl} data collected over a period of almost 3 years shows that several continuous gaps exist due to the maintenance procedure when all oceanographic sensors were taken to laboratory for inspection and clearance (Figure 3). The total period of maintenance corresponds to approximately 27% of the entire period. From the 73% of $F_{chl-raw}$ data, only 1.3% was filtered out by the QARTOD data quality control procedure, which confirms the high quality of the fluorescence data. The F_{chl} time series spans from Feb 2017 to Nov 2019 (Figure 3). Table 5 shows a statistical description of qualified and C_{flu} data.

Figure 3 – Temporal series of hourly F_{chl} data (black dots) approved by the SiMCosta data quality control system. The gaps (blue stripes) correspond to 35.6% of the entire dataset, and usually they are associated with maintenance of sensors and/or electrical failure of the power system of the SiMCosta-SC01 buoy.

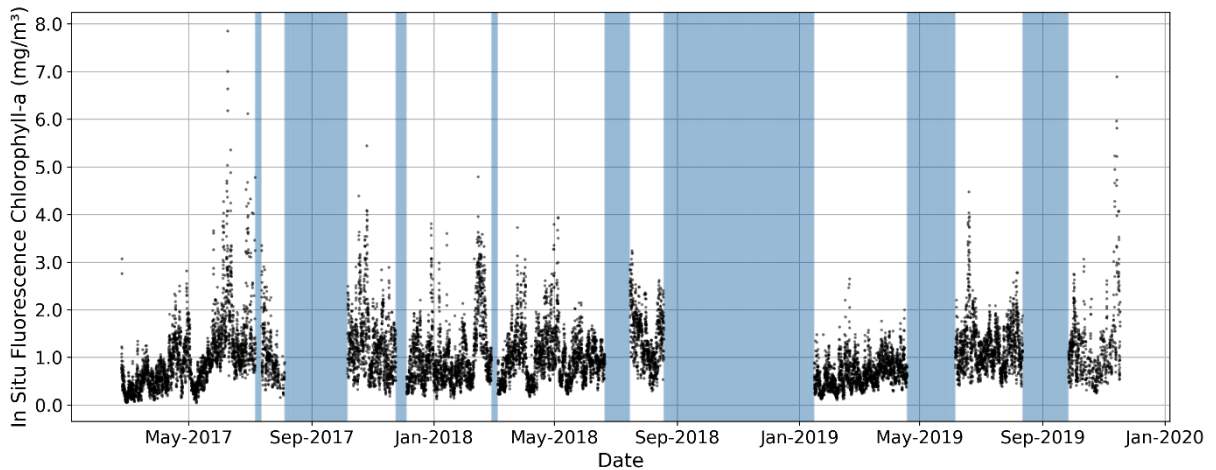


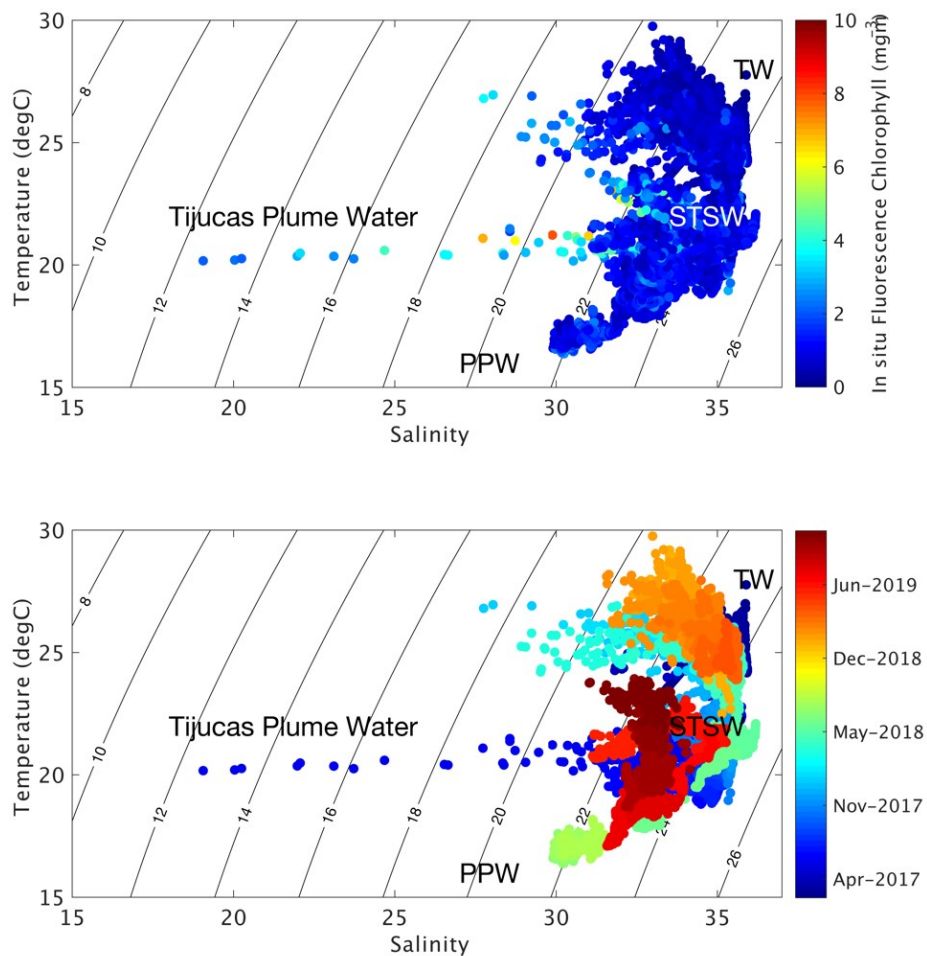
Table 5 – Number of F_{chl} measurements, minimum, mean, maximum and standard deviation of F_{chl} data in 2017, 2018 and 2019. The period of data collection spans from Feb 2017 to Nov 2019.

