UNIVERSITÉ DU QUÉBEC À RIMOUSKI



DYNAMIQUE DU PHYTOPLANCTON DANS LE SYSTÈME DE LA BAIE DHUDSON : UNE PERSPECTIVE PAR CAPTEUR SATELLITAIRE DE LA COULEUR DE LOCÉAN

« Phytoplankton dynamics in the Hudson Bay System: an ocean color satellite perspective »

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PAR

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Dedicated to my family.

To recognize all the love, patience, and support on this great journey. I thank my parents José Flávio and Ruth Maria, my wife Daniela, my daughter Nicole, Melissa, and the arrival of my son Caetano.

| "Rien à craindre | "Nada a temer |
|---------------------------|------------------------|
| Sinon, la fuite du combat | Senão o correr da luta |
| Rien à faire | Nada a fazer |
| Mais oubliez la peur" | Senão esquecer o medo" |
| | |

Fragment of "Caçador de mim", a music of Milton Nascimento, original composition in Portugues by Sérgio Magrão and Luiz Carlos Sá.

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Résumé

Dans l'océan Arctique et les mers sub-Arctiques, le réchauffement et les pertes de glace de mer constituent des changements climatiques marquants de cette nouvelle Ère que l'on nomme désormais l'Anthropocène. Ces changements spectaculaires imposent un ajustement de la dynamique du phytoplancton, ce qui affecte l'ensemble du réseau trophique marin, la fonctionnalité des écosystèmes et la pompe à carbone. Dans le système de la baie d'Hudson, la plus grande mer intérieure du monde, la perte de glace de mer est deux fois plus importante que celle observée dans l'océan Arctique, et les taux de réchauffement atmosphérique sont plus rapides que ceux enregistrés à la fin de la dernière période glaciaire, il y a environ 12 000 à 11 000 ans. La radiométrie satellitaire de la couleur de l'océan (OCR) est l'outil le plus approprié pour l'observation systématique du phytoplancton, en particulier dans les environnements difficiles d'accès et les mers infestées de glace. Cependant, les communautés d'algues adaptées à une faible luminosité solaire, la persistance d'un maximum de chlorophylle en profondeur et la production sous la glace remettent en question les algorithmes de couleur de l'océan. Le drainage continental des constituants terrigènes optiquement actifs et les doubles efflorescences (c'est-à-dire les efflorescences dans la zone marginale de glace de mer et d'automne) renforcent la complexité bio-optique. Les interactions entre le climat, les processus océanographiques, les propriétés bio-optiques et la dynamique du phytoplancton restent un sujet ouvert. Dans le chapitre 1, deux décennies d'observations par satellite ont révélé comment les téléconnexions planétaires influent sur l'équilibre entre les efflorescences sous la glace, les algues de la banquise et les efflorescences dans les zones de glace marginale. Dans le chapitre 2, en utilisant en parallèle les données issues de modèles couplés océan-atmosphère-glace de mer, de réanalyses climatiques, d'observations de la Terre par satellite (OCR), nous avons étudié le contrôle des processus atmosphériques et océaniques sur les efflorescences automnales. Dans le chapitre 3, nous avons présenté une analyse de sensibilité de la production primaire nette de phytoplancton (NPP) dérivée du satellite aux paramétrisations et aux processus océanographiques dans l'est de l'Arctique canadien. Les principales contributions de cette thèse à la dynamique du phytoplancton des mers polaires du Nord sont les suivantes : i.) l'efflorescence de phytoplancton dans la zone marginale de glace, c'est-à-dire le pic de [Chla] trouvé immédiatement après le retrait de la glace de mer, présente une variabilité spatiale et interannuelle substantielle. Cependant, en règle générale, un retrait précoce de la glace de mer entraîne une intensification de l'efflorescence de la lisière de la glace, car le phytoplancton sous la banquise a moins de temps pour épuiser l'inventaire des nutriments de la couche supérieure de la colonne d'eau ; ii.) dans la polynie de Kivalik, dans le nord-ouest de la baie d'Hudson, une zone de forte production primaire et d'agrégation de la faune marine, la corrélation entre les indices climatiques de l'oscillation nord-atlantique, de l'oscillation arctique (NAO/AO) et de la concentration de chlorophylle-a indique que l'efflorescence répond à la circulation atmosphérique à grande échelle dans l'hémisphère nord. Comme le vortex polaire est fort pendant les phases positives de NAO/AO, la force des vents d'ouest favorise la dynamique de la polynie, la production/exportation de glace de mer, le rejet de saumure et la reconstitution des nutriments. Par conséquent, le climat hivernal préconditionne la couche supérieure de la colonne d'eau pour le développement ultérieur des efflorescences à la lisière des glaces. Dans le contexte d'un déclin de la NAO/AO, la polynie de Kivaliki devrait subir une diminution de sa productivité avec des conséquences sur l'ensemble de la HBS ; iii.) le mélange convectif, forcé principalement par le refroidissement atmosphérique et dans une moindre mesure par la turbulence due au vent, étend la couche mélangée, ventile la pycnocline et érode probablement la nitracline, ce qui déclenche les efflorescences de phytoplancton tôt à l'automne. La variabilité saisonnière de l'état de photo-acclimatation estimé par satellite OCR et du carbone phytoplanctonique (c'est-à-dire le rapport carbone-chlorophylle) suggère que ces efflorescences automnales sont productives en terme de fixation du carbone organique; et iv.) Le réglage régional des modèles de production primaire et la modélisation des adaptations photo-physiologiques du phytoplancton sont essentiels pour améliorer l'évaluation satellitaire de la NPP. La production d'algues peut renforcer la pompe à carbone et atténuer le réchauffement de l'Arctique en éliminant les gaz à effet de serre (dioxyde de carbone). Toutefois, la capacité biochimique des mers arctiques et subarctiques à assimiler la forte teneur en matières organiques déversées par les rivières et produites in situ par les efflorescences de phytoplancton dans ce scénario arctique en évolution rapide reste un sujet ouvert.

Abstract

In the Arctic Ocean and adjacent north-polar seas, warming and sea-ice losses are the most prominent footprint of climatic changes in the Anthropocene. These dramatic changes force an adjustment of phytoplankton dynamics, affecting the whole marine trophic web, ecosystem functionality, and the Carbon pump. In the Hudson Bay System (HBS), the world's largest inland sea, the sea-ice loss is twice that observed in the Arctic Ocean, and atmospheric warming rates are faster than recorded at the end of the last glacial period about 12,000–11,000 years ago. Satellite ocean color radiometry (OCR) is the most suitable tool for systematic phytoplankton observation, even in harsh environments and ice-infested seas. However, algae communities adapted to low sun declination, the persistence of subsurface chlorophyll maximum, and production under-ice challenge ocean color algorithms. Continental drainage of terrigenous optically-active constituents and double-blooms (i.e., marginal-ice and fall blooms) enhance the bio-optical complexity. The interplays between climate, oceanographic processes, marine bio-optics, and phytoplankton dynamics remain an open topic. In chapter 1, two decades of satellite observations unveiled how planetary teleconnections impact the balance between under-ice blooms, sea-ice algae, and ice-edge blooms throughout the marginal-ice zones. In Chapter 2, using a broad synergy between oceanic sea ice models, climate reanalysis, remote sensing, in situ bio optics, and radiometry, we investigated the control of atmospheric and oceanic processes on fall blooms. In Chapter 3, we presented a sensitivity analysis of satellite-derived net phytoplankton primary production (NPP) to parametrizations and oceanographic processes in the eastern Canadian Arctic. The main contributions of this thesis to the phytoplankton dynamics of north polar seas are: i.) the ice-edge bloom, i.e., the peak in chlorophyll-a concentration, [chla], immediately found after the sea-ice retreat, has substantial spatial and inter-annual variability. However, as a general rule, early sea-ice-retreat resulted in ice-edge bloom intensification because under-ice blooms have less time to deplete the upper layer nutrient inventory; ii.) in the Kivalik polynya in the northwest Hudson Bay, a marine wildlife hot-spot, the correlation between the climate indices of the North Atlantic Oscillation, Arctic Oscillation (NAO/AO), and [chla] indicated that the bloom responds to large-scale atmospheric circulation patterns in the North Hemisphere. As strong the polar vortex is during positive NAO/AO phases, the strength of westerly winds favors the polynya dynamics, sea-ice production/export, brine rejection, and nutrient replenishment. As a result, the winter climate preconditioned the upper layer of the HBS for the subsequent development of ice-edge blooms. In the context of a decline in the NAO/AO, the Kivaliki polynya should drive a decrease in productivity in the whole HBS; iii.) the convective mixing, forced mainly by atmospheric cooling and to a lesser extent by wind-driven turbulence, expands the mixed layer, ventilates the pycnocline, and likely erodes the nitracline, which trigger pelagic fall blooms. Seasonal variability of satellite-derived photo-acclimation state and phytoplankton carbon (i.e., carbon-to-chlorophyll ratio) unveil the potential productivity of organic carbon fixation in fall blooms; and iv.) regional tuning and resolving photo-physiology are essential to improve NPP satellite assessment. Algae production can enhance the carbon pump and mitigate Arctic warming by removing greenhouse gases (carbon dioxide). However, the biochemical capability of the Arctic and sub-Arctic seas to assimilate high content of organic matter discharged by rivers and produced in situ by phytoplankton blooms in this rapidly changing Arctic scenario remains an open topic.

Keywords:

Marginal ice zone, ocean color radiometry, optically complex waters, inherent optical properties, phytoplankton photo-physiology, atmosphere-ocean processes, and climatic indexes.

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Global introduction

0.1 The origin of ecosystems and the direction we are guiding the Earth's future.

The planetary-scale processes that underpinned profound-ecosystem changes dateline the Earth's life. In the Proterozoic Ocean, the evolution of ancient-cyanobacteria photosynthesis drove the composition of the ocean and atmosphere to the Great Oxidation Event around 2.45 billion years ago. This milestone in natural history allowed the Earth to support complex life and ecosystems (Planavsky et al., 2011; Luo et al., 2016). In the last centuries, after a stable period of 10,000 years during the Holocene, Human activity has impacted the Earth's ecosystems into a new geological era, recently referred to as the Anthropocene (Rockström et al., 2009). The industrial revolution, fossil combustive burning, expansion of cities, and agriculture, for instance, have driven unacceptable damage to the natural ecosystems. In the last decades, one of the most prominent footprints of human-driven climatic changes on the Earth's surface is the pan-Arctic sea-ice loss (Liu et al., 2021; Brennan et al., 2020; Barber et al., 2018; Stroeve and Notz, 2018; Comiso et al., 2017). The pan-Arctic air temperature has arisen two-fold the global trend. This warming is fast and comparable to the abrupt changes observed during the last glacial period about 12,000–11,000 years ago, known as the Dansgaard-Oeschger events (Jansen et al., 2020). As a consequence, the Arctic is changing at a rate faster than any marine ecosystem can naturally adapt (Giesbrecht et al., 2019).

The Earth System is driven by complex interactions between the cryospheric, atmospheric and oceanic processes that eventually control light, nutrients, and stratification, i.e., the drivers of phytoplankton

dynamics. In turn, interplays of phytoplankton and marine ecosystem impact all-trophic levels, as well as the earth's climate by controlling primary production, the coupling of sympagic, pelagic and benthic realms, marine diversity and abundance, ecological borders, and the biological carbon pump (Trudnowska et al., 2021; Kearney et al., 2013; Ji et al., 2010; Leu et al., 2011; Wassmann et al., 2011; Boyce et al., 2010).

This thesis aims at understanding the interaction between climate variability and phytoplankton in the north polar region. It focuses on a particular region, the Hudson Bay and the Canadian Arctic, where rapid changes occur and limited knowledge about the phytoplankton dynamic is currently available. In the following section, I present an overview of this region.

0.2 The Hudson Bay System, a north polar sea in transition

In the Hudson Bay System (HBS), the large inland sea of the word, climatic changes can be even more accentuated than observed in the Arctic Ocean. The trend of air temperature is about 3.7° C since the postindustrial era, almost double that observed over the Arctic Ocean (2°C) (Brand et al., 2014). Sea ice concentration losses reached -15.1% in northwest and -20.4% in south bay per decade since 1980 (Hochheim et al., 2011). For the next decades, prognostics of climate models indicate a decrease of ~20% in sea-ice concentration in winter (Lukovich et al., 2021), resulting in dramatic impacts on key regional ecosystems for polar life, such as, for example, the Nelson river plume (Smith et al., 2017; Sergeant, 1973), James Bay (Macdonald et al., 2021), and the Kivalliq Polynya in the northwestern Hudson Bay (Bruneau et al., 2021; Matthes et al., 2021; Landy et al., 2017).

The Hudson Strait is the main connection between the Hudson Bay and the Global ocean. It is where the bay waters outflow toward the Labrador Sea (Sutherland et al., 2011). As exposed by Dmitrenko et al. (2020), HBS is a large-scale subarctic estuarine system because of the high content of freshwater from continental drainage (Stadnyk et al., 2020), sea-ice melting (Kirillov et al., 2020; Landy et al., 2017), and intrusions of Arctic waters from Pacific origin entering in the bay throughout the Hudson Strait (Florindo-López et al., 2020), and Fury and Hecla Strait in the Foxe Basin (Webb, 2014; De-
fossez et al., 2012). Riverine freshwater input is about 713 km³ year⁻¹ (Kuzyk et al., 2010), which represents 12% of the total Pan-Arctic runoff (St-Laurent et al., 2011). Stream flow has raised about 0.31 km³ year⁻¹ between 1964 and 2008 (Déry et al., 2016, 2011). Despite a large amount of riverine input, the melting of seasonal sea-ice, which covers the whole HBS except in some coastal polynyas (Kirillov et al., 2020; Landy et al., 2017), supplies about twice the total riverine input in a short melting period during the spring-to-summer transition (Mysak et al., 1996).

HBS receives a large amount of dissolved organic carbon (DOC) every year (around 5.5 Tg) (Mundy et al., 2010), equivalent to 25% of total Arctic riverine input. Dark-water color, commonly attributed to a high concentration of chromophoric dissolved organic matter (CDOM), is dominant in most HBS making this region optically-complex waters (Burt et al., 2016; Heikkila et al., 2016; Xi et al., 2013; Guéguen et al., 2011; Mundy et al., 2010; Granskog et al., 2007). The Hudson Bay watershed has stocked a massive amount of organic matter since the Holocene in peatlands, the second continuous large lowlands ecosystem on Earth. Peatlands occupy an area of 37,200 km³ that stocks 27.6 Pg of carbon from glacial-marine deposits. As a result, as in other Arctic Regions (Connolly et al., 2020), the largest source of dissolved organic carbon (DOM) in the HBS is from terrigenous sources, which overlap autochthonous marine production. The Hudson Bay shoreline embraces many ecosystems like the Arctic tundra, boreal forest, Canadian shield, Peatland, wetland, and grassland (Yang et al., 2021; Packalen et al., 2014; Preston et al., 2012; Pelletier et al., 2007). The role of climatic changes on composition and marine bio-optical properties in the Hudson Bay System is complex because its domain embraces a heterogeneity of ecosystems and hydro-physiographic domains.