Year	Number of samples	Minimum (mg/m ³)	Mean (mg/m ³)	Maximum (mg/m ³)	Standard deviation (mg/m ³)
2017	5139	0.11	1.73	9.58	1.00
2018	4724	0.31	1.88	7.43	0.94
2019	4237	0.22	1.61	9.01	0.82
Total	14100	0.11	1.74	9.58	0.93

3.2 SURFACE WATER MASSES

The collection of data by the WQM sensor also includes both sea surface temperature and salinity. Figure 4 shows TS diagrams with F_{chl} (Figure 4a) and date (Figure 4b) as a third variable in the diagrams. Most of salinity values were above 32, therefore, estuarine waters rarely reach SiMCosta-SC01 buoy. Only in April 2017 when Tijuca river plume reaches the buoy, salinity values were of about 17 units. Salinity values were higher than 32 most (92 %) of the recorded time.

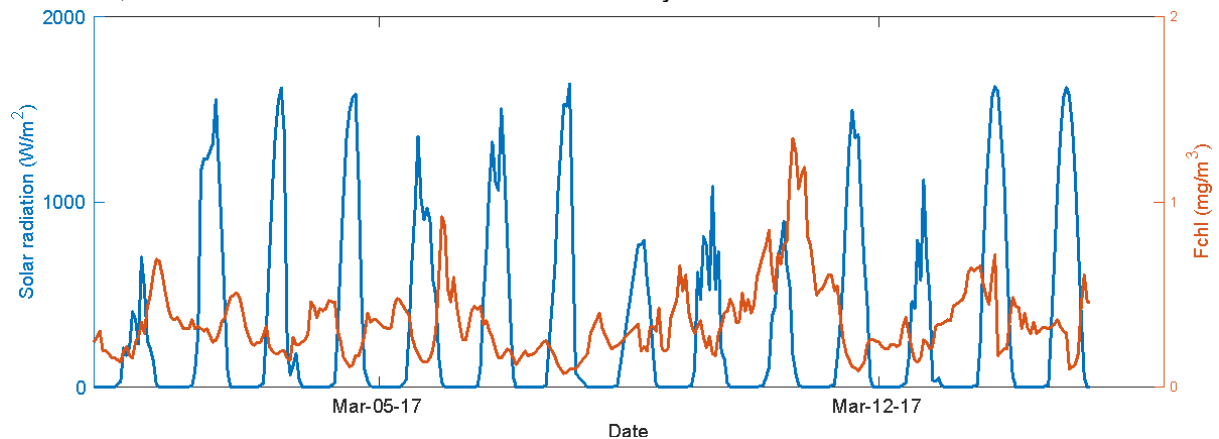
Figure 4 – TS-fluorescence (a) and TS-time (b) diagrams. TW, STSW and PPW stand for Tropical Water, Subtropical Shelf Waters and La Plata Plume Water. The effect of the plume of Tijuca river on the local thermohaline properties is also shown.



3.3 THE QUENCHING CORRECTION PROCEDURE

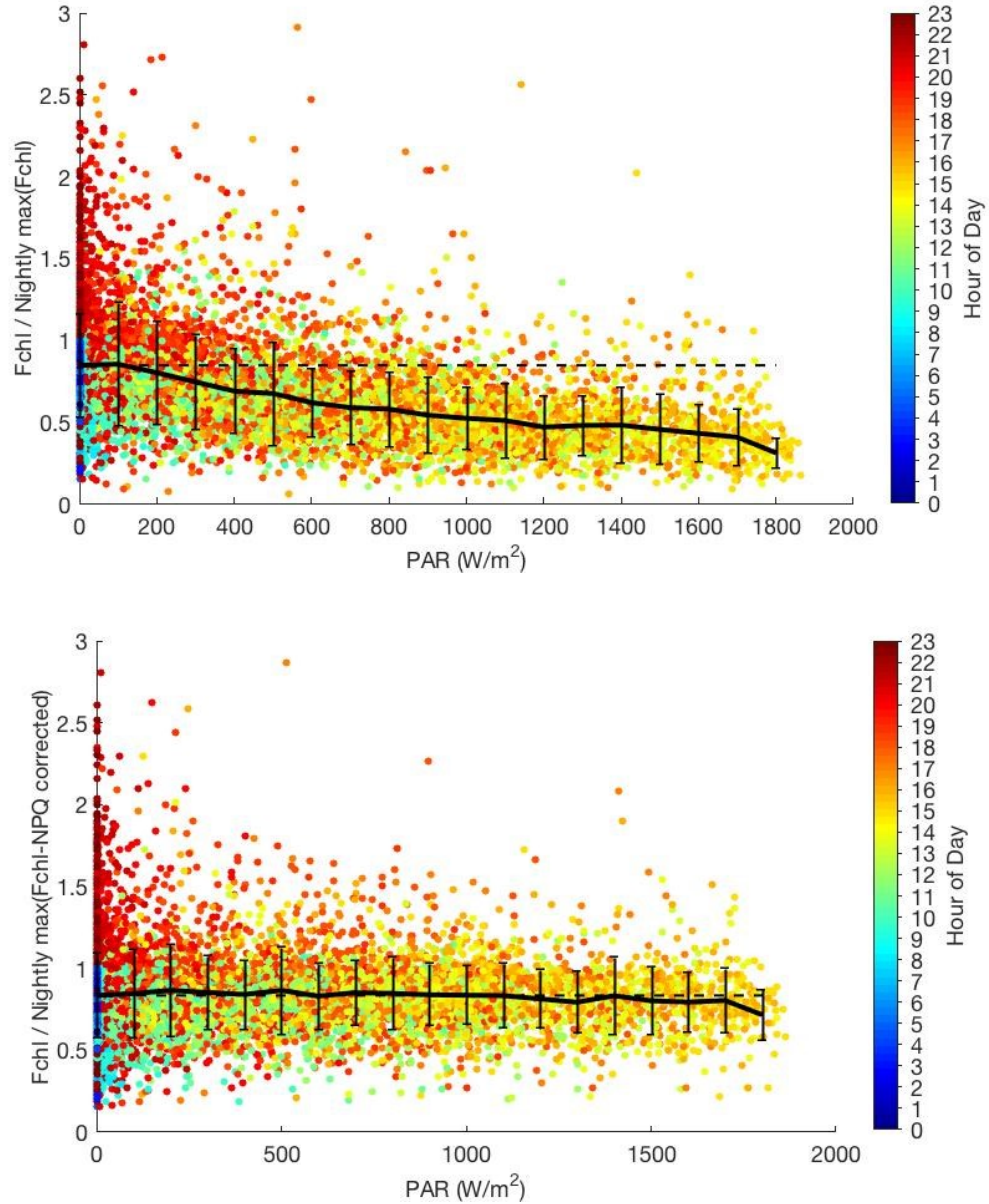
The observed decrease in fluorescence values in nature appears when the phytoplankton cells absorb sunlight energy but photoprotective mechanisms present in phytoplankton cells avoid photodamage under excessive sunlight. Therefore, daylight F_{chl} values are usually smaller than nighttime values (Figure 5).

Figure 5 – Evolution of hourly solar radiation and *in situ* chlorophyll-a fluorescence (F_{chl}) from March 1 to 14, 2017. The NPQ effect can be observed in daytime when fluorescence values decrease.



The influence of NPQ on F_{chl} estimates can be also clearly seen when each F_{chl} measurement is normalized by their respective nightly maximum value (Carberry et al., 2019). Figure 6 shows an example of the NPQ effect on daytime F_{chl} recorded by the WQM sensor at SiMCosta SC01. The dependence of F_{chl} on PAR was noticeable when PAR values were above 200 Wm^{-2} . Furthermore, such dependence is not contingent on the hour of day (Figure 6a), since measurements can be made in very cloudy days when PAR measurements are relatively low. On the other hand, after NPQ correction, the ratio of F_{chl} to its respective maximum nighttime value, showed only a small dependence on PAR after 1200 Wm^{-2} (Figure 6b). The overall behavior of NPQ-corrected F_{chl} with solar irradiance data (Figure 6b) suggests a successful approach to correct quenching on *in situ* fluorescence chlorophyll-a values.

Figure 6 – The ratio maximum nighttime F_{chl} to F_{chl} for non-quenching (a) and quenching-corrected (b) measurements as function of incident PAR over SiMCosta SC01. The dashed line represents the mean value of the ratio at nighttime when solar radiation is null. Median and standard deviation of F_{chl} values are shown by solid black line and error bars, respectively, at PAR intervals of 100 W/m^2 . The colors are associated with the hour (GMT time) of the day.



3.4 EVALUATION OF OPERATIONAL CHLOROPHYLL CONCENTRATION ALGORITHMS

The validation criteria adopted here to evaluate operational Chl-a algorithms allowed us to obtain 506 paired of C_{flu} and C_{sat} data being 222 pairs for MODIS and

284 for VIIRS. This relatively high number of paired chlorophyll values was achieved when flags ATMFAIL, LAND, CLDICE, HILT were applied. The frequency distribution of C_{flu} and C_{sat} paired data are quite similar (Figure 7), where mean and standard deviation values for C_{flu} and C_{sat} were 1.83 ± 0.86 and 1.76 ± 0.87 mg m^{-3} , respectively. Table 6 provides the basic statistical data C_{flu} and C_{sat} paired data for MODIS and VIIRS sensors. If we use the STRAYLIGHT flag, there is a substantial reduction in the number of C_{sat} data. For instance, if we consider that at least 5 out of 9 pixels (window size) are not contaminated by straylight, then the number of paired chlorophyll data decreases to 56 pairs for MODIS and 64 for VIIRS, and the mean and standard deviation values for C_{flu} and C_{sat} were 1.76 ± 0.72 and 1.82 ± 0.82 mg m^{-3} , respectively.

Figure 7 – Distribution of 506 paired data which were considered valid for the match-up procedure between C_{flu} (blue color) and C_{sat} (orange color). The mean and standard deviation values for C_{flu} and C_{sat} were 1.83 ± 0.86 and 1.76 ± 0.87 mg m^{-3} , respectively.

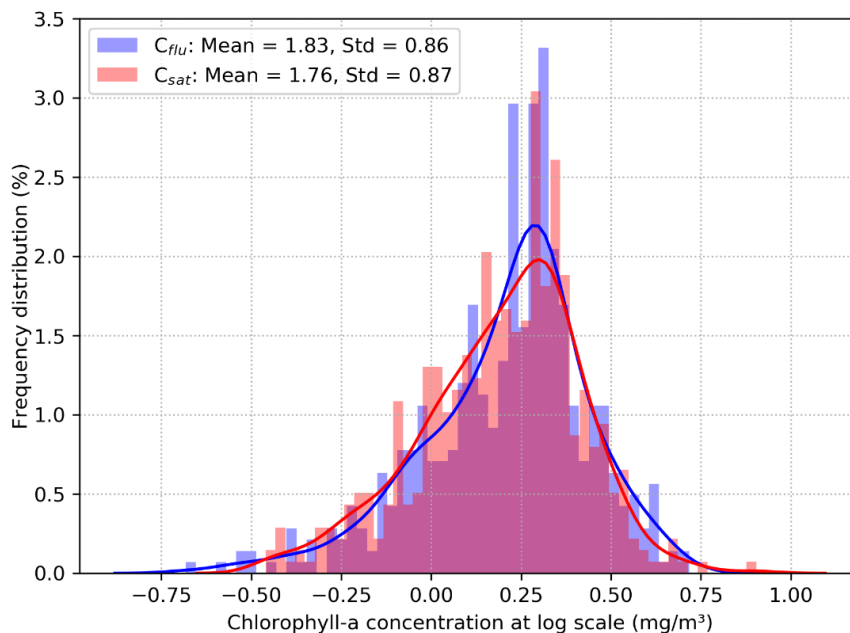


Table 6 – Description of matchup results by each sensor.