0.3 Planetary teleconnections to Hudson Bay System, what do we know?

Global processes and regional feedbacks amplify Arctic warming (Levine et al., 2021). For example the sea-ice albedo, the permafrost organic carbon release (Bader, 2014); the lapse-rate-feedback (Pi-than and Mauritsen, 2014); tropospheric processes like atmospheric blocking events, and the poleward transport of moisture and heat from cyclones (Henderson et al., 2021; Serreze and Barry, 2011); the dynamics of Rosby waves (Riboldi et al., 2020); and large-scale oceanographic processes like Arc-

tic Borealization (Polyakov et al., 2020); and the dynamic of Beaufort Gyre (Morison et al., 2021; Solomon et al., 2020; Hill et al., 2018).

Due to its shallow topography and relative isolation from global ocean circulation and sea-ice exchanges, the HBS is more sensitive to atmospheric processes than other polar seas. Large-scale atmospheric variability and planetary teleconnection should be coupled tightly to marine conditions in the HBS. For example, satellite altimeters, in situ data, and ocean model simulations showed that cyclonic winds intensify Hudson Bay's water cyclonic circulation and transport of water in the Hudson Strait (Dmitrenko et al., 2021). In the Fall season, atmospheric cyclonic systems passing over Hudson Bay toward the Baffin Bay and the Labrador Sea amplify water masses exchange in Hudson Strait, which reduces the residence time of riverine and ice-melt waters in Hudson Bay (Dmitrenko et al., 2020). In winter, atmospheric-forcing controls the sea-ice thickness spatial distribution (Kirillov et al., 2020) and ice production in the Kivalliq Polynya (i.e., the northwest Hudson Bay polynya; Bruneau et al., 2021; Landy et al., 2017).

Studies dedicated to planetary teleconnections utilize climatic indices to express global processes. For instance: the North Atlantic Oscillation (NAO) ties pressure gradients between the Atlantic Tropical and the Arctic, the northward heat transport, and the Gulf Stream dynamics, while the Arctic Oscillation (AO) ties circumpolar jets, strength/waving of the north polar vortex, and the dynamic of westerly winds (Moritz et al., 2002); and El Nino-Southern Oscillation (ENSO) is related to the Ocean Pacific warming/cooling (McCrystall and Screen, 2021; Liu et al., 2004).

Planetary teleconnections influence the atmospheric circulation pattern throughout polar cell variability, which affects the Pan-Arctic and sub-polar North America (Meleshko et al., 2016; Francis et al., 2009). For example, in the northern hemisphere, poleward/southward shifts and wave amplitude of polar jet streams over Canada influence weather patterns (Hall et al., 2015), extreme events (Francis and Vavrus, 2015) like storms, heatwaves, droughts, and even burning in Boreal forest (Jain and Flannigan, 2021; Girardin et al., 2006). In Hudson Bay System, sea-ice anomalies, temperature, precipitation, and NAO covariate (Qian et al., 2008). AO and HBS river discharges are strongly correlated (Déry et al., 2016, 2011; Déry and Wood, 2004). According to Shabbar et al. (1997), El Nino influences the dynamic of the jet stream across North America. El Nino produces positive (negative) precipitation anomalies in north-central (southern) Canada in late winter. On the other hand, in the La Nina situation, the jet stream activity causes near-normal climatological rainfall over southern Canada (Lee et al., 2007). The control of the Arctic Polar vortex and the planetary waveguide on regional marine processes can also impact phytoplankton dynamics in north polar seas (Morison et al., 2021; Armitage et al., 2020; Carmack et al., 2016; Overland et al., 2012; Beuermann et al., 2002). Arctic phytoplankton production is the subject of the next section.

0.4 Pan-Arctic phytoplankton pelagic production

Global phytoplankton production ranged from 38.8 to 42.1 Gt Carbon year⁻¹ between 1998 and 2018 (Kulk et al., 2020) and, according to Boyce et al. (2010), declined over the past century at a rate of ~1% per year since 1899 in response to climatic fluctuations and sea surface warming. On the other hand, in the Arctic Ocean, chlorophyll-*a* concentration ([*chla*]) has increased by 21.5% and integrated annual production by 56.5% between 1998 and 2018 (Lewis et al., 2020).

Arrigo and Van Dijken (2011) reported that Arctic production rise by 0.77 Tg C per year for each drop of 10^6 km^2 of sea-ice coverage. Arctic sea ice declined ~ $2.0 \times 106 \text{ km}^2$ during the satellite era between 1979 and 2017 (Brennan et al., 2020) at a rate of -4.57% per decade (Comiso et al., 2017). Besides the sea-ice coverage, the timing of the Arctic-wide melt season has decreased at a rate of 5 days per decade since 1979 (Stroeve et al., 2014). Sea ice is melting earlier and freezing later, resulting in an extended open water season (Ardyna and Arrigo, 2020). A decrease in sea ice thickness, snow layer depth, and timing shifts of melt and pond onsets allow more light to penetrate the ice-pack and reach the upper ocean layer (Tedesco et al., 2019; Horvat et al., 2017; Leu et al., 2015). Although sea surface releases water vapor and heat, when sea-ice retreats, increase cloudiness and fog reduce the light reaching ice-edge zones (Bélanger et al., 2013), and the continuum of water-column heating during the open water season forces a convey of atmospheric radiation transmission (Laliberté et al., 2021). The lengthening of the open water season augmented the annual light incoming into the Arctic

pelagic ecosystems (Ardyna and Arrigo, 2020; Arrigo et al., 2020; Lewis and Arrigo, 2020; Stroeve et al., 2020; Horvat et al., 2017; Bélanger et al., 2013).

The Arctic arisen of phytoplankton abundance and production are sustained by an influx of new nutrients from processes like vertical mixing Randelhoff et al. (2020), Pacific and Arctic waters intrusions (Polyakov et al., 2020), drainage of the Pan-Arctic watershed, permafrost thawing, and coastal erosion (Terhaar et al., 2021; Guéguen et al., 2011). According to (Terhaar et al., 2021), continental drainage processes and coastal erosion fuel up to 28–51% of the current annual increase of phytoplankton production (Arrigo et al., 2020; Connolly et al., 2020; Lewis et al., 2020).

0.5 Algae and ecosystem feedback

As exposed by Wassmann (2011), monitoring and predicting the pan-Arctic ecosystem remain a huge challenge. This is due to the complexity and fast nature of physical and biological alterations and a lack of information on polar marine ecosystems. Understanding how planetary processes affect biologic production is critical for predicting the future of Arctic ecosystem functioning (Armitage et al., 2020). We recognize that regional interplays between the atmosphere, ocean, cryosphere, and phytoplankton are distinct among the Arctic bio-regions and north polar seas (Carmack et al., 2016). The Arctic Borealization (Polyakov et al., 2020), i.e., the expansion of the Atlantic and Pacific domains into the Arctic Basin, is an example of how ecological secession of species, ecosystem functioning, and ecological borders are distinct between north polar seas.

In the Bering and Chukchi Sea shelves, the balance of Arctic water and saltier and nutrient-rich Pacific water affect the whole food web. An ecological succession from a high productivity ecosystem sustained by Pacific Water Intrusion, primary production of large diatoms, low zooplankton grazing pressure, tight pelagic–benthic coupling, and abundant benthic-feeding marine mammals, toward Arctic Waters domains favoring high zooplankton grazing, pelagic-fish, and scaling down of the benthic realm (Hirawake et al., 2021; Ji et al., 2019; Coupel et al., 2015; Grebmeier et al., 2006). In the Eastern Arctic Sector, in the Barents Sea, satellite-ocean color revealed a significant increase in annual trends of spring bloom productivity reaching 60 mg C m⁻² day⁻¹ year⁻¹ as a consequence of early sea-ice retreat and intensification of northward intrusion of Atlantic Water between 2003 to 2013 (Vernet et al., 2019; Renaut et al., 2018). An intensification of northward currents and the presence of *Emiliania huxleyi*, a proxy of Atlantic Water intrusion (Oziel et al., 2020) and keystone species due to its ability to form massive blooms (Gafar et al., 2019), confirm the expansion of the Atlantic water domain through the Europe Arctic corridor. Recent bio-optical observations from satellite ocean color also suggest a significant role in increasing the frequency of Phaeocystis blooms in the Barents sea (Orkney et al., 2020).

Phytoplankton phenology time shifts, e.g., delay or early bloom initiation and peak (Vargas et al., 2009; Jönsson and Eklundh, 2004), influence all trophic levels (Michel et al., 2006; Post, 2016). Upper-trophic level species during recruitment stages are sensitive to time-shifts in phytoplankton phenology (Ramírez et al., 2017; Post, 2016; Thackeray et al., 2016; Diez et al., 2014; Yamashita et al., 2013; Platt et al., 2003; Drolet et al., 1991). For example, phytoplankton bloom timing synchronization with organisms in early-life and sensitive development stages (eggs or larval) is essential for species survival and recruitment (match/mismatch hypothesis: Cushing 1990). Therefore, the ecological timing impact on fish larval recruitment produces a bottom-up control with a cascade effect on survival rates of a wide range of species (Platt et al., 2003) and impacts fisheries of economical-valuable species (Tremblay et al., 2012; Friedland et al., 2012; Chassot et al., 2010).

In spring or summer time, the timing of the ecological process throughout the marginal ice zone affects marine-snow morphology/composition, the biological carbon pump, and coupling between pelagic and benthic realms (Trudnowska et al., 2021; Leu et al., 2011). Therefore, climate and phytoplankton feedback potentially impact all polar sea life and Earth's climate (Trudnowska et al., 2021; Terhaar et al., 2021; Leu et al., 2011). An enhancement of phytoplankton production can mitigate the greenhouse effect throughout the biological carbon pump. On the other hand, the organic matter accumulation in the pelagic system, high sedimentation, and denitrification can have ecological consequences for further production in Arctic shelves ecosystems overwhelming the Earth's self-regulatory capacity (Lannuzel et al., 2020; Arrigo, 2013; Lovelock, 2003).

The future prevalence of a fall bloom could have significant impacts on consumers who exploit this windfall to increase recruitment and winter survival (Hill et al., 2018). Sigler et al. (2014) reported that large crustacean zooplankton taxa *Calanus spp*. respond to inter-annual variability in the time interval between spring and fall blooms in the Eastern Bering Sea. Fall blooms can also increase the survival rates of important species, especially in phases of development. For example, Friedland et al. (2008) reports that the largest recruitment events of haddock *Melanogrammus aeglefinus* in George banks recorded in its assessed history are associated with the dynamics of the fall phytoplankton bloom in the year prior to spawning. Fall blooms can supply extra-energy stocks to polar species overwintering (Rho and Whitledge, 2007).

0.6 Revisiting phytoplankton phenology and pre-conditioning in north polar seas

Seasonal phytoplankton abundance and production are known as phenology. Increasing pieces of evidence point out that phytoplankton phenology responds to global warming in north polar seas (Ardyna et al., 2014; Wassmann, 2011; Ardyna and Arrigo, 2020). Algae bloom occurs when the ecosystem goes toward a noun-equilibrium state, resulting in high phytoplankton growth rates trespassing the losses. Phytoplankton phenologies are distinct among world oceans because of the wide range of physical processes that co-exist in bioregions (D'Ortenzio and D'Alcalà, 2009). Events preceding a phytoplankton bloom (i.e. the pre-conditioning), if well-characterized, supply important information for quantifying, understanding, and predicting impacts on the phytoplankton dynamic.

In winter, sea-ice production and thickness regulate brine rejection and consequently nutrient replenishment in upper layers by vertical mixing through deep convection. Therefore, sea-ice dynamics affect the balance of nutrient consumption between under-ice and pelagic components of marginal ice zones. The nutrients that remained after under-ice blooms sustain a subsequently eventual pelagic bloom in spring. Heat accumulated during the open waters season and freshwater input affects the sea ice thickness in the subsequent winter, which in turn, is going to control phytoplankton dynamics. In extension, the interactions of solar energy incoming with optical components influence the energy transfer among hydrosphere, atmosphere, and oceanographic processes (Bruneau et al., 2021; Eastwood et al., 2020; Landy et al., 2017).

Over recent decades, changes in pelagic and under sea-ice primary production have been driven by a sea-ice coverage decreasing and shifts in sea-ice seasonal thermodynamics in marginal-ice zone (Arrigo et al., 2008). Sea ice losses forced by Arctic amplification have increased the frequency of massive under-ice blooms in the Arctic Ocean (Arrigo et al., 2012). Sea-ice thermodynamic stages control the balance between under-ice and pelagic production throughout the marginal ice zone. This balance also depends on timing concerning the seasonal cycle of photosynthetic available radiation and nutrient availability (Horvat et al., 2017; Kahru et al., 2016). A decrease in sea ice thickness, leads, and a change in the timing of the melt, ponds, and drainage onsets allow more light to penetrate the ocean through the ice, increasing the occurrence of under-ice bloom. For example, melt-ponds increase considerably the light transmission throughout the ice pack determining the beginning of the under-ice production season (Mundy et al., 2009, 2014; Lannuzel et al., 2020; Assmy et al., 2017; Horvat et al., 2017; Arrigo et al., 2014; Frey et al., 2011). Massive under-ice blooms can consume nutrients and leave oligotrophic conditions, hindering a possible subsequent open-water phytoplankton bloom (Matthes et al., 2021). Arrigo et al. (2012) reported that massive under-ice blooms can occur even in high sea-ice coverage in the Chukchi Sea. In the Canadian archipelago, such under-ice blooms have been documented in several places (Mundy et al., 2014, 2009; Galindo et al., 2002). On the other hand, spring blooms have been onset early in north polar seas because of the sea-ice early melting (Kahru et al., 2011). Despite the occurrence of under-ice bloom appearing as a predominant feature in the Arctic, Perrette et al. (2011), using satellite ocean color observations of 2007, showed that ice edge bloom was a nearly ubiquitous feature in the Arctic ocean.

In the summer, production is highly limited by nutrient availability and stratification imposed by freshwater coming from rivers and ice melting. This phenomenon has also been observed in Hudson Bay in late summer (Ferland et al., 2011). Nutrient depletion and high light incoming forces an oligotrophic set up with the small cells in the upper layer (Li et al., 2009) and in sub-surface chlorophyll maximum large diatoms with high intra-cellular pigments content (Martin et al., 2010). In the fall season, after a stable oligotrophic set up in the summer season, atmospheric forcings favor the development of a secondary fall bloom because the convective and wind-driven turbulence force nutrients replenishment in the upper layer from the deep nutrient pool (Ardyna et al., 2014). The biomass amplitude in autumn may respond to the summertime pre-conditioning on vertical water structure and stratification stretching (Ardyna and Arrigo, 2020; Waga and Hirawake, 2020; Hill et al., 2018).

In Fall, blooms became more frequent in north polar seas because the expansion of open water areas also allows a delay of sea-ice retreat, an increase in light incoming in the upper layer, and storms (Ardyna et al., 2014). Carbon flux measured in sediment trap evidence the importance of blooms in the summer-to-fall transition in the Bering Sea (Rho and Whitledge, 2007). Greenan et al. (2004) discussed the importance of short-term physical events in the phenology of spring and fall blooms in the Nova Scotia Shelf. Kim et al. (2007) report the relation between wind speed and bloom initiation in the sub-polar frontal area of the Japan/East Sea. Fall blooms occurred in a wide area of the Pacific Arctic, and larger phytoplankton was predominant during fall blooms (Waga and Hirawake, 2020).

Previous studies have shown that the impact of storms on the upper ocean is becoming prominent due to a drastic increase in the ice-free period over the Arctic (Rho and Whitledge, 2007; Kim et al., 2007; Greenan et al., 2004). This process alleviates the strength of stratification forced by rivers and ice melt in the upper layer (Wassmann, 2011; Déry and Wood, 2004), which favors the transport of nutrients from the deep-nutrient pool upward to the euphotic zone (Crawford et al., 2020; Randelhoff et al., 2020; Waga and Hirawake, 2020; Ardyna et al., 2014). On the other hand, intense mixing can disrupt the water column structure leaving a not organized phytoplankton vertical structure advecting large cells adapted to high stratification and low light acclimated phytoplankton with intracellular content from subsurface chlorophyll-a maximum to upper ocean layer.

0.7 Ocean color satellite observations in north polar seas: strengths and limitations

As there isn't any marine-pelagic life without light, we can not "see" or understand the interplays of Earth and life without a deepen-perspective on the interaction of light, algae, and bio-optical properties within seawater. Understanding the climatic implications on the sea's food web and ecosystem structure relies on deepen-investigation of the interactions among phytoplankton, atmospheric, continental, and oceanographic processes. The advance in oceanographic and satellite methods provide us with tools to understand the past, monitor ongoing changes, and build prognostic about the future of north polar (Fischer et al., 2014). The synergy of ocean color satellites (optical), active and passive microwave remote sensing (e.g., scatterometers, synthetic aperture radar, passive microwave), ocean-sea-ice dynamic models, climatic reanalysis, and oceanographic fieldwork are essential to studying complex ecological components, and ecosystem feed-backs at all spatial scales.

Satellite oceanography sustains the continuum and systematic monitoring of polar seas. The ocean color satellite constellation has unique characteristics of time-spatial coverage and frequency of revisit dedicated to phytoplankton dynamics and bio-optical properties (Groom et al., 2019). However, in situ samples must constrain remote sensing to well-represent the complexity of ecosystems algorithms (Werdell et al., 2018; Matsuoka et al., 2017; Demidov et al., 2017; Babin et al., 2015; Lee et al., 2015; Bélanger et al., 2007, 2008).

How satellite ocean color can be employed to better understand the impact of climatic changes on phytoplankton phenology? In spring, ice edge pelagic cells and under-ice production balance the production in marginal ice zones. Ocean color satellite range is restricted by ice-pack, and clouds, and confined into a thin-superficial layer where light is back-scattered out of the sea surface. Therefore, low pelagic production observed by remote sensing may not mean low annual production in marginal ice zones because an important component of phytoplankton biomass can be escaping from the remote sensing range at depth (i.e., in the sub-surface chlorophyll-*a* maximum; Martin et al. 2010). Low biomass signatures early detected by ocean color satellites during open water onset may indicate or at least be a proxy of previous under-ice blooms, as suggested by some authors (Lewis et al., 2019; Hill et al., 2018; Horvat et al., 2017; Arrigo et al., 2012; Palmer et al., 2011).

Ocean carbon fluxes quantification is a major field of research in marine science in the context of the global carbon cycle and global warming (Richardson et al., 2016). To constrain the global ocean carbon cycle, it, therefore, becomes necessary to obtain precise estimates of photosynthetic production rates in the global ocean (Richardson et al., 2016). High latitude plankton communities are among the most productive, seasonally dynamic, and rapidly changing ecosystems in the global ocean (Behrenfeld et al., 2017). In this way, phytoplankton must adjust its photosynthetic machinery and pigments composition to acclimate to severe transitions of light levels and nutrient availability (Lewis et al., 2019; Lacour et al., 2017; Arrigo and Brown, 1996). Strategies include non-photochemical quenching (NPQ), fluorescence (O'Malley et al., 2014; Behrenfeld et al., 2009), production of photoprotective pigments like xanthophyll (Graff and Behrenfeld, 2018; Brunelle et al., 2012; Matsuoka et al., 2009), packaging effect (Cota et al., 2004; Ben Mustapha et al., 2012), carbon to chlorophyll ratio (Graff and Behrenfeld, 2018; Lacour et al., 2017), ecological-succession of community size structure and taxonomy (Gafar et al., 2019; Lewis et al., 2019; Richardson et al., 2016; Uitz et al., 2008; Palmer et al., 2013; Claustre et al., 2005). The strategies affect the photosynthetic maximum production and light saturation of the phytoplankton community, as observed in the global ocean and the Canadian Arctic (Matthes et al., 2021; Bouman et al., 2017; Huot et al., 2013, 2007). These processes have proven extremely challenging to detect from ocean color satellites and they could impact the satellite-derived phytoplankton primary production estimations in north polar seas (Bouman et al., 2020; Demidov et al., 2020; IOCCG, 2015; Behrenfeld et al., 2009).

Figure 1 shows the expected seasonal photoacclimation process of phytoplankton with productive cells in marginal ice zone, small cells acclimated to summer oligotrophy, and development of sub-surface chlorophyll maximum populated with large cells with high pigment content, and the fall bloom phenomenon in a low stratified water column. Satellite-derived observations of the Carbon-to-Chlorophyll ratio, C_{phy} :[*chla*], can account for the photo-physiology to support the quantifying of ocean productivity and carbon cycling (Graff and Behrenfeld, 2018). Emergent literature has applied satellite measures of inherent optical properties and [*chla*] to assess carbon content, community size structure, and photoacclimation in production. The particle backscattering coefficient (b_{bp}) has been proposed to estimate carbon phytoplankton from space (Behrenfeld et al., 2005). However, b_{bp} is also composed of non-algal particles (NAP) like zooplankton, bacteria, viruses, fecal pellets, cell debris, and mineral particles. NAP and a_{CDOM} have high seasonal and spatial-temporal variability, are dominant in north polar seas and do not co-vary with [*chla*] in optically complex water (Bellacicco et al., 2020, 2019, 2018).



Figure 1: Phytoplankton photo-acclimation and ecological succession in Hudson Bay. In spring, phytoplankton communities in the upper layer, under ice, and sympagic algae balance the production of the marginal ice. In summer, an oligotrophy setup takes place with small cells with low intracellular chlorophyll-*a* content in the upper layer and the development of sub-surface chlorophyll-*a* maximum. In the fall bloom phenomenon, large cells with high intracellular content are possibly advected from sub-surface chlorophyll-*a* maximum or/and summer communities are photo-acclimated to fall conditions.

0.8 Research questions, hypotheses, and main objectives

What is the impact of climatic changes on algae dynamics in the marginal-ice zone, summer oligotrophy, and fall bloom phenomenon in Hudson Bay? How do interplays of the cryosphere, atmosphere, and oceanographic processes trigger, maintain, and module the magnitude and timing of phytoplankton blooms in Hudson Bay? How climatic changes can affect the balance between under-ice and pelagic production? How phytoplankton fall blooms are triggered and maintained? In fall, what is the consequence of loss of stratification on fall productivity? How does satellite-ocean color perform to measure phytoplankton production, abundance, community size and taxonomic structure, and photophysiology in north Polar Seas? To address these questions, my thesis is structured into three chapters, and, in the end, two sections dedicated to future perspectives and global conclusions.

Firstly, in chapter 1, we focused on the actual role of environmental processes and climatic teleconnections on phytoplankton in ice edge zone using two decades of ocean color for phytoplankton chlorophyll-*a* and passive microwave for sea-ice concentration. Next, in chapter 2, we investigated how atmospheric forcing (winds and heat-flux) and water column vertical structure evolution affect the seasonal phytoplankton biomass and photo-acclimation, summer oligotrophy, and fall bloom phenomenon using a synergistic approach that integrates the satellite ocean color time series, in situ biooptics, atmospheric reanalysis, and ocean-sea-ice dynamic model in Hudson Bay. Lastly, in chapter 3, we assess the performance of satellite-derived primary production (PP) based on in situ observations obtained in the Canadian Arctic in 2016 (Baffin Bay) and 2018 (Hudson Bay). To do so, a sensitivity analysis is performed to quantify the propagation of errors of each PP model input or parameters, and to orient future work to improve the satellite estimation of PP.

The chapters are systematized in three original full-length research papers produced in the scope of my doctorate in oceanography and approved by the scientific committee. For these three articles, for which I am the first author, I participated in all stages of development and drafted the first version (the design, written, data analysis, figure plots, and scientific discussions). However, I must highlight the contribution from other co-authors, and journal reviewers, that greatly improved the quality of the manuscripts. The collaboration and even severe criticism allowed me to build a bridge of excellence

toward scientific questions about bio-optics and the dynamic of phytoplankton in the north polar seas. The hypotheses, main objectives, and references are briefly presented below for each Chapter.

Chapter 1: Climate control of ice edge phytoplankton blooms in the Hudson Bay System.

Autors: Barbedo, L., Bélanger, S., and Tremblay, J.-É.

Peer-reviewed journal: Elementa: Science of the Anthropocene 8 (1) 2020.

Hypothesis:

- I. An inheritance effect (pre-conditioning) of winter on sea-ice production impacts the level of phytoplankton production that will occur in the spring-to-summer transition.
- II. Global atmospheric circulation patterns strongly influence phytoplankton ice-edge blooms in Hudson Bay.

Objectives:

- to evaluate the impact of the climatic changes and atmospheric teleconnections on algae phenology throughout the marginal ice zones and pelagic system in HBS;
- to explore the variability of [*chla*] in the ice-edge zone in terms of potential physical forcing that control nutrient availability and incoming light in the upper layer and consequently the magnitude of the bloom;
- To understand the sensitivity of Hudson Bay Northwestern (Kivalliq) polynya to large-scale climate forcing.
- to identify impacts of climatic changes and river regulation by hydroelectric power plans on phytoplankton phenology;

Chapter 2: Atmospheric forcing and photoacclimation of phytoplankton fall blooms in Hudson Bay.

Authors: Barbedo, L., Bélanger, S., Lukovich, J., Myers, P., and Tremblay, J.-É.

Peer-reviewed journal: Elementa: Science of the Anthropocene 10 (1) (2022).

Hypothesis:

I. In the fall season, atmospheric forcing promotes excessive vertical mixture. Consequently, it forces a process of subsurface chlorophyll maximum seeding of the upper layer with phytoplankton communities, composed of larger cells with high intracellular chlorophyll content. Therefore, phytoplankton communities with high intracellular chlorophyll-*a* content in an environment of low solar elevation and excessive turbulence can result in overestimation of ocean color satellite-derived phytoplankton carbon production and biomass.

Objectives:

- to understand the role of atmospheric forcings (winds and heat flux) and water column structure on fall blooms;
- to evaluate the ability of ocean color radiometry to detect fall blooms;
- to assess the photo-physiological state of phytoplankton communities blooming in the fall season using the satellite-derived optical proxies carbon-to-chlorophyll ratio (C_{phy} :[chla]).

Chapter 3: Sensitivity of satellite-derived phytoplankton production in eastern Canadian Arctic.

Authors: Barbedo, L., Bélanger, S., and Babin, M.

Publication: Biogeoscience (in preparation)

Hypothesis:

- I. Reconciling of satellite-derived phytoplankton production and photo-acclimation models can be done using ocean color measurements of chlorophyll-specific phytoplankton backscattering coefficient $(b_{b\phi}^{*})$ to resolve light-induced variation of carbon to chlorophyll ratio $(C_{phy}:[chla])$ in optically complex waters.
- II. In north polar seas, the performance of satellite-derived phytoplankton production relies on how a model based on phytoplankton spectral signatures on absorption coefficient $(a_{\phi}(\lambda))$ can resolve the ecological succession of phytoplankton functional groups.

Objectives:

- to tune a satellite-derived phytoplankton production model to marginal ice zones in the Canadian eastern Arctic.
- to assess the performance of parameterizations photosynthetic production vs. irradiance curves (E_k) , chlorophyll-*a* concentration vertical distribution, phytoplankton absorption, and light profiles using in situ bio-optics and radiometry collected during the BaySys expedition in Hudson Bay (2018) and the GreenEdge expedition in the Baffin Bay (2016).

In the last sections, future perspectives and the thesis general conclusions, I presented: i) what is our thesis contribution to north polar sea science, phytoplankton dynamics, and satellite ocean color; ii) revisited phytoplankton phenology of Hudson Bay, iii) perspective of the research line: what questions remain open; iv) the applicability of methodology from a pan-Arctic perspective; and v) future perspectives about the synergy of ocean color satellites and sea-ice dynamic models.

Climate control of sea-ice edge phytoplankton blooms in the Hudson Bay System

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Abstract

The Hudson Bay System (HBS), the world's largest inland sea, has experienced disproportionate atmospheric warming and sea-ice decline relative to the whole Arctic Ocean during the last decades. The establishment of almost continuous positive atmospheric air temperature anomalies since the late 1990s impacted its primary productivity and, consequently, the marine ecosystem. Here, four decades of archived satellite ocean color were analyzed together with sea-ice and climatic conditions to better understand the response of the HBS to climate forcing concerning phytoplankton dynamics. Using satellite-derived chlorophyll-a concentration ([chla]), we examined the spatio-temporal variability of phytoplankton concentration with a focus on its phenology throughout the marginal ice zone. In recent years, phytoplankton phenology was dominated by two peaks of [chla] during the ice-free period. The first peak occurs during the spring-to-summer transition and the second one happens in the fall, contrasting with the single bloom observed earlier (1978–1983). The ice-edge bloom, i.e., the peak in [chla] immediately found after the sea-ice retreat, showed substantial spatial and inter-annual variability. During the spring-to-summer transition, early sea-ice retreat resulted in ice-edge bloom intensification. In the northwest polynya, a marine wildlife hotspot, the correlation between climate indices, i.e., the North Atlantic Oscillation and Arctic Oscillation (NAO/AO), and [chla] indicated that the bloom responds to large-scale atmospheric circulation patterns in the North Hemisphere. The intensification of westerly winds caused by the strong polar vortex during positive NAO/AO phases favors the formation of the polynya, where ice production and export, brine rejection, and nutrient replenishment are more efficient. As a result, the winter climate pre-conditions the upper layer of the HBS for the subsequent development of ice-edge blooms. In the context of a decline in the NAO/AO strength related to Arctic warming, primary productivity is likely to decrease in the HBS and the northwest polynya in particular.