Sensor	Number of samples	C_{flu} (mg/m^3)				C_{sat} (mg/m^3)			
		Min	Max	Mean	Std	Min	Max	Mean	Std
MODIS	222	0.21	4.60	1.81	0.83	0.37	5.79	1.97	0.85
VIIRS	284	0.26	5.22	1.84	0.88	0.35	8.02	1.59	0.84

4 DISCUSSION

4.1 THE CORRECTION FOR NONPHOTOCHEMICAL QUENCHING

The correction of F_{chl} for nonphotochemical quenching (NPQ) in ocean surface waters is not a simple task. In cases where F_{chl} is available for the entire water column in open ocean waters, one can assume that fluorescence signal does not suffer from NPQ in deep water and the decrease of F_{chl} occurs only at mixed layer ([Sackmann et al., 2008](#)). For instance, Xing et al (2018) have corrected the NPQ effect in thousands of fluorescence profiles measured by instrumented elephant seals in the Kerguelen region (Southern Ocean) by making an extrapolation of the deep fluorescence value toward the surface. In coastal waters, if advection of surface waters plays an important role in phytoplankton biomass variability within the diurnal cycle, then a complex procedure should be used to correct for the advection of water within the tidal cycle. Carberry et al. (2019) used the unquenched nighttime observations and measured current velocity data to correct for both NPQ effect and local advection in a tidally dominated narrow inlets that comprise Casco Bay in Maine (USA).

[Dalbosco et al. \(2020\)](#) analyzed the contribution of tidal and meteorological forcing on the alongshore and cross-shore components of currents obtained by an ADCP installed close (< 5 nm) to the SiMCosta-SC01 buoy in the Rebio Arvoredo region. They concluded that a predominance of southward flow (68.5%) was found in the alongshore component, with an average of 0.18 m/s. The decomposition in variance of the barotropic component of current has shown that only 13% is due to tidal forcing, and 87% of the energy was on the subtidal frequency where winds are the most important forcing mechanism driving these shallow waters. This suggests that the variability of phytoplankton biomass at SiMCosta-SC01 is expected to occur on

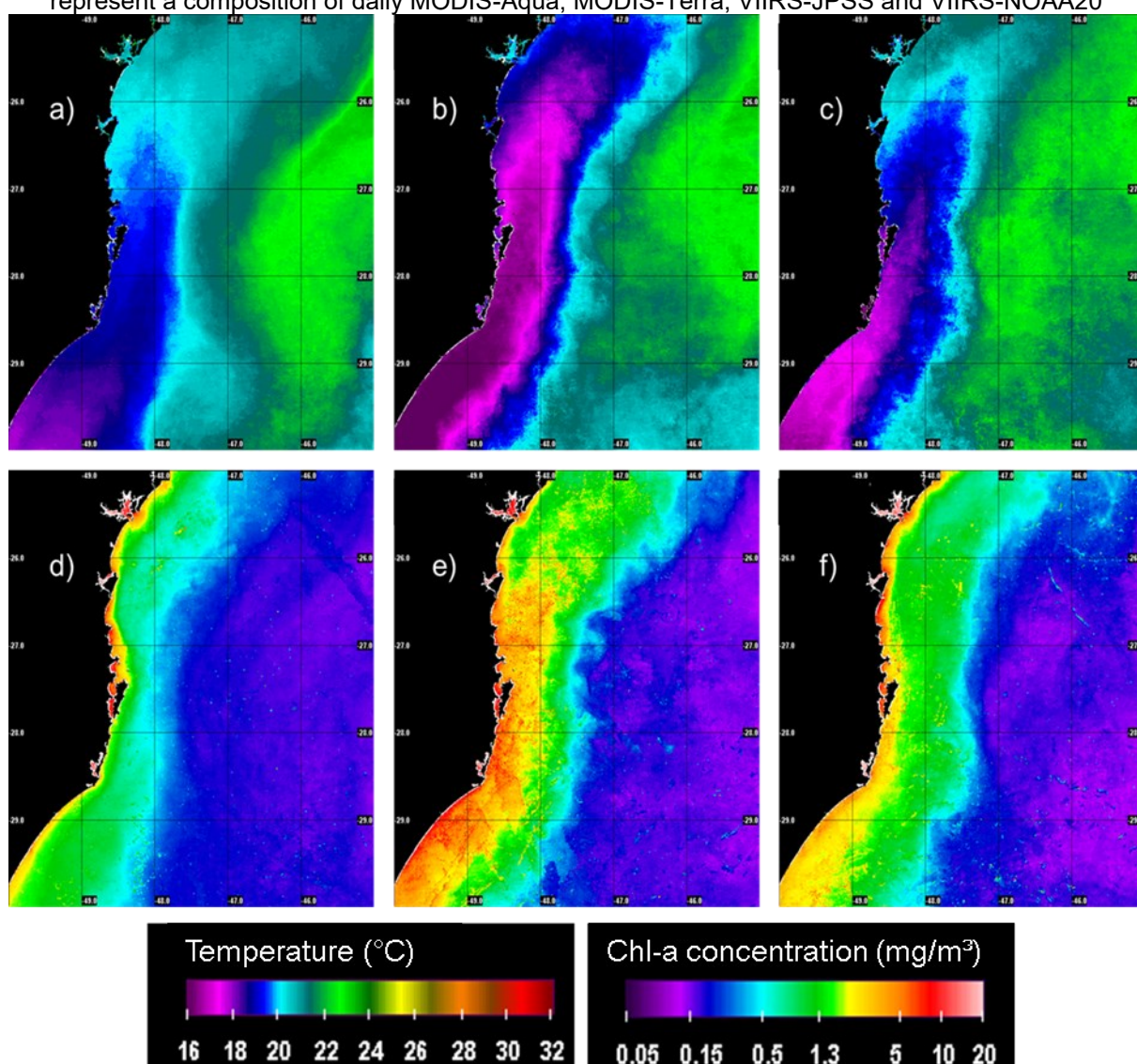
timescales longer than the diurnal cycle. Therefore, daylight fluorometric measurements could be replaced to a first approximation by interpolation between F_{chl} measurements at sunrise and sunset on a daily basis, which was successfully done in this study (see Figure 7b) to correct the NPQ effect on F_{chl} measurements.