Résumé

Contrôle climatique des efflorescences phytoplanctoniques en bordure de la glace de mer dans le système de la baie d'Hudson

Le système de la baie d'Hudson (HBS), la plus grande mer intérieure du monde, a connu un réchauffement atmosphérique et un déclin de la glace de mer disproportionnés par rapport à l'ensemble de l'océan Arctique au cours des dernières décennies. L'établissement d'anomalies positives presque continues de la température de l'air atmosphérique depuis la fin des années 1990 a eu un impact sur sa productivité primaire et, par conséquent, sur l'écosystème marin. Ici, quatre décennies d'observations de la couleur des océans archivées par satellite ont été analysées avec la glace de mer et les conditions climatiques afin de mieux comprendre la réponse du HBS au forçage climatique concernant la dynamique du phytoplancton. En utilisant la concentration de chlorophylle-a [chla] estimée par satellite, nous avons examiné la variabilité spatio-temporelle de la concentration de phytoplancton en mettant l'accent sur sa phénologie dans la zone marginale de glace. Ces dernières années, la phénologie du phytoplancton a été dominée par deux pics de [chla] pendant la période sans glace. Le premier pic se produit pendant la transition entre le printemps et l'été et le second à l'automne, ce qui contraste avec l'efflorescence unique observée au début des années 1980s. L'efflorescence en marge de la glace, c'est-à-dire le pic de [chla] trouvé immédiatement après le retrait de la glace de mer, a montré une variabilité spatiale et interannuelle substantielle. Pendant la transition entre le printemps et l'été, le retrait précoce de la glace de mer a entraîné une intensification de l'efflorescence en bordure de la glace. Dans la polynie nord-ouest, une zone primordiale pour la biodiversité marine, la corrélation avec les indices climatiques, c'est-à-dire l'oscillation nord-atlantique et l'oscillation arctique (NAO/AO), et la [chla] indique que l'efflorescence répond aux modèles de circulation atmosphérique à grande échelle dans l'hémisphère nord. L'intensification des vents d'ouest provoquée par le fort vortex polaire pendant les phases positives de la NAO/AO favorise la formation de la polynie, où la production et l'exportation de glace, le rejet de saumure et la reconstitution des nutriments sont plus efficaces. Par conséquent, le climat hivernal conditionne la couche supérieure du HBS pour le développement ultérieur des efflorescences en bordure des glaces. Dans le contexte d'une diminution de la force de la NAO/AO liée au réchauffement de l'Arctique, la productivité primaire est susceptible de diminuer dans le HBS et la polynie nord-ouest en particulier.

1.1 Introduction

The Arctic Ocean and its surrounding seas are facing the most pronounced climatic changes on Earth. Several regional positive feedback processes amplify the warming of the Arctic (Overland et al., 2004; Serreze et al., 2009), such as the sea-ice albedo (Screen and Simmonds, 2010), a decline of sea ice in all seasons (Stroeve and Notz, 2018), the lapse-rate and the thermal radiative balance (Pithan and Mauritsen, 2014). Those changes also increase the frequency of extreme climatic events in the northern latitudes (Pithan and Mauritsen, 2014). As a consequence, the timing of the Arctic-wide sea-ice melt season has advanced at a rate of 5 days per decade since 1979 (Stroeve et al., 2011, 2014). Arctic sea-ice volume has declined at a rate of $-513 \text{ km}^3 \text{y}^{-1}$ and $-287 \text{ km}^3 \text{y}^{-1}$ during winter and fall seasons, respectively, between 2002 and 2018 (Kwok, 2018). Climatic changes have been even more accentuated in the Hudson Bay System (HBS), a complex ecosystem embracing Hudson Bay, James Bay, Foxe Basin, and Hudson Strait, which forms the world's most extensive inland sea (1.24×10^6) km²). For example, Stroeve and Notz (2018) showed that Hudson Bay sea-ice cover in September decreased at the rate of $-1046 \text{ km}^2 \text{ y}^{-1}$ between 1979 and 2018, a loss of -93.6% relative to the average of 45.2% for the whole Arctic. As reported by Hochheim et al. (2011), sea-ice concentration (SIC) losses range from -15.1% to -20.4% per decade since 1980 in the northwest and southwest sectors of Hudson Bay (HB), respectively. As a consequence, the duration of the open water season increased by 12 days per decade between 1980 and 2005, which is almost twice the rate observed in the Arctic Ocean, i.e., 6.4 days per decade (Markus et al., 2009). Finally, the mean annual sea surface temperature trend is about 3.7°C since the post-industrial era, which is much larger than the trend observed over the Arctic Ocean, approximately 2°C (Brand et al., 2014).

The ongoing changes in the sea-ice cover extent and thickness have impacted the primary producers of the arctic and subarctic marine ecosystems (Kahru et al., 2016). Changes in the cryosphere have resulted in an imbalance in primary production between ice algae, under-ice, and open water phytoplankton in the Arctic Ocean and adjacent polar seas (Arrigo et al., 2012; Leu et al., 2015). This imbalance has been driven by decreasing sea-ice coverage and time shifts in seasonal sea-ice dynamics (i.e., ice and snow thickness, melt onset, pond onset, etc.; Arrigo et al. 2014; Horvat et al. 2017). Recent field observations (Arrigo et al., 2012) and model simulations (Horvat et al., 2017) suggest

that the warming trends at high latitudes may have increased the occurrence of under-ice blooms as a consequence of the rise in under-ice solar radiation during the spring season due to thinner first-year ice, early melting, a significant fraction of leads, and melt ponds at the ice surface (Mundy et al., 2009, 2014; Palmer et al., 2014; Leu et al., 2015; Assmy et al., 2017; Horvat et al., 2017).

High phytoplankton biomass and primary production rates in the marginal ice zone (MIZ), as defined hereafter as the area along the edge of the ice pack that is affected by open ocean processes, have been reported in the literature over several decades (Barber et al., 2015, and references therein). Physical, chemical, and biological processes occurring at the MIZ trigger important ecological successions in the marine ecosystem and impact the coupling between sympagic, pelagic, and benthic realms (Leu et al., 2015). Satellite ocean color observations have proven a handy tool to map chlorophyll-a concentration ([chla]), a proxy for sea surface pelagic phytoplankton biomass and abundance, in open waters found in the edge zone of the MIZ (see Barber et al., 2015) in both poles since the launch of the Coastal Zone Color Scanner (CZCS) (Maynard and Clark, 1986, 1987; Mitchell et al., 1991). Recently, Perrette et al. (2011) developed a method to assess the phytoplankton bloom along the edge of the ice pack, which is referred to as ice-edge bloom hereinafter, at the pan-Arctic scale using the Sea Wide Field-of-view Sensor (SeaWiFS). Based on the year 2007, they concluded that the ice-edge blooms were ubiquitous in the northern latitudes (> 66.6° N). Also using SeaWiFS, Lowry et al. (2014) reported that ice-edge blooms on the Chukchi Sea shelf depend on the timing of sea-ice retreat and further speculated that massive under-ice blooms were widespread in nutrient-rich waters of Pacific origin. Renaut et al. (2018) applied the method of Perrette et al. (2011) to 11 years of chlorophyll-a observation of the Moderate-Resolution Imaging Spectrometer Sensor (MODIS) and reported an intensification and a northward expansion of the ice-edge bloom in many subarctic seas. Altogether, these results suggest that non-linear processes regulate ice-edge blooms. Among them, sea-ice production and snow cover thickness affect convective mixing and nutrient replenishment during winter, light availability at the onset of the growing season, and the amount of meltwater available for the subsequent emergence of meltwater-stratification.

Are ice-edge blooms a recurrent feature throughout the HBS? To our knowledge, ice-edge blooms in

the HBS have not been examined explicitly, using satellite ocean color or with field observations. The HBS was excluded from recent ocean color analyses conducted in the Arctic (Perrette et al., 2011; Renaut et al., 2018). Except in river plumes and some upwelling spots in Hudson Strait and near the Foxe Peninsula and the Belcher Islands, the HBS has been assumed to be a low-productivity oligotrophic system (Ferland et al., 2011; Tremblay et al., 2019). A few studies investigated under-ice phytoplankton and pelagic community interactions during the spring season in a few coastal locations (i.e., near the Belcher Islands and Great Whale River in the southeastern coastal HB; Michel et al., 1988, 1993; Runge et al., 1991; Monti et al., 1996). These land-fast ice camp-based studies reported many critical ecological processes occurring during the transition from the under-ice to a pelagic-dominated system: photo-adaptation of ice-algal communities (Michel et al., 1988); ice-algal communities seeding the pelagic ecosystem (Michel et al., 1993); the coupling between under-ice grazers, inter-facial and pelagic communities (Runge et al., 1991); and the impact of river plume dynamics on algal community composition (Monti et al., 1996). None of these studies found evidence of under-ice phytoplankton blooms during the melting season at the Hudson Bay basin scale. Model-based investigations by Sibert et al. (2010, 2011), however, reported that under-ice production timing is mainly controlled by surface melting (snow and ice) processes that determine the light levels, even under conditions of sufficient nutrient availability. A bay-wide assessment of [chla] is needed to obtain a large-scale perspective of the phytoplankton productivity of the HBS.

In summary, there are many indications that the MIZ is a biologically productive feature in the HBS. Still, no systematic observations of ice-edge phytoplankton blooms have been reported in this subarctic region. The main objective of this study was to assess the temporal and spatial variability of the ice-edge bloom based on a systematic analysis of available satellite time series. Therefore, we analyzed two decades of satellite remote sensing data combining ocean color observation of [*chla*] and passive microwave imagery for sea-ice concentration (SIC). First, we compared the phytoplankton phenology assessed from archived observations of the CZCS (1978–1983) to the modern phenology obtained from MODIS-Aqua (2002–2014). Next, we characterized phytoplankton dynamics based on the temporal evolution of satellite [*chla*] and timing of sea-ice retreat to obtain climatological conditions, trophic categories, and phytoplankton phenological types in marginal ice zones. We documented the inter-annual variability of the surface [*chla*] at the MIZ and examined how it is impacted by the timing of sea-ice retreat and winter air temperature. Finally, we examined the influence of large-scale climate variability patterns, particularly the Arctic Oscillation (AO) and North Atlantic Oscillation (NAO), on oceanographic processes and ice-edge bloom intensity in the HBS.

1.2 Materials and Methods

1.2.1 Satellite data

1.2.1.1 Ocean color

Multi-sensor merged [*chla*] Level-3 (i.e., binned and mapped) 8-day composites from the Globcolour Project (http://www.globcolour.info/) were used as a proxy for phytoplankton biomass. Globcolour products have a spatial resolution of 4.63 km and cover 1998–2018 period. The merged product was selected to improve the spatial-temporal coverage diminishing gaps due to cloud cover and sea-ice coverage (Maritorena et al., 2010). The binning methodology combines the normalized water-leaving radiances from different ocean color sensors whenever they are available, which includes: SeaWiFS (1998-2010), MODIS-Aqua (2002–2018), Medium-Resolution Imaging Spectrometer (MERIS: 2002–2011), and Visible Infrared Imaging Radiometer Suite (VIIRS: 2012–2018). [*chla*] was estimated from normalized water-leaving radiances merged using the Garver-Siegel-Maritorena (GSM) semi-analytical model (Garver and Siegel, 1997; Maritorena et al., 2002). GSM also yields particle backscattering (b_{bp}) and colored detrital matter (CDM) coefficients at 443 nm.

Colored dissolved organic matter (CDOM) and non-algal particles can deteriorate the performance of ocean color algorithms because, as phytoplankton pigments, they absorb the blue part of the visible spectrum (Bricaud et al., 1981). Consequently, in Arctic and sub-Arctic seas, [*chla*] overestimates (underestimates) in the lower (higher) range of [*Chla*] have often been reported (Cota et al., 2004; Hi-rawake et al., 2012; IOCCG, 2015). CDOM is known to be a dominant optical component in most of the HBS, making this region optically complex (Granskog et al., 2007; Mundy et al., 2010; Guéguen et al., 2011; Xi et al., 2013; Burt et al., 2016; Heikkila et al., 2016). As discussed by Ben Mustapha et al. (2012), Bélanger et al. (2013), and Lewis and Arrigo (2020), the GSM algorithm can minimize

the impact of other optical constituents on [*chla*] retrievals because the more mechanistic GSM algorithm is able to take into account seasonal and regional variability of bio-optical properties compared to empirical algorithms for Polar shelves. Therefore, the GSM was selected because it can better represent the optically complex waters of the HBS (Xi et al., 2013, 2014, 2015), and data from depths shallower than 50 m were excluded from the analysis to avoid turbid or CDM-rich waters and river plumes.

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We performed a cluster analysis (see below) on 8-day composites (multi-year averages) of [*chla*] to detect potential changes in phytoplankton phenology between the 1980s and the 2000s. We used the CZCS for the period 1978–1983 and MODIS from 2002—2014. For consistency in the data processing for these two ocean color missions, [*chla*] was calculated using the case-1 waters standard empirical Ocean Color algorithm CZCS OC3 and MODIS OC3v5 (O'Reilly et al., 1998, 2000). The use of band ratio algorithms allows a better interconnection between distinct sensors (Antoine et al., 2005; McClain, 2009). We tested the sensitivity of the cluster analysis to the choice of [*chla*] algorithms and available ocean color products. Specifically, we used the Globcolour merged chlorophyll-*a* products obtained using both GSM (as above) and empirical algorithms for the same period as MODIS OC3v5 alone (2002–2014). We found some spatial discrepancy in the cluster distribution between products, but the main conclusion drawn from the analysis remained unchanged (i.e., increased occurrence of double bloom, see Results section).

1.2.1.2 Sea-ice concentration

Sea-ice concentration (SIC) was obtained from the National Snow and Ice Data Center (NSIDC). It is based on daily passive microwave radiometry processed using the Bootstrap algorithm (Comiso, 2000) at 25 km resolution. The Bootstrap technique clusters the multichannel passive microwave sensors: Scanning Multichannel Microwave Radiometer on the Nimbus-7 satellite, Special Sensor Microwave/Imager and Special Sensor Microwave Imager/Sounder from the Defense Meteorological Satellite Program's satellites, and the Advanced Microwave Scanning Radiometer (Comiso et al., 1997). SIC was interpolated onto the same [*chla*] grid using the nearest neighborhood scheme implemented in Matlab.

1.2.2 Climate index and reanalysis

The Arctic Oscillation is a climate pattern characterized by winds circulating counterclockwise around the Arctic at around 55°N latitude. The AO index is calculated from the first component of the empirical orthogonal function of monthly anomaly variations in sea-level atmospheric pressure north of 40°N, which explains 22% of total variance (Thompson and Wallace, 1998). The North Atlantic Oscillation index is extracted from the difference between monthly anomaly variations in sea-level atmospheric pressure over Greenland (low pressure) and The Azores Island (high pressure) (Hurrell et al., 2001, 2003; Qian et al., 2008). NAO/AO data were obtained from the Climatic Prediction Center/the National Oceanic and Atmospheric Administration (CPC/NOAA: http://www.cpc.ncep.noaa.gov). Here we used the average index for the winter months of January, February, and March.

We obtained the monthly air temperatures from the National Centers for Environmental Prediction/National Center for Atmospheric Research (NCEP/NCAR) Reanalysis Project. Anomalies of air temperature were calculated as the difference between each monthly average and its corresponding monthly climatology and normalized by the standard deviation, both of which were calculated using data from the 1948 to 2018 period.

1.2.3 Data analysis

1.2.3.1 Phytoplankton phenology during the ice-free season

We investigated the potential changes in phytoplankton phenology between the 1980s and 2000s using a K-means cluster analysis applied on the annual time series of [*chla*]. The approach used here is similar to that adopted by D'Ortenzio and D'Alcalà (2009) in the Mediterranean Sea, D'Ortenzio et al. (2012) at the global scale, Ardyna et al. (2017) in the Southern Ocean, and Marchese et al. (2017) at regional Arctic scales.

Briefly, we analyzed the seasonal variability (or shape) of the annual [*chla*] time series (i.e., a multiyear average of 8-day [*chla*] available for a given period, hereafter referred to as *climatology*) to determine the number of phytoplankton blooms during the annual cycle, as well as their timing. Therefore, we focused on the relative change in [*chla*] over the year rather than the absolute values of [*chla*]. In addition, we standardized the individual climatologies, $Chl_{clim}(x, y, t)$, for each 4.60-km pixel (x, y), as:

$$Chl_N(x, y, t) = \frac{Chl_{clim}(x, y, t) - Chl(x, y)}{\sigma_{Chl}(x, y)}$$
(1.1)

where *t* is the time referring to the 8-day composite; $Chl_N(x, y, t)$ is the normalized time series; and $\overline{Chl}(x, y)$ and $\sigma_{Chl}(x, y)$ are the annual mean and standard deviation values of climatological time series for the pixel (x, y). $Chl_{clim}(x, y, t)$ was calculated with a temporal resolution of 8 days for CZCS and MODIS-Aqua. Data applied to phenology analysis were also filtered by a spatial-temporal median filter $(3 \times 3 \times 3)$, and the gaps were filled using the data interpolating empirical orthogonal functions scheme implemented in R (DINEOF; Beckers and Rixen, 2003). The ideal number of clusters was determined by the Davies-Bouldin criterion, and cluster stability was accessed by Jaccard, Bootstrap, and Noised coefficients (Hennig, 2007; D'Ortenzio and D'Alcalà, 2009; D'Ortenzio et al., 2012).

1.2.3.2 Phytoplankton phenology at the marginal ice zone

To assess the impacts of sea-ice retreat timing on MIZ phytoplankton blooms (also refers to phytoplankton spring blooms or ice-edge blooms), we analyzed both [*chla*] and SIC variability in parallel. The method is similar to that of Perrette et al. (2011), which was also adopted by Lowry et al. (2014) and Renaut et al. (2018). The sea-ice retreat, t_R , is defined as the day at which SIC is below 10% for at least 24 days. This time interval is longer than the 20 days applied by Perrette et al. (2011) and Renaut et al. (2018), and the 14 days by Lowry et al. (2014) because we used 8-day composites instead of daily maps. However, to avoid sub-pixel contamination in ice-infested regions near the ice edge (Bélanger et al., 2013), we opted to be more conservative by applying a 10% threshold on SIC, as did Perrette et al. (2011) and Renaut et al. (2018) instead of 50% as applied by Lowry et al. (2014). The maximum [*chla*] observed in the MIZ was extracted for each pixel for each year, yielding one map of MIZ [*chla*] per year.

We recognized that sea-ice cover hides an important component of phytoplankton phenology that is

out of the reach of ocean color satellites (Arrigo et al., 2012). To address this problem, we developed a trophic predictor of under-ice and pelagic phytoplankton phenology throughout the MIZ by analyzing a seasonal time series of satellite-derived SIC and [*chla*]. This trophic predictor is defined by the temporal evolution of [*chla*] since the sea-ice retreat (t_R).

Figure 2 illustrates five typical [*chla*] phenologies expected during the spring-to-summer transition at the MIZ, assuming that the temporal evolution of [*chla*] during phytoplankton blooms has a Gaussianlike curve (Jönsson and Eklundh, 2004; Platt et al., 2009). Each of these phenologies is defined in terms of three metrics: 1) the very first [*chla*] observation after the sea-ice retreat ([*chla*($t_{1,2,3,...}$)_{max}]), 2) the maximum [*chla*] reached within five weeks after the sea-ice retreat ([*chla*($t_{1,2,3,...}$)_{max}]), and 3) the minimum reach within five weeks after the sea-ice retreat ([*chla*($t_{1,2,3,...}$)_{min}]). Table 1 presents the criteria that define each type of MIZ phenology. The bloom threshold, *B*, was set at 0.5 mg m⁻³ as in Perrette et al. (2011). The oligotrophy threshold, *Ol*, was set at 0.2 mg m⁻³. We applied these criteria to each pixel and for each year, yielding one thematic map per year.

1.2.3.3 Correlation analysis between MIZ [chla] and environmental forcing

To investigate the impact of climate and environmental forcing on ice-edge blooms, we calculated the Pearson coefficient of correlation (r) of the linear relationships between the MIZ [chla] and (1) the annual values of the AO, (2) the sea-ice retreat day (t_R) and (3) the winter (December–January–February, DJF) air temperature anomaly. The analysis was made on each grid cell of the HBS between 1998 and 2018. We standardized the maximum [chla] values in the MIZ (Perrette et al., 2011) using climatology mean and standard deviation as above. Only significant slopes, obtained from a least-squares fit at an interval of confidence of 95% (P > 0.05) and for pixels having more than ten valid years between 1998 and 2018, were mapped.

Table 1: Remote sensing criteria defining the types of phytoplankton phenology throughout marginal ice zones.

| Phenology type ^{<i>a</i>} | Criteria ^b | |
|---|--|--|
| I – Oligotrophic or old under-ice bloom | $[Chla(t_R)] < B$ | |
| | $[Chla(t_R)] < [Chla(t_{1,2,3\dots})_{max}] < B$ | |
| II – Probable (recent) under-ice bloom | $Ol < [Chla(t_R)] < B$ | |
| | $[Chla(t_{1,2,3\dots})_{max}] < [chla(t_R)]$ | |
| III – Mesotrophic/nutrients replenished | $[Chla(t_R)] \ge B$ | |
| | $[chla(t_{1,2,3\dots})_{max}] \ge B$ | |
| | $[chla(t_{1,2,3\dots})_{min}] \ge B$ | |
| VI – Bloom triggered in ice-free waters | $[chla(t_R)] < [chla(t_{1,2,3})_{max}]$ | |
| | $[chla(t_R)] < B$ | |
| | $[chla(t_{1,2,3\dots})_{max}] \ge B$ | |
| V – Bloom triggered under-ice | $[chla(t_R)] > [chla(t_{1,2,3})_{min}]$ | |
| | $[chla(t_R)] \ge B$ | |
| | $[chla(t_{1,2,3\dots})_{min}] < B$ | |

^{*a*} defined based on the time evolution of [*chla*] after the sea-ice retreat (with [*chla*] in mg m⁻³).

^{*b*} *B* is the bloom threshold (*B*), here set to 0.5 mg m⁻³; The oligotrophic threshold (*Ol*) was set to 0.2 mg m⁻³; t_R is the day of sea-ice retreat defined as the day at which sea-ice concentration (SIC) is below 10% for at least 24 days; $t_{1,2,3...}$ refers to weeks after the sea-ice retreat.



Figure 2: Schematic of phytoplankton phenologies throughout marginal ice zones. The five possible phenologies are: consistently low biomass indicating undetectable (old) under-ice bloom or an oligotrophic set up (I: blue line or dotted); probable (recent) under-ice bloom (II: red line); consistently high biomass indicating efficient nutrient replenishment (III: green line), bloom triggered in ice-free waters after the sea-ice retreat (VI: orange line); and bloom triggered under-ice which develop a peak just after the sea-ice retreat (V: cyan line)

1.3 Results

1.3.1 Air temperature and phytoplankton phenology: CZCS versus MODIS era

Warmer air temperatures in the HBS began around 1998 (Figure 3), which coincides with the beginning of the modern era of ocean color radiometry (i.e., the launch of SeaWiFS in August 1997). This recent period contrasted with the CZCS era (1978–1983), which was characterized by the predominance of a negative air temperature anomaly (T_{air}) relative to the average air temperature calculated over the 1948–2018 period. One extreme cold event was observed at the beginning of the CZCS era in 1978. During the MODIS observational era, T_{air} was mainly positive, but colder winters were often seen, as in 2002, 2003, 2004, 2011, 2014, 2015, 2016, and 2018. In contrast, most summers showed positive anomalies, except for 2004, 2007, 2011, and 2018. The latter stands out in the modern era with a noticeable negative T_{air} during most of the year.

The distinct T_{air} between the CZCS and MODIS eras coincided with remarkable changes in phy-



Figure 3: Surface air temperature anomalies and ocean color satellite coverage. Monthly anomalies of air temperature (T_{air}) spanning the period from 1948 to 2018 (negative anomalies in blue and positive in red bars). The temporal coverage of CZCS (1978–1983), MODIS (2002–2014), and Globcolour (1998–2018) [*chla*] observations are marked. During the modern era of ocean color radiometry, positive values for T_{air} were often observed during the spring-to-summer transition.

toplankton phenological patterns in the HBS (Figure 4). Our analysis resulted in three statistically distinct bio-regions characterized by the shape and the number of observable [*chla*] peaks, hereafter referred to as phytoplankton "blooms", over an annual cycle. The spring-summer bloom (SB) type (red pixels and curve in Figure 4) exhibited only one [*chla*] peak, which reached its maximum a few weeks after the summer solstice (21 June). The double bloom (DB) type (green pixels) was characterized by a first [*chla*] peak occurring in late May/early June, and a second peak at the very end of the open water season, when ocean color observations were still available (i.e., mid-October). The last type, the fall bloom (FB) (blue pixels), was initiated in mid-summer, peaked in mid-September, and declined until the sea-ice-recovered (Figure 4C). FB contrasted with the second peak of the DB phenology, in which [*chla*] increased continually until the sea-ice recovery.

Three types of bloom were observed during the CZCS era, but with no distinct spatial patterns (Figure 4A). Of 65873 valid observations over that period, the SB, DB, and FB occupied 28%, 38%, and 24%, respectively. During the MODIS era, for which 70972 valid pixels were found, SB remained at about 28%, but DB increased to 54%, and FB decreased to 18% of the total surface area. This result

| Cluster ^a | MODIS SB | MODIS FB | MODIS DB |
|----------------------|----------|----------|----------|
| CZCS SB | 39 | 24 | 34 |
| CZCS FB | 27 | 15 | 21 |
| CZCS DB | 24 | 18 | 23 |

Table 2: Changes in the number of days (Δt) of open water season between the CZCS (1978–1983) and MODIS (2002–2014) eras, according to the phenological cluster.

^a SB indicates spring bloom; FB, fall bloom; and DB, double blooms.

suggests that a remotely sensed spring or summer bloom is a common feature in the HBS. Whether this increase in [chla] at the beginning of the open water season is an actual ice-edge bloom or not is examined further in the next sections.

Single [*chla*] peak phenology (SB and FB) might be seen as a variation of DB phenology. The start date and the peak amplitude of a single SB occurred shortly after the spring bloom of DB phenology. Similarly, the single FB peak occurred before the fall bloom of the DB phenology. The fact that the DB phenology has become a predominant feature in the HBS implies that an earlier spring–summer bloom is now occurring. We examined whether or not the duration of the open-water-season (OW), which was defined as the number of days with SIC below 10% during an annual cycle, could explain the fact that more DB are now observed. The OW duration increased from 15 to 39 days between CZCS and MODIS eras, reaching about 125 days (4 months) in modern times (Figure 4D, Table 2). The regions where SB in the CZCS era was replaced by DB in the MODIS era had an increase in OW of 34 days (Table 2). The OW duration in areas where FB was replaced by DB or remained as DB had increased by 21 and 23 days, respectively. However, these increases in OW were not more significant than for pixels showing SB in both CZCS and MODIS eras (39 days). Therefore, no clear link was identified between the OW duration and the change (or the lack of change) in the phytoplankton phenology patterns.



Figure 4: Phytoplankton phenology changes between CZCS (1978–1983) and MODIS eras (2002–2014).Cluster-derived maps of phytoplankton phenological regimes for the (A) CZCS era (1978–1983) and the (B) MODIS era (2002–2014). (C) The plot shows the three types of phenology obtained using the K-means cluster analysis. (D) Open water season duration (number of days with a sea-ice concentration lower than 10%) for each phenological domain in the CZCS era (blue boxplots) and MODIS era (yellow boxplots). The boxplots show the median (red lines), 25^{th} and 75^{th} percentiles at the hinges, and the whiskers extend to show \pm 1 standard deviation.

1.3.2 Marginal ice zone blooms between 1998 and 2018

Figure 5A shows the climatology of the 8-day bins of [chla] for the whole HBS from the Globcolour dataset (1998–2018), together with the average daily percentage of OW in the HBS (blue bars). Interestingly, we observed two distinct peaks in [chla]: one in spring around day-of-year (DOY) 75 (mid-March) and a second around DOY 150 (beginning of June). The first peak, reaching values around 0.7 mg m⁻³, is observed when sea ice covers the bay almost entirely (90% of the area). During that time, we noted early phytoplankton blooms in very restricted locations known as polynyas, such as the northwestern part of Hudson Bay (Ferguson et al., 2010). The second increase in [chla] begins as soon as the OW area started to increase and can be considered as an ice-edge bloom, which is a typical feature along the marginal ice zone during the spring-to-summer transition (Mitchell et al., 1991). During this transition period, the [*chla*] reached a relatively high level (1.0 mg m^{-3}) with lower variability, as depicted by the lower standard deviation (grey-shaded area on Figure 5A) compared to the rest of the year. This bloom is probably productive, as it is synchronized almost perfectly with the peak of incident photosynthetic available radiation (PAR(0+), where 0+ indicates PAR just above the sea surface) (Figure 5B). The end of the OW season is characterized by a continuous increment of [chla], referred to as the fall bloom, which ended when sea ice recovered in late October (DOY 300). The high standard deviation during this season indicates extremes of low and high [chla], pointing toward high spatial variability.

To illustrate the recurrence of ice-edge blooms in the HBS, we plotted the frequency distribution of [chla] (N ~ 10⁶ pixels) as a function of the number of days after the sea-ice break-up between 1998 and 2018 (Figure 6). Higher [chla] values are generally restricted to the first 8-day period after the sea-ice retreat, with [chla] values ranging from 1 to 3 mg m⁻³. In contrast, observations of high chlorophyll-*a* later during the open water season were relatively low. These results suggest that ice-edge blooms, which are characterized by an increase in phytoplankton abundance propagating along the ice edge, could be observed frequently by ocean color satellites in the HBS. However, spatial analysis is required to confirm whether ice-edge blooms are present everywhere in the HBS or whether they are restricted to some parts of the Bay, where ocean conditions are more favorable, as suggested by the phenology analysis based on the climatology (Figure 4).