4.2 VARIABILITY OF SURFACE WATER MASS

The studied region is regularly occupied by Subtropical Shelf Water (STSW) (Bordin et al, 2019) – a mixture of La Plata Plume Water (PPW) and Tropical Water (TW) (Moller et al, 2008) – with higher influence of PPW (TW) in wintertime (summertime) (Moller et al, 2008; Bordin et al 2019). The influence of PPW in the thermohaline properties occurred during wintertime (Figure 4b), when a series of cold frontal passages crossed the southern portion of Brazil and brought cold and less saline waters from the Uruguayan coast northwards along the Brazilian coast. The presence of colder and less saline waters of the La Plata plume over the southern Brazilian coast has been extensively studied (Piola et al, 2005; Moller et al, 2008, Garcia and Garcia, 2008; Bordin et al, 2019). The incursion of these waters along the southern inner shelf depends on the magnitude of the La Plata discharge and the intensity, direction and duration of the wind stress (Piola et al, 2005). TS-diagrams have shown that La Plata plume waters had a more pronounced influence in 2018 than in 2019 (Figure 4b). A close inspection of monthly mean of sea surface temperature and Chl-a surface concentration images of July 2017, 2018 and 2019 (Figure 8) showed that indeed the stronger intrusion of cold and less saline waters happened in 2018. Most of the time, the studied region was occupied by STSW water, with influence of TW in summer and PPW in wintertime. The Tijucas river outflow was reduced to the

vicinities of its mouth, reaching the position of SiMCosta-SC01 buoy in a very rare occasion (Figure 4a and Figure 4b). Therefore, in almost the entire period of study, the organic and inorganic material derived from Tijucas outflow did not reach the near surface waters sensed by buoy SiMCosta-SC01.

Figure 8 – Monthly mean MODIS/VIIRS composite of daily sea surface temperature (SST) in July 2017 (a), July 2018 (b) and July 2019 (c) and monthly mean MODIS/VIIRS composite of daily chlorophyll-a surface concentration in July 2017 (d), July 2018 (e) and July 2019 (f). The SST images were derived from the NLSST algorithm and represent a composition of daily MODIS-Aqua, MODIS-Terra, VIIRS-JPSS and VIIRS-NOAA20



4.3 ON THE VALIDATION OF SATELLITE ESTIMATES OF CHLOROPHYLL-A CONCENTRATION

In this work, an effort was made to infer the consequences of using pixels contaminated and not contaminated by straylight. The overall values of the metrics used in the validation procedure here are quite similar (Table 7), either if we consider STRAYLIGHT flag off (Figure 9) or we use at least 5 pixels (in the 3x3 pixels window) not contaminated with STRAYLIGHT (Figure 10).

Table 7 – The values of the metrics used to evaluate existing operational chlorophyll-a algorithms. The results from the linear regressions between C_{flu} and C_{sat} , either in linear or logarithm form, presented statistical significance at 90% level when straylight flags was not applied. Linear and Log10 stand for RMA linear regressions between C_{flu} and C_{sat} and $\log_{10}(C_{flu})$ and $\log_{10}(C_{sat})$, respectively.

Sensor matchup statistics	Valid Straylight Flag	N	Slope	Intercept	R ²	MAE (mg/m ³)	RMSE (mg/m ³)	BIAS (mg/m ³)	APD (%)	RPD (%)
MODIS Linear	Not applied	222	1.02	0.13	0.96	0.50	0.16	0.16	33.40	17.97
	5	56	0.99	0.21	0.93	0.38	0.20	0.20	27.21	18.59
VIIRS Linear	Not applied	284	0.96	-0.17	0.92	0.59	0.25	-0.25	30.95	-5.29
	5	64	1.37	-0.63	0.86	0.54	0.04	0.04	32.73	10.24
MODIS Log	Not applied	222	0.92	0.06	0.96	1.34	0.05	1.11	115.78	-30.25
	5	56	0.86	0.08	0.93	1.25	0.06	1.14	79.12	7.65
VIIRS Log	Not applied	284	0.97	-0.06	0.88	1.41	0.06	0.86	149.99	1.51
	5	64	0.96	0.02	1.00	1.34	0.01	1.01	174.25	-115.26

Figure 9 – Comparisons between C_{flu} and C_{sat} for sensor MODIS and VIIRS at linear (a and b) and logarithm (d and e) scales using no straylight flag. The star plots of the metrics used to compare C_{flu} and C_{sat} at linear (c) and logarithm (f) scales are also shown.

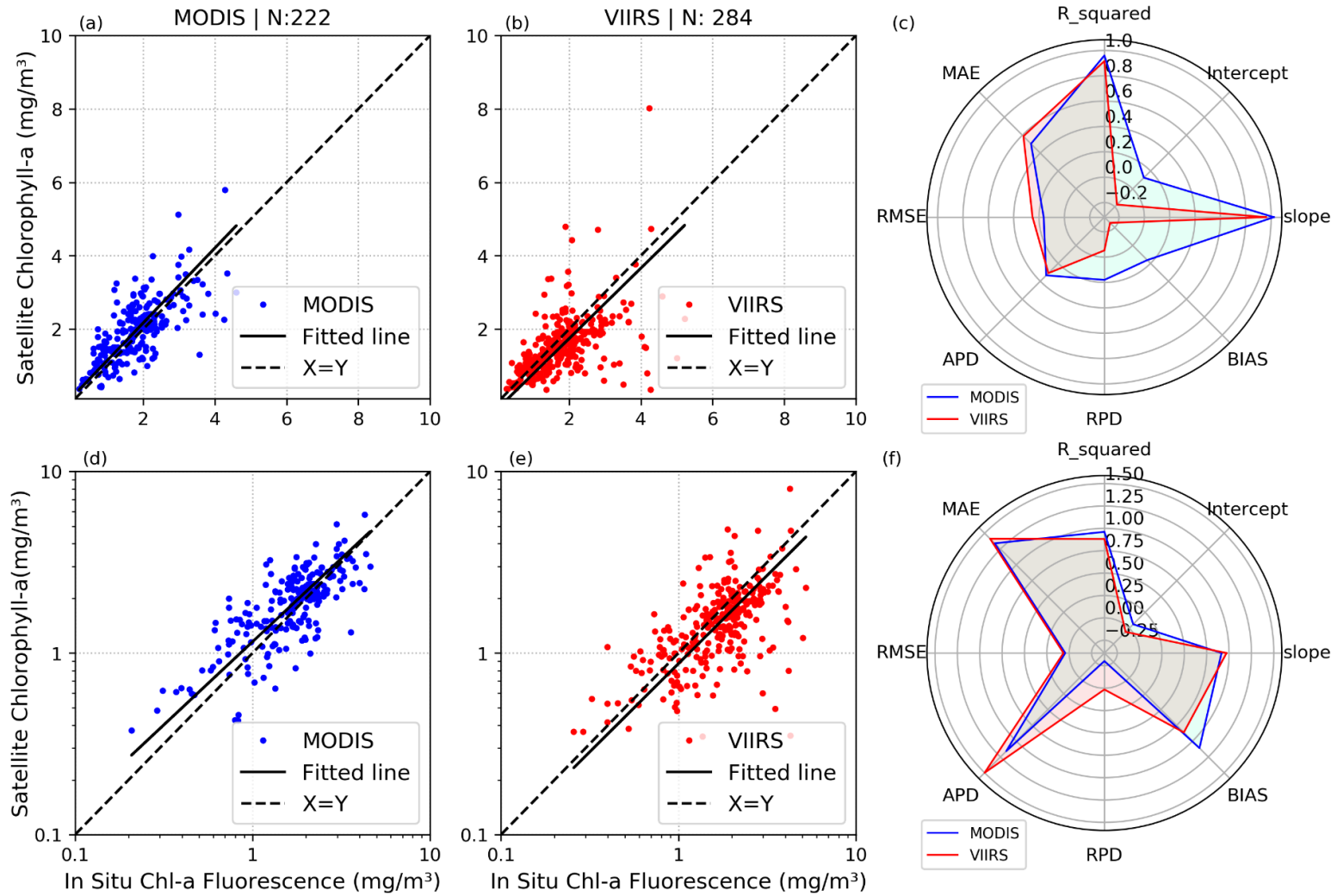
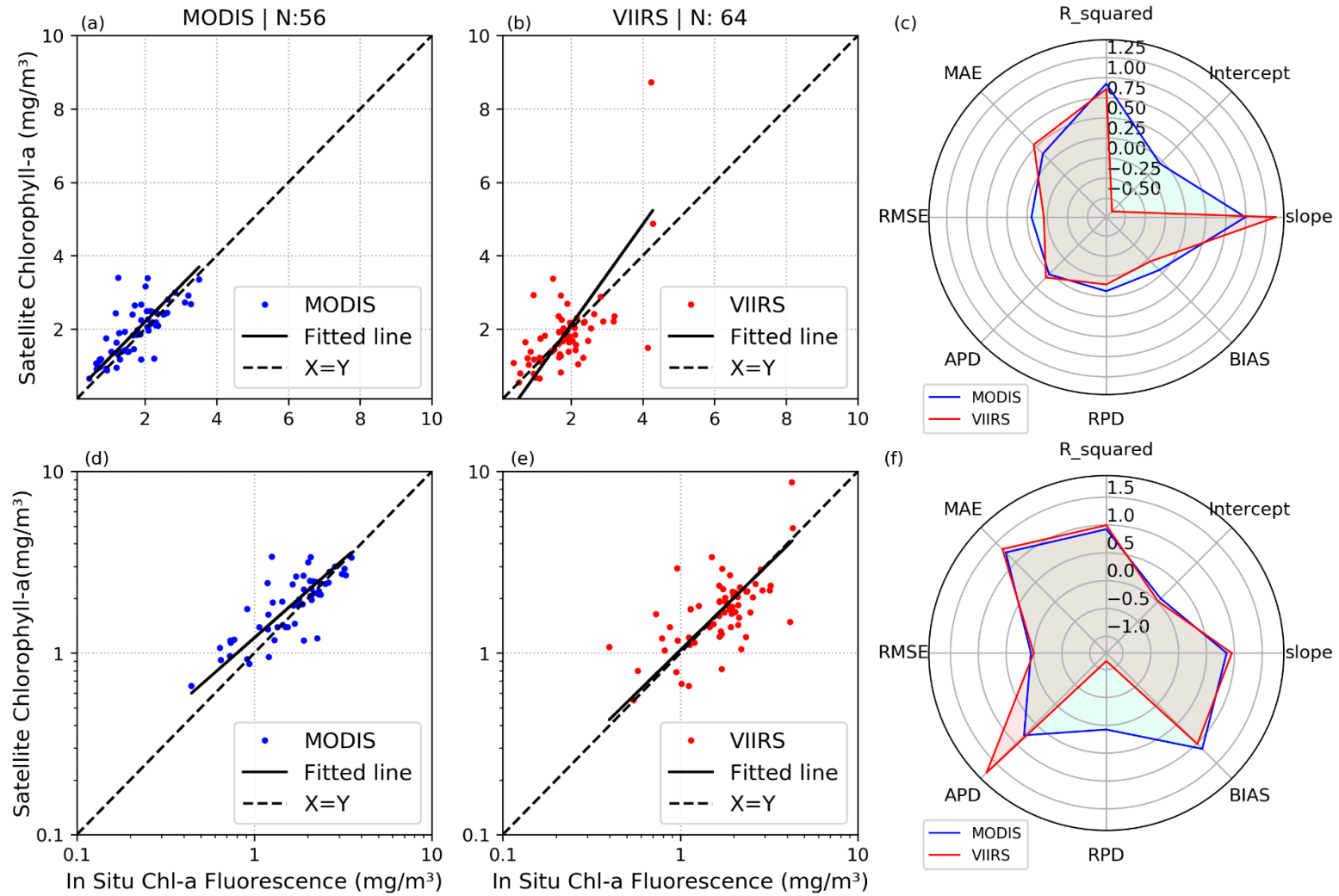