Figure 5: Climatologies of [*chla*], percentage of open water and photosynthetic active radiation (PAR). (A) [*chla*] climatology from Globcolour (GSM; merged product) and open water fraction (blue area) as a function of day of the year (DOY). (B) *PAR*(0+) climatology (Bélanger et al., 2013; Laliberté et al., 2016) (black lines) their respective standard deviation (shaded) observed between 2003 and 2010 in HBS. The sea-ice retreat was typically followed by a pelagic bloom during the spring-to-summer transition with a broad peak in early June (DOY 152) that was preceded by a smaller peak in February (DOY 120) and followed by a peak in the fall (DOY 243).



Figure 6: Frequency distribution of [*chla*] after the sea-ice retreat. Frequency distribution of [*chla*] as a function of the number of days after the sea-ice retreat. The marginal ice zone (red box) is defined by the first 24 days after the sea-ice retreat (Perrette et al., 2011). The subsequent days define the open water season. Relations are extracted from the annual time series of [*chla*] for all pixels and all years between 1998 and 2018 in the HBS.

Panels A and B of Figures 7 show maps of the average and the standard deviation of the maximum [*chla*], respectively, observed in the ice-edge zone of the MIZ between 1998 and 2018. The statistics were calculated using the 21 annual maps depicted in Figure 16. The limits of the sub-regions are those used by Landy et al. (2017) who reported satellite-based sea-ice thickness and snow depth in the HBS. In general, we noted higher [*chla*] in the surrounding of the Bay, with the highest values found in the Hudson Strait (HS) and Southeastern (SE) HB. These two regions also show a higher standard deviation (STD) in the maximum [*chla*] at the MIZ, indicating relatively high inter-annual variability. We also observed a high STD in the northwestern (NW) polynya. Southwestern (SW) and
Northeastern (NW) HB have moderate to high [*chla*] (around 1 mg m⁻³) in the MIZ and relatively low interannual variability. The central HB shows both low [*chla*] (< 0.5 mg m⁻³) and STD interannual variability, suggesting that ice-edge blooms are not a dominant feature offshore. Figures 7C and D illustrates the average and standard deviation of sea-ice retreat date (t_R) for the same period (1998–2018) based on annual maps shown in Figure 17 (in supplementary material). The central HB had the latest t_R , ranging from DOY 180 to 210 (month of July), with relatively low interannual variability (STD < 10). The highest (lowest) interannual variability of t_R occurred in the coastal (offshore) areas of SW and NE Hudson Bay. Interestingly, the t_R and [*chla*] were somewhat very similar, suggesting that the magnitude of the ice-edge bloom is linked to the timing of sea-ice retreat, as explored further below.

Table 3 presents the statistics and frequency of occurrence of the surface extension (in km² and % of the total surface area) for four sub-categories of [*chla*], which is a good proxy for the trophic state of the MIZ. On average, an ice-edge bloom (0.5 to 2.0 mg m⁻³) or major ice-edge bloom (here major bloom is defined as [*chla*] > 2 mg m⁻³) occupied 46.3% of the Bay, but blooms can range from 27.9% (1999) and 56.2% (2008) of the total area (see also Figure 16). High interannual variability was also observed in the area of major blooms ranging from 2.3% (2010) to 9.0% (2015) (Figure 8). During the study period (1998–2018), the surface area of the ice-edge blooms increased by 10.5% (i.e., 0.5% per year times 21 years). In 2015, a major ice-edge bloom occupied as much as 7200 km² (or 9.0% of the HBS surface) but was found in the polynyas (Figure 8). In 2018, the timing of the sea-ice break-up showed large spatial variability with an early break-up in the NW and a late break-up in the NE (Figure 8). The ice-edge bloom occupied a large portion of the NW, but with a modest [*chla*] compared to 2015. This result suggests that the magnitude of the ice-edge bloom is explained not only by the timing of the sea-ice retreat.

Figure 8 shows annual maps of the maximum [*chla*] observed during the MIZ time window for selected years (2008, 2011, 2015, and 2018) showing interesting features in terms of ice-edge blooms. Several key observations can be made from these maps. First, the [*chla*] in the central HB remained relatively low (< 0.5) after the break-up for most of the years, except in 2005, 2008, 2012, and 2016,



Figure 7: Climatic maps of maximum [*chla*] in the ice-edge zone and of sea-ice retreat timing. Average (A) and standard deviation (B) of the maximum [*chla*] during the 24-day period after the sea-ice retreat. The statistics were calculated using the annual maps between 1998 and 2018 (n = 21 for each grid cell) shown in Figure 16. Similar statistics (C and D) were made for the DOY of sea-ice retreat (t_R) shown in Figure 17.

which means that no ice-edge blooms occurred in the central HB for most of the years analyzed. Moderate to high values of [*chla*] were observed during the MIZ period along the surrounding of the bay with obvious variability in both northwestern and northeastern parts of the bay, which sometimes showed opposite patterns (e.g., compare 2015 and 2016; Figure 16). Higher [*chla*] in the MIZ was observed systematically in the Hudson Strait, where mixing and nutrient replenishment are more intense relative to the rest of HB (Ferland et al., 2011). However, the largest ice-edge bloom was observed in the NW HB in 2015 with [*chla*] higher than 2.0 mg m⁻³.

To gain insight into the variability in the MIZ [*chla*] (Figure 8), we considered the timing of the sea-ice retreat. Figure 17 depicts the DOY of the sea-ice break-up or, in other words, the beginning of the MIZ period in the HBS for each year between 1998 and 2018. The break-up occurred within a wide range of four months, i.e., from DOY 120 to 240. An early break-up can be found either in the NW or NE HB, where polynyas are common. Sea ice often accumulated in the southern part of HB delaying the break-up to the end of the summer, as observed in 2000, 2004, 2008, 2009, and 2015. A visual comparison of the annual maps presented in Figures 8, 16, and 17 suggest that, at least in some parts of Hudson Bay, early sea-ice break-up resulted in more intense ice-edge blooms observable from space. This relationship, however, is far from applicable to the whole HBS, which we examine further in the next section.

Figure 9 shows maps of the frequency of occurrence of the four trophic states in the ice-edge zone defined above (Table 3). These maps provide an additional point of view about the spatial and interannual variability of ice-edge blooms in the HBS between 1998 and 2018. Oligotrophy occurrence ($< 0.2 \text{ mg m}^{-3}$) was more frequent offshore, covering a vast region in the central part of HB in 30% of the years analyzed. On the other hand, the occurrence of oligotrophy conditions across the bay was less than 5% (Figure 9A). As observed in Figure 9B, moderate oligotrophy ($0.2 <= [chla] < 0.5 \text{ mg m}^{-3}$) conditions were more frequent in the central HB with a frequency higher than 60% covering a large proportion of the bay (almost half of it). Ice-edge bloom ($0.5 < [chla] <= 2.0 \text{ mg m}^{-3}$) occurrence in the surrounding of the bay and HS generally surpassed 65%. A presence higher than 80% was reached in the domains of the NW polynya, proximal areas of the most significant river plumes, the



Figure 8: Maximum [*chla*] in the ice-edge zone and ice-retreat timing during extreme years and the BaySys expedition. Annual map of maximum [*chla*] following the sea-ice retreat (left panels), and the timing (DOY) of sea-ice retreat (right panels) for selected years (same as Figures 16 and 17). The top panels are for 2008 and 2000, which showed the largest and smallest ice-edge bloom extension, respectively, as reported in Table 2. The bottom panels are for 2015, the year showing the largest ice-edge bloom in the NW polynya, and 2018, the year of the BaySYS expedition.

Table 3: Annual extension of distinct trophic states in the ice-edge zone estimated using [*chla*] thresholds and sea-ice retreat between 1998 and 2018 in the HBS

| Ice-edge zone trophic state | | Extension in 10^4 km^2 (% ^{<i>a</i>}) and extreme years ^{<i>b</i>} | | | | |
|------------------------------|----------------------|---|--------------------|--------------------|----------------------|--------------------|
| Categories | $[chla] (mg m^{-3})$ | Median | max., year | min., year | trend ^{c,d} | rms.e ^e |
| Oligotrophy | < 0.2 | 3.7 (4.6%) | 18.2 (22.7%), 1999 | 0.5 (0.6%), 2008 | -0.4 (-0.4%) | 4.3 |
| Moderate oligotrophy | 0.2-0.5 | 28.8 (35.9%) | 36.4 (45.4%), 2000 | 13.6 (17.0%), 2015 | -0.2 (-0.3%) | 4.9 |
| Bloom | 0.5-2.0 | 33.1 (41.3%) | 45.0 (56.2%), 2008 | 22.3 (27.9%), 1999 | +0.4(+0.5%) | 5.6 |
| Major bloom | > 2.0 | 4.0 (5.0%) | 7.2 (9.0%), 2015 | 1.8 (2.3%), 2010 | 0.0(0.0%) | 1.5 |
| Sea-ice retreat ^f | | 183 | 194, 2004 | 174, 2006 | +0.1 | 5.7 |

^{*a*} % of total area of Hudson Bay and Hudson Strait deeper than 50 m: 80×10^4 km² (Amante and Eakins, 2009);

^bextreme events are reported according to year of maximum and minimum coverage;

^c in an interval of confidence of 95% (P < 0.05) for the extension of trophic states;

^d in an interval of confidence of 99% (P < 0.01) for the day of sea-ice retreat;

^e root mean square error;

^f first day of year when sea-ice concentration is below 10%.

eastern bay, and HS (Figure 9C). Recurrently productive hot spots (> 50% of occurrence; Figure 9D) were found in relatively small regions, south of Belcher Island, some places in the northern HS, and river-influenced coastal areas. We also observed occurrence above 10% in the NW HB polynya and south of Southampton Island.

1.3.3 Phytoplankton phenology at the MIZ

We performed a time series analysis of SIC and [*chla*] at the pixel level to assess the potential that under-ice blooms escaped satellite range. We considered four scenarios for the temporal evolution of [*chla*] at the MIZ, as shown in Figure 2. Applying the criteria of Table 1 resulted in 21 thematic maps presented in Figure 18. To synthesize the results, we calculated the frequency of occurrence of each type based on 21 years of observations. Figure 10 shows the frequency of occurrence of the five phenology types between 1998 and 2018.

Consistently low biomass observed in the MIZ after the ice retreat (Figure 10A) could be due to an under-ice bloom that escaped the satellite range entirely or to an oligotrophic state at the sea surface. Similarly, the probable (recent) under-ice bloom (Figure 10B) may also indicate that oligotrophic domains remain in the ice-edge zone. However, these domains involve moderate concentrations between 0.2 and 0.5 mg m⁻³ after the sea-ice retreat followed by a decline in [*chla*]. Oligotrophy/old under-ice bloom (type I) and probable (recent) under-ice blooms (type II) can be considered similar



Figure 9: Frequency of occurrence of four trophic stages in the ice-edge zone. Maps of frequency of occurrence of four categories of chlorophyll-*a* concentration in the ice-edge zone based on 21 years (1998 to 2018) of ocean color observations defining MIZ trophic conditions: (A) oligotrophy, (B) moderate oligotrophy, (C) bloom, and (D) major bloom.

features, though with distinct magnitudes and bloom-timing. This scenario (types I and II) dominated the whole central HB, extending north of Southampton Island with a frequency of occurrence ranging from 50 to 100%. In contrast, the situation characterized by [*chla*] consistently above 0.5 mg m⁻³ (Figure 10C), suggesting mesotrophic conditions where surface waters are efficiently replenished in nutrients, was frequent only in coastal waters or at the ends of the Hudson Strait. The last scenario, i.e., when the bloom is triggered in ice-free waters, was infrequent, except at the margin between the coastal domains and the central HB, from Churchill to NE HB (Figure 10D). Finally, the typical ice-edge bloom scenario, i.e., when [*chla*] peaks just after the ice-break-up and then vanishes to low concentration, was relatively frequent (30% to 70% of the time) all around HB and in the central part of HS (Figure 10E).

1.3.4 The magnitude of the ice-edge bloom and timing of sea-ice break-up

As shown above, a high spatio-temporal variability characterized the dynamic of the MIZ, both in terms of [*chla*] and sea-ice break-up in HBS (Figures 8, S1, and S2). Here we examined the potential link between these two variables by aggregating data in the seven sub-regions presented above (Figure 11): northwestern (NW), southwestern (SW), central and offshore (Central), narrows at the Hudson Bay entrance (Narrows), Hudson Strait (HS), northeastern (NE), and southeastern (SE). The box-plots of Figure 11 show the [*chla*] in the MIZ as a function of the date of the sea-ice retreat (t_R). The frequency occurrence of t_R is also shown on top of each box-plot. These distributions allow an understanding of the dynamic of the ice-edge bloom in each sub-region of the HBS.

The western part of the bay (NW and SW; Figure 11) showed a similar relationship between the timing of the ice-break up and the magnitude of the ice-edge bloom. The sooner the sea ice breaks up, the higher the [*chla*] in the ice edge. The NW sub-region, known to host wind-driven polynyas (Landy et al., 2017), shows more frequent sea-ice-retreat in June (86.4% of the time), though it was also often observed in May (21.7% of the time). The median [*chla*] values were > 1 mg m⁻³ when the break-up was in May, and ~ 0.7 mg m⁻³ if it occurred during the first half of June. We observed oligotrophic conditions whenever the ice melt happened after June 15, with [*chla*] well below the threshold of 0.5



Figure 10: Frequency of occurrence of five phytoplankton phenological types throughout the marginal ice zone. Maps of frequency of occurrence for the five types of MIZ phenology between 1998 and 2018, as depicted in Figure 2: (A) Oligotrophy/old under-ice blooms; (B) probable (recent) under-ice bloom; (C) mesotrophic/nutrient replenished; (D) bloom triggered in ice-free waters; and (E) bloom triggered under-ice.



Figure 11: Influence of sea-ice retreat timing on [chla] along the ice edge in Hudson Bay sub-systems. Boxplots of maximum chlorophyll-*a* concentration ($[chla]_{max}$) in the marginal sea-ice zone (MIZ) in relation to day of the year of sea-ice retreat (t_R) in each sub-region of the Hudson Bay System. The central red line-mark is the $[chla]_{max}$ median, the edges of the blue boxes are the 25th and 75th percentiles, and the whiskers extend to the most extreme data points between $\pm 0.26 \sigma$ considering a normal distribution, and the percentage of valid pixels for each boxplot in relation to each sub-region is marked above the respective upper whisker. The significant differences between these boxes were ensured by the ANOVA statistical test at a confidence interval of 99.9%. [*chla*] above the threshold of 0.5 mg m⁻³ (green line) defines the marginal ice bloom occurrence (Perrette et al., 2011).

mg m⁻³. In the SW in May, however, ice-edge blooms only occurred 4.2% of the time. The sea-ice break-up happened mainly between mid-June and mid-July (60.3% of the time) and showed ice-edge [*chla*] very close to the 0.5 mg m⁻³ threshold. The influence of the Churchill and the Nelson rivers may explain the larger [*chla*] in summer compared to the NW sub-region where river inputs were minimum in the North. The increase in [*chla*] in the ice edge after 1 August only represented 0.3% and 2.1% of the time in the NW and SW, respectively, and thus was negligible.