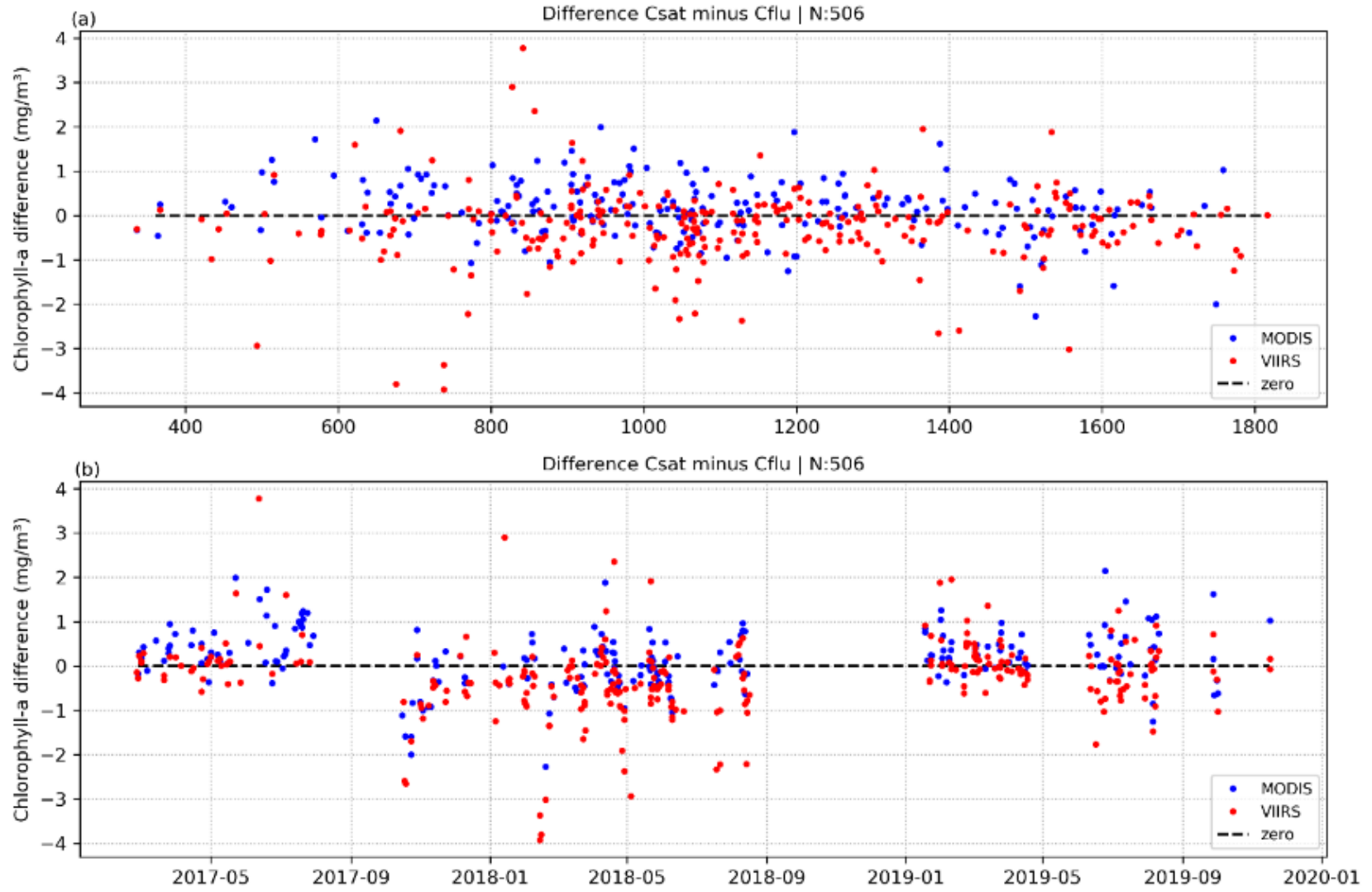
Figure 10 – Comparisons between C_{flu} and C_{sat} for sensor MODIS and VIIRS at linear (a and b) and logarithm (d and e) scales using straylight flags (at least 5 valid pixels). The star plots of the metrics used to compare C_{flu} and C_{sat} at linear (c) and logarithm (f) scales are also shown.