The Narrows of the HB entrance and the central HB (Figure 11) showed a similar relationship between the timing of the break-up and the magnitude of the ice-edge bloom. First, the sea-ice retreat happened mainly in late June (~ 50% of the time) or early July (~ 30% of the time), but never before mid-May. Second, when the sea-ice retreat between mid-May and mid-June (~ 11% of the time), moderate phytoplankton blooms characterized the ice edge with a median [*chla*] around 1.0 mg m⁻³. Third, when the sea-ice retreat occurred after mid-June, it was followed by [*chla*] ~ 0.5 mg m⁻³. Lastly, a slightly higher [*chla*] was found in the ice edge when the sea ice retreated in late July, but this scenario represents only 7 or 8% of cases.

In the eastern part of the bay (NE and SE; Figures 11), [*chla*] remained well above the bloom threshold regardless of the date of the sea-ice retreat. We found higher [*chla*] in the SE, compared to NE, just south of the Belcher Islands (Figure 7A). Similarly, the Hudson Strait should be considered a highly productive system because the median [*chla*] in the ice-edge zone remained close to 1.5 mg m⁻³ when sea ice retreated between mid-May and the end of July. There, early ice retreat (before mid-May) resulted in lower [*chla*] compared to the rest of the season.

In summary, the timing of sea-ice retreat seems to play a crucial role in setting the magnitude of the ice-edge bloom observed from space in most of the HBS (NW, SW, Central, and Narrows), except in the eastern part of the bay (SE, NE, and HS). Significant ice-edge blooms were more restricted to May in the NW and SW sub-regions where the sea-ice retreat was earlier compared to the rest of the HBS (Figure 7C).



Figure 12: Relationships between the timing of sea-ice retreat and the maximum [*chla*] along the ice edge. Linear regressions between t_R and the maximum [*chla*] in the ice-edge zone (i.e., [*chla*]_{*IEZ*}(*x*, *y*) = *slope*(*x*, *y*) $t_R(x, y) + offset(x, y)$) were performed for each grid cell (*x*, *y*) using the annual maps shown in Figures 16 and 17 (n = 21 for each grid cell). The slope of the regressions is presented in A and its associated root mean square error (rms.e) in B.

The response of ice-edge blooms to the timing of sea-ice retreat showed some distinct spatial patterns. Figure 12A shows the slope $(\frac{\partial Chla_{IEZ}}{\partial t_R})$ of the linear regression between the maximum [*chla*] in the ice-edge zone and t_R on a pixel basis. The negative (positive) slope indicates that the sooner (later) the ice retreat, the higher the [*chla*] in the ice-edge zone. Interestingly, we found strong negative slopes in the Northwest HB, the Narrow at the HB entrance, and the central HS. Negative slopes were also found in about half of the pixels in the NE sub-region. Some coastal spots in the south presented positive slopes, which are associated with river discharge. The increment of [*chla*] with delays in the sea-ice retreat was also observed southeast of Belcher Islands, where tidal mixing is particularly intense (Webb, 2014). However, these domains were also associated with relatively high root mean square errors (*rms.e* above 1.00 mg m⁻³), suggesting large uncertainty in the relationship. Finally, we noted a neutral response of ice-edge blooms to t_R in most of the central HB.

1.3.5 The magnitude of the ice-edge bloom and atmospheric forcing

We computed a winter temperature index using the normalized air temperature anomalies relative to 1948–2018 mean (T'_{air}). A similar approach was used by Hochheim and Barber (2014) to investigate the impact of surface air temperatures on sea-ice break-up in the HBS. Here the response of ice-edge bloom magnitude is discussed in terms of the positive, negative, and neutral slope of the relationship between the winter air temperature anomaly and the maximum [*chla*] in the ice-edge zone ($\partial Chla_{IEZ}/\partial T'_{air}$) (Figure 13A). The positive (negative) slope indicates the warmer (colder) the winter, the higher (lower) the [*chla*] in the ice-edge zone in the spring–summer season. Based on this analysis, we found a positive relationship between air temperature and ice-edge bloom in the Hudson Bay entrance and NE (red pixels in Figure 13A), with NW and SE sub-regions appearing more sensitive than the rest of the bay (blue pixels). This positive relationship means that higher magnitude ice-edge blooms are expected after a cooler winter. Some spots, e.g., near large river plumes (Churchill, Nelson), had a negative relation between ice-edge blooms and T'_{air} but were also associated with the highest *rms.e*. This result may be related to river discharge variability (timing or volume). In contrast to the HB, the Hudson Strait presented a complex spatial distribution concerning the relation between ice-edge [*chla*] and T'_{air} , with strong negative slopes observed in most of the area.

We subsequently examined the impact of climatic teleconnections, such as the North Atlantic Oscillation and Arctic Oscillation, on the phytoplankton dynamic in MIZ, by correlating the maximum [*chla*] in the ice-edge zone with the NAO/AO index (Thompson and Wallace, 1998). As illustrated in Figure 14A and B, the main pattern observed is a positive correlation between NAO/AO and ice-edge zone [*chla*] in the NW and south of Belcher Islands polynyas, where sea ice usually retreats earlier (Landy et al., 2017). As reported in Figure 14C (D), the time series of normalized ice-edge [*chla*] and NAO (AO) index correlated significantly, with a Pearson correlation coefficient of 0.27 (0.29) in a confidence interval of 95% for the whole HBS and 0.46 (0.41) for the NW polynya. The correlation maps between ice-edge blooms, AO (Figure 14A) and NAO (Figure 14B) showed a similar pattern: a vast region of high correlation controlled by the NW polynya dynamic, negative correlation in the HB and NE bay, and high correlation south of Belcher Island. The maximum value of both [*chla*], AO, and NAO indices during 1998–2018 period occurred in 2015 when we observed a massive phyto-



Figure 13: Relationships between anomalies of winter air temperature and maximum [*chla*] in the marginal ice zone. Linear regressions between the winter air temperature anomaly (T'_{air}) and the maximum [*chla*] in the ice-edge zone (i.e., [*chla*]_{*IEZ*}(*x*, *y*) = *slope*(*x*, *y*)*t_R*(*x*, *y*) + *offset*(*x*, *y*)) were performed for each grid cell (*x*, *y*) using the annual map shown in Figures 16 (n = 21 for each grid cell). The slope of the regressions is presented in A and its associated root mean square error (rms.e) in B. Note that a single value of T'_{air} (Figure 19) was used for the whole HBS due to the lack of spatial variability.

plankton bloom in the whole HBS and the NW polynya (Figure 8 and 14C, D). In contrast, the lowest NAO/AO indices occurred in 2010, preceding a negative anomaly in ice-edge [*chla*] in the HBS by one year, but simultaneous with a local minimum in the NW polynya (Figure 14C versus 14D). The primary mismatches with NAO/AO indices occurred in 2005 and 2017 (Figure 14C) when considering the whole HBS, and 2000 and 2017 in the NW polynya (Figure 14D).

1.4 Discussion

We first discuss the inherent limitations of ocean color data for describing the phytoplankton dynamic in an ice-infested region under the influence of significant riverine inputs. Then, we explore the variability of [*chla*] in the ice-edge zone in terms of potential physical forcings that control nutrient availability and incoming light in the upper layer, and consequently the magnitude of the bloom. We further examine the impact of climatic changes on the phytoplankton dynamic throughout the MIZ. To achieve this objective, we explore the relationships between ice-edge bloom intensity and climate indices (NAO/AO), winter air temperature, and sea-ice retreat. Climate indices are used to describe the planetary teleconnections between the northern polar vortex. Finally, we focus on the HB NW polynya, an essential hotspot for marine life, as it shows high sensitivity to large-scale climate forcing.

1.4.1 Satellite Ocean Color of the HBS

Satellite remote sensing provides high revisit frequency, global coverage, and continued operational monitoring capability for access-limited regions such as HBS (Babin et al., 2015; Lee et al., 2015). Despite inherent limitations (IOCCG, 2015), i.e., restricted vertical range to the first optical depth $(1/K_d)$, lack of data under clouds or sea ice, presence of terrigenous optical components, and sea-ice contamination of ocean color products, satellite data have proven efficient to describe the phytoplankton dynamic at high latitudes, including in the MIZ (Maynard and Clark, 1986, 1987; Perrette et al., 2011; Lowry et al., 2014; Renaut et al., 2018).

Notwithstanding, standard empirical [*chla*] algorithms for global ocean data, and even Arctic-adapted ones, can be biased (IOCCG, 2015), calling into question the choice of a fixed threshold to detect



Figure 14: Teleconnection between climatic indices (NAO/AO) and phytoplankton ice-edge blooms. Map of correlation coefficients (P > 95%) between [*chla*] maxima in the ice edge zone and AO (A) and NAO (B) between annual 1998 and 2018 generated using the [*chla*] GSM algorithm from Globcolour and climatic indexes obtained from CPC/NOAA. Pearson's correlation with a t-test smaller than the 95% confidence interval was removed. A 95% confidence interval was applied to the time series of climatic indexes AO and NAO, and normalized mean values of annual [*chla*] maxima in the ice-edge zone for the whole HBS (C) and in the Northwest Hudson Bay polynya (D).

phytoplankton blooms. In the Arctic and sub-Arctic seas, empirical algorithms tend to overestimate (underestimate) [*chla*] in the lower (higher) range (Cota et al., 2004; Hirawake et al., 2012; IOCCG, 2015).

In particular, CDOM and non-algal particles can diminish the performance in these algorithms because, as phytoplankton pigments, they absorb the blue part of the visible spectrum (Bricaud et al., 1981). CDOM is known to be a dominant optical component in most of the HBS, making this region optically complex (Granskog et al., 2007; Mundy et al., 2010; Guéguen et al., 2011; Xi et al., 2013; Burt et al., 2016; Heikkila et al., 2016). The GSM algorithm can better deal with the presence of CDOM compared to empirical algorithms and was selected to minimize the impact of other optical constituents on [chla] retrievals (Ben Mustapha et al., 2012). The nearshore region where river inputs contribute more to the water reflectance variability than phytoplankton was avoided by masking shallow water pixels (i.e., depth < 50 m). Granskog et al. (2009) found that river runoff and CDOM are constrained within the coastal domain (100–150 km from the shore), where they are transported along the coast counterclockwise around the HBS. Xi et al. (2013) reported that phytoplankton was the main optically significant component driving the seasonal variability of light absorption in the HBS, while CDOM remained relatively stable over the annual cycle. These results provide confidence in the present [chla] time-series analyses. However, we cannot exclude an influence of riverine-derived CDOM on [chla], in particular along the eastern coast of HB, where most river runoff is transported before its exit through the Hudson Strait (Saucier et al., 2004). A high CDOM background in the east of HB (Xi et al., 2013) explains the relatively high [chla] observed in the ice edge regardless of the sea-ice break-up in the eastern part of HB (NE and SE in Figures 11). An evaluation of the GSM algorithm based on *in situ* measurements in the HBS beyond the scope of this study but would be necessary to evaluate the potential bias in [chla] and consequently the choice of 0.5 mg m⁻³ as a threshold for detecting pelagic blooms.

Here we adopted a fixed [*chla*]-based threshold of 0.5 mg m⁻³ to detect the ice-edge bloom (Perrette et al., 2011) instead of dynamic methods like, for example, rate of change method, cumulative biomass-based thresholds (Brody et al., 2013), or model fitting (Ardyna et al., 2014; Marchese et al.,

2017). Because the ice-edge bloom can reach its peak just after the sea-ice retreat (Figure 2 and type V in Figure 10), the pelagic cycle often began with the highest annual values, without a well-defined Gaussian-like seasonal evolution in [*chla*]. Therefore, we could not apply the Gaussian fitting method to the HBS.

1.4.2 Winter air temperatures and ice retreat impact on ice-edge blooms

What role do winter air temperatures (T'_{air}) and sea-ice retreat (t_R) play in the magnitude and variability of ice-edge blooms? Can these relationships be affected by climate change? We used 21 years of SIC and [*chla*] to address these questions.

As illustrated in Figures 12 and 13, t_R and T'_{air} can have a very strong but local impact on the balance between under-ice and pelagic production throughout the MIZ (Palmer et al., 2014). This impact can be explained by the interactions of various oceanographic processes in the MIZ, such as tidal resonance (Webb, 2014), water mass exchange throughout the Hudson Strait (Sutherland et al., 2011), polynya dynamics (Landy et al., 2017), and freshwater inputs (St-Laurent et al., 2011). Notably, the relatively strong negative correlation between [*chla*] and t_R in the northern part of the HBS illustrated in Figure 12 is very similar to the Arctic water intrusion pattern in the system depicted by Wang et al. (1994), Saucier et al. (2004), and Piecuch and Ponte (2015).

In winter, primary production in the HBS is limited by photosynthetic available radiation, as confirmed by the absence of dinoflagellate cysts (a proxy for under-ice production) reported by Heikkila et al. (2016) in two coastal sites in both west and east HB. On the other hand, physical processes controlling the cryosphere, i.e., brine production and vertical mixing, are essential to bringing deep nutrient-rich waters to the upper ocean. These processes can be critical in the HBS because it is a relatively shallow sea (Stewart and Lockhart, 2005; Granskog et al., 2011). Also, compared to other polar domains of the Arctic, the sea ice is thinner, which may result in less brine rejection and relatively weak vertical mixing and nutrient replenishment during winter.

Winter air temperature is a good proxy for sea-ice production and the overall winter severity. Hochheim and Barber (2014) reported that a positive anomaly of only 1°C decreased the sea-ice coverage by 14% and advanced the break-up by one week. However, this generalization can be ambiguous concerning its effect on phytoplankton productivity because winter air temperature can impact many different key processes. Those include the nutrient replenishment due to sea-ice or brine production (Landy et al., 2017) or winter convection in the open waters (Stewart and Lockhart, 2005; Granskog et al., 2011; St-Laurent et al., 2011), the PAR attenuation by sea ice and snow cover (Horvat et al., 2017), the timing and length of the open water season (Ardyna et al., 2014; Hochheim and Barber, 2014), the riverine input (Déry and Wood, 2004; Déry et al., 2005). The latter controls the amount of CDOM and nutrients (Granskog et al., 2007), which have a contrasting impact on phytoplankton production.

The complexity of air, sea and ice interactions at high latitude makes the interpretation of the relationship between ice-edge [*chla*] and winter air temperature difficult (Figure 13A). Indeed, various feedbacks are in play between polynya dynamics, air temperature, vertical mixing, brine production, and phytoplankton blooms (Chaudhuri et al., 2014). For example, Saucier et al. (2004) reported that the NW polynya dynamic causes significant sensible heat loss at a rate of 100 W m⁻² in winter. The presence of a polynya during the cold season tends to intensify the sea-to-air heat flux, which potentially warms the atmosphere locally (Saucier et al., 2004). Similarly, the Weddell Sea polynya, Antarctica, can effectively heat the atmosphere at the regional scale (Campbell et al., 2019). However, the polynya may only affect local air temperatures, which may be difficult to assess given the coarse resolution of the NCEP/NCAR reanalysis data (Winsor and Björk, 2000).

The strong negative relationship between ice-edge [*chla*] and winter air temperature in the HB polynyas (i.e., NW and Belcher Island) reflects the intensification of polynya dynamics that lead to efficient nutrient replenishment in the euphotic zone (Figure 13). Atmospheric cooling of the ocean also influences the amount of ice and brine production, which further increases vertical mixing and weakens the under-ice stratification (Stewart and Lockhart, 2005; Granskog et al., 2011). Consequently, the nutrient stock available at bloom onset may be greater (Nguyen et al., 2009; Barthélemy et al., 2015). Indeed, thick sea ice stocks a large quantity of fresh water, which provides low-density water and

stabilizes the upper ocean upon sea-ice melting (Galbraith and Larouche, 2011).

In summary, an inheritance effect of winter sea-ice production could indirectly impact the level of phytoplankton primary production that will occur in the spring–summer seasons. Therefore, we conclude that cooler air temperatures intensify the wind-driven polynyas of the HB due to steady atmospheric cooling of the ocean, which supports ice (and brine) production, vertical mixing, and deep nutrient replenishment during winter. As a result, as soon as the stratification is reestablished and light becomes available in spring, phytoplankton can reach higher biomass.

1.4.3 Ice-edge phytoplankon blooms response to global and local forcing

A warmer climate has already been established in the HBS due to warmer air and less frequent cold and dry polar air masses (Leung and Gough, 2016). Based on air temperature analysis between 1948 and 2018 (Figure 3), positive anomalies have been predominant in most seasons since 1998. Impacts on the cryosphere dynamics have been observed: thinner sea-ice cover, early sea-ice retreat, late ice recovery, and longer open water season (Hochheim and Barber, 2014; Kowal et al., 2017). These changes in the sea-ice dynamics may have driven significant changes in the marine ecosystems, with potential cascading impacts on all trophic levels in the HBS (Hoover et al., 2013; Keller et al., 2014; Andrews et al., 2017).

Mechanisms controlling the spring–summer and fall blooms are distinct. Our results suggest that pelagic production may have increased in the HBS since the open water season has increased in duration and double blooms are more frequent (Figure 3). Sea-ice dynamics and incoming PAR in the upper ocean layer control the spring–summer bloom. Kahru et al. (2011) reported a pronounced trend toward earlier phytoplankton blooms in about 11% of the North Polar seas area between 1997 and 2009, including the northern part of the HBS. The latter can be related to earlier ice break-up trends (Kowal et al., 2017). In contrast, the lengthening of the open water season and the increase in nutrient pumping by wind-driven turbulence (Ardyna et al., 2011) and the inversion of heat fluxes drive the fall blooms. Notwithstanding, the increase in annual phytoplankton primary production is correlated with

the length of the open water season (Arrigo and van Dijken, 2015).

The HBS is located in a transition between sub-polar and polar domains. However, its complex topography and its semi-confined configuration by the continental shelf result in relative isolation with regard to global ice exchange and ocean circulation (Sutherland et al., 2011). Its primary connection to the global ocean takes place through Hudson Strait. Therefore, HBS trends and dynamics are especially impacted by local atmospheric processes (Hochheim and Barber, 2010, 2014; Hochheim et al., 2011) and by climatic teleconnections (Déry and Wood, 2004). Therefore, climatic forcing and global scale teleconnections (e.g. NAO/AO) can impact both sea-ice retreat and recovery in HBS (Hochheim and Barber, 2010; Hochheim et al., 2011).

Climate indices express global or hemispherical teleconnections (Carmack et al., 2006). Part of the atmospheric and oceanic variability of the HBS has been correlated with both AO (Déry and Wood, 2004; Hochheim and Barber, 2010; Hochheim et al., 2011) and NAO indices (Qian et al., 2008). NAO is recognized as a significant descriptor of the winter-to-winter variability over northeastern America (Wallance, 2007; Qian et al., 2008). It accounts for the direct North-South dipole patterns between the North Atlantic and the Arctic oceans. Meanwhile, AO (annular paradigm) also includes the Pacific sector processes, such as the Aleutian High (Wang et al., 2005; Wallance, 2007). Nevertheless, there is an overlap between NAO and AO patterns in the Atlantic sector. Therefore, NAO and AO are highly correlated and related to similar phenomena (Ambaum et al., 2001; Wallance, 2007), especially during winter (Rogers and McHugh, 2002). Both NAO and AO indices are associated with the intensity of the north polar vortex (Wallance, 2007), with a positive phase reflecting the strengthening of the winter-time polar vortex and westerly intensification between 50°N and 70°N (Moritz et al., 2002). For example, Hurrell et al. (2001) reported that positive NAO strongly affects the Atlantic Ocean, causing substantial changes in surface wind patterns with stronger westerly winds encircling the North Pole. In contrast, Arctic warming and a wavier polar jet resulting in an intensification of southward advection of polar air masses in North America were observed during negative NAO/AO phases (Baldwin and Dunkerton, 1999; Ding et al., 2014; Francis and Vavrus, 2015; Leung and Gough, 2016; Meleshko et al., 2016). We found that the ice-edge zone [chla] and NAO/AO indices are relatively well correlated, especially in the NW polynya (Figure 14). The extreme event of the highest (lowest) NAO/AO in 2015 (2010) corresponded to a strong (weak) ice-edge bloom in NW HB polynya (Figure 14). These results suggest that global atmospheric circulation patterns, depicted by the NAO/AO, strongly influence phytoplankton blooms in the NW HB polynya.

Figure 15 illustrates schematically how the strength of westerlies affects the NW HB polynya processes controlling ice-edge blooms during winter and spring-to-summer transition. As discussed by Saucier et al. (2004) and Landy et al. (2017), the NW polynya is maintained by strong westerly winds opening up areas of water along the northwestern coast by coastal divergence and enhancing ice production. In winter, the NW polynya acts as an "ice factory", where ice growth is favored by thermodynamic processes (ocean cooling) and then the ice is exported by winds (Landy et al., 2017). Brine rejection due to sea-ice production plays a fundamental role in vertical stratification and deep convection (Prinsenberg, 1988) and results in the nutrient replenishment of the euphotic zone through vertical mixing. Meanwhile, we found that early sea-ice retreat results in more intense ice-edge blooms (NW in Figures 12 and 11). This finding suggests that nutrient stocks set up in winter and the timing of polynya expansion in the spring-to-summer transition are the main drivers of the balance between pelagic and under-ice production throughout the MIZ. Notably, NAO/AO events can control the feedback between westerlies, the NW HB polynya dynamic, and the ice-edge blooms, because initially, brine rejection forced by ice production and export sets up the pre-conditions of nutrients stocks in the euphotic zone. After that, early polynya expansion due to intensification of westerlies results in ice-edge bloom intensification during the spring-to-summer transition (Figure 11-NW).

Déry and Wood (2004) highlighted that AO could explain 70%–90% of the variance in HBS river discharge anomalies. According to Déry and Wood (2004), the origin of dominant air masses over the HBS controls this pattern. During the positive (negative) AO index north easterly (north-westerly) winds that advect relatively warm (cool), moist (dry) air from the Labrador Sea to the HBS increases the river discharge (Déry and Wood, 2004; Hochheim and Barber, 2014). We found weak correlations between AO and ice-edge zone [*chla*] in the southern HB, where riverine input into the HBS is more important (St-Laurent et al., 2011). We also found no significant correlations between the maximum



Figure 15: Conceptual model of teleconnections of NAO/AO to phytoplankton dynamics in the NW HB Polynya.

[*chla*] in the ice-edge zone and riverine discharge, even at local scales (results not shown), suggesting a marginal role of rivers in the primary productivity of the HBS.

1.4.4 Potential role of under-ice blooms

Recent observations have suggested that under-ice phytoplankton blooms can draw down the surface nutrient pool before the open water season starts (Mundy et al., 2009; Arrigo et al., 2014). Then, the sub-surface chlorophyll-*a* maximum sinks near the nitracline before or just after the ice retreat, allowing the phytoplankton to achieve a balance between PAR and nutrients, as illustrated in Figure 15. As a result, the ocean color satellites detect a low [*chla*] in the ice-edge zone (Horvat et al., 2017) (blue and red curves in Figure 2). The frequency occurrence map depicting this situation (Figure 10A and B) suggests that a vast portion of the central-western part of the HBS is experiencing under-ice blooms. However, this scenario may also reflect the oligotrophic nature of the system.

Only in situ observations or model simulations can help to resolve the above situation (under-ice bloom versus oligotrophy). Most field observations before the BaySys project were based on ice camps, which focused more on ice algae or open waters later in summer. Michel et al. (1993) and Michel et al. (1988) reported a maximum of vertically integrated ice-algal [*chla*] of 23.6 mg m⁻² in April, while Monti et al. (1996) reported algal concentrations at the ice/water interface as high as 100.6 mg m⁻² between April and May. High ice-algal concentrations were followed by an increase of water column [*chla*] reaching moderate concentrations (i.e., 2 and 4 mg m⁻³) in May during the ice melt (Runge et al., 1991; Michel et al., 1993), suggesting initiation of the bloom under ice (type V in Figure 2). Model simulations also suggest that nutrient draw-down in the surface waters begins in May, but the maximum diatom biomass is reached after the ice retreat in June or July (Sibert et al., 2011). Recently, however, Tremblay et al. (2019) concluded that, except in river plumes and some upwelling spots (e.g., Foxe Peninsula, Belcher Islands, and Hudson Strait), the HBS should be considered an oligotrophic system. More observations in the MIZ during the spring-to-summer transition are still needed.

1.5 Conclusions and perspectives

We showed that phytoplankton phenology in the HBS is subject to substantial spatio-temporal variability and closely linked to large-scale atmospheric forcings. In recent years, the phenology has been characterized by two peaks in [*chla*], one after the sea-ice break-up in the marginal ice zone (May– June) and one in the fall. Here we focused our effort on the ice-edge bloom. In the western part of the HB, the magnitude of the ice-edge bloom depends on the timing of ice break-up, with more intense blooms occurring when the ice retreats early. The northwestern polynya stands out as a significant feature in the HBS in terms of primary production, and its variability is highly coupled to the northern hemisphere climate variability (NAO and AO indices). At the bay scale, we found no direct evidence that river discharge, which can supply the surface waters with nutrients and impact the vertical stratification influenced the MIZ.

The relative contributions of the under-ice, MIZ, and fall blooms to total annual primary production remain to be established. Regionally tuned satellite-derived primary production models (Ardyna et al., 2013; Bélanger et al., 2013; Lee et al., 2015) could be used at least to assess the contribution of the MIZ and fall blooms. The combination of *in situ* observations, satellite monitoring (e.g., ocean color in synergy with sea-ice thermodynamic stages and/or albedo), and 3D ocean models coupled with biological models will be most promising to predict how all components of the HBS marine ecosystem will be impacted by climate change, including primary productivity.

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Additional information: http://umanitoba.ca/faculties/environment/departments/ceos/ research/BaySys.html. 1.7 Supplementary material



Figure 16: Ice-edge blooms between 1998 and 2018 in the Hudson Bay System. Ice-edge blooms were detected by the maximum [*chla*] during the 24 days after sea-ice retreat (first day of continuous SIC < 10%) (Perrette et al., 2011) between 1998 and 2018. Days of the year and their respective calendar date: 120 (Apr 30), 135 (May 15), 150 (May 30), 165 (Jun 14), 180 (Jun 29), 195 (Jul 14), 210 (Jul 29), 225 (Aug 13), and 240 (Aug 28).



Figure 17: Sea-ice retreat between 1998 and 2018 in the Hudson Bay System. Sea-ice retreat is detected when SIC (Comiso, 2000) reaches the threshold of 10% (Perrette et al., 2011).



Figure 18: Maps of four phytoplankton phenological categories throughout marginal ice zone between 1998 and 2018. Annual classification maps of MIZ phenology based on the evolution of [*chla*] following sea-ice retreat (t_R). The four categories are oligotrophic state or old under-ice bloom (blue); probable (recent) under-ice bloom (red); a mesotrophic system where efficient nutrient replenishment is in place (green), bloom triggered in ice-free waters (orange); and bloom triggered under ice (cyan).



Figure 19: Winter air temperature anomalies in the Hudson Bay System. Winter anomalies of surface air temperature (T'_{air}) calculated using air temperatures from National Centers for Environmental Prediction/Atmospheric Research (NCEP/NCAR) Reanalysis Project as the difference between each winter (January, February and March) average and its corresponding climatology and normalized by the standard deviation, using data from the 1948 to 2018 period.



Atmospheric forcing and photo-acclimation of phytoplankton fall blooms in the Hudson Bay

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Abstract

Pulses of ocean primary productivity during the fall season are frequent in the mid-latitudes when ocean cooling and wind-driven turbulence erode the surface stratification and allow the injection of nutrients into the euphotic zone. This phenomenon is often referred to as a phytoplankton fall bloom and can play an essential role in the survival of marine species during winter. In Hudson Bay, we found that pelagic fall blooms are triggered when the convective mixing, forced mainly by atmospheric cooling and to a lesser extent to wind-driven turbulence, expands the mixed layer, ventilates the pycnocline, and likely erodes the nitracline. Ocean color observations were used to assess the seasonal variability of phytoplankton photo-acclimation state from the ratio of phytoplankton carbon (C_{phy}) to chlorophyll-*a* concentration ([*chla*]). C_{phy} was estimated using the satellite-derived particulate backscattering coefficient (b_{bp}) after subtraction of the non-algal backscattering background. We found a systematic increase in C_{phy} and C_{phy} :[*chla*] from mid-summer to fall season indicating that fall blooms are potentially productive in terms of organic carbon fixation.

Résumé

Forçage atmosphérique et photo-acclimatation des efflorescences automnales de phytoplancton dans la baie d'Hudson

Les pics de productivité primaire océanique pendant l'automne sont fréquents aux latitudes moyennes lorsque le refroidissement de l'océan et la turbulence due au vent érodent la stratification de surface et permettent un apport de nutriments dans la zone euphotique. Ce phénomène est souvent appelé "floraison automnale de phytoplancton" et peut jouer un rôle essentiel dans la survie des espèces marines pendant l'hiver. Nous avons étudié les interactions entre la dynamique du phytoplancton (abondance et photo-acclimatation), les processus océanographiques et le forçage atmosphérique dans la baie d'Hudson en automne. En