The high quality L2 images provided by the operational chlorophyll algorithm for MODIS and VIIRS sensors uses a 7x5 pixel window around the pixels classified as cloud to mask the straylight contamination (Feng and Hu, 2016). Usually the straylight can be noticeable in the vicinity of pixels masked as cloud or land and can extend for several pixels from the source. This 7x5 pixels straylight window in the masking method has been subject of analysis by several researchers (Sterckx et al, 2011; Jiang and Wang, 2013; Feng and Hu, 2016). Feng and Hu (2016) suggested that the current MODIS straylight masking 7x5 pixels window may be relaxed to 3×3 without losing data quality. Essentially, for MODIS and VIIRS (most sensors in fact) the STRAYLIGHT flag is effectively a dilation of the CLDICE (and/or HILT) flags.

Our results reinforce such change in the window size used by NASA operating chlorophyll algorithms to mask pixels contaminated by straylight. In addition, our results have also shown that the differences between C_{sat} and C_{flu} do not depend on PAR measurements (Figure 11a) and time of year (Figure 11b), which reflects the good correction for nonphotochemical quenching in the measurements of *in situ* chlorophyll-a fluorescence data.

Figure 11 – Dependence of the difference between C_{sat} and C_{flu} on PAR measurements (a) and along the almost 3-year period (b).



5 CONCLUSION

In this study, we investigated the uncertainties of standard chlorophyll-a algorithms in the southern Brazilian inner shelf using *in situ* chlorophyll-a fluorescence data provided by a WQM sensor placed on the SiMCosta-SC01 buoy located in Rebio Arvoredo. Prior to any analysis, a rigid quality data control was used on both *in situ* fluorescence and satellite-derived chlorophyll concentration based on SiMCosta/QUARTOD and NASA data quality control, respectively. The surface water in the area under investigation is mainly composed of Subtropical Shelf Waters with little influence of nearby river outflows which could insert a complexity on the optical properties of surface waters. After the successful removal of the NPQ effect on fluorescence readings, their values were calibrated with laboratory chlorophyll-a concentration. We ended up with a time series of 14,100 hourly *in situ* chlorophyll-a concentration to be compared with satellite-estimates. Among the tested ocean color algorithms used on MODIS and VIIRS sensors, the MODIS algorithm yielded the best performance results, although VIIRS presented relatively good performance. Overall, the time series analysis of the *in situ* and satellite-derived Chl-a values agreed well, which suggest the use of the standard MODIS and VIIRS chlorophyll algorithms for the region. The procedure adopted here to evaluate existing operational algorithms can be applied to other Brazilian coastal regions with relatively low turbid waters. Despite our results, the collection of *in situ* spectral reflectance data in conjunction with chlorophyll-a concentration is highly desirable to create a regional algorithm to monitor Chl-a with higher accuracy.

6 ACKNOWLEDGEMENTS

This work received funding from the Brazilian Coastal Monitoring System (SiMCosta) team and their support is gratefully acknowledged. SiMCosta is funded by Fundo Clima, the Ministry of Environment and the Ministry of Science, Technology and Innovation. A number of field assistants were involved in the deployment of the buoy SiMCosta SC01 and we are particularly grateful to all of them. A special thank you to Ella S. Pereira, national manager of SiMCosta. To A.M. Ciotti and C. Belinni for the data of relationship between extracted chlorophyll-a and in situ WQM measurements and to A.M. Ciotti for previously revised this manuscript. The US NASA space agency and Ocean Biology Processing Group (OBPG) is thanked for the easy access to MODIS and VIIRS data.. A crucial and indispensable thank you to the Federal University of Santa Catarina and to the Postgraduate Program in Oceanography that provided Gabriel S. de M. Silva the opportunity for a public and high-quality academic training. This scientific article is a contribution resulting from public investment in oceanography and emphasizes the importance of promoting R&D in Brazil. The manuscript was previously revised by A.M. Ciotti.

7 AUTHOR CONTRIBUTION STATEMENT

G.S.M.S and C.A.E.G. conceived of the presented idea of comparing satellite data with fluorescence time series collected at buoy SiMCosta-SC01. Both authors analyzed water mass and proposed correction on quenching. G.S.M.S. performed all comparisons

between in situ and satellite images, including statistical analysis. Both authors discussed the results and contributed to the final manuscript.

3 CONCLUSÃO

Neste estudo, investigamos as incertezas dos algoritmos de clorofila-a, utilizados por padrão pela NASA, na plataforma interna do sul do Brasil usando dados de fluorescência da clorofila-a in situ fornecidos por um sensor WQM colocado na boia SiMCosta-SC01 localizada em Rebio Arvoredo. Antes de qualquer análise, um controle rígido de dados de qualidade foi usado na fluorescência in situ e na concentração de clorofila derivada de satélite com base no controle de qualidade de dados SiMCosta / QUARTOD e NASA, respectivamente. A água superficial na área sob investigação é composta principalmente de Águas Subtropicais de Plataforma com pouca influência das vazões de rios próximos, o que poderia inserir uma complexidade nas propriedades ópticas das águas superficiais. Após a remoção bem-sucedida do efeito NPQ nas leituras de fluorescência, seus valores foram calibrados com a concentração de clorofila-a de laboratório. Terminamos com uma série de tempo de 14.100 horas de concentração de clorofila a in situ para ser comparada com estimativas de satélite. Entre os algoritmos de cor do oceano testados usados em sensores MODIS e VIIRS, o algoritmo MODIS apresentou os melhores resultados de desempenho, embora o VIIRS tenha apresentado desempenho relativamente bom. No geral, a análise das séries temporais dos valores de Chl-a derivados de satélite e in situ concordaram bem, o que sugere o uso dos algoritmos de clorofila MODIS e VIIRS padrão para a região. O procedimento aqui adotado para avaliar algoritmos operacionais existentes pode ser aplicado a outras regiões costeiras brasileiras com águas turvas relativamente baixas. Apesar de nossos resultados, a coleta de dados de refletância espectral in situ em conjunto com a concentração de clorofila-a

é altamente desejável para criar um algoritmo regional para monitorar Chl-a com maior precisão.

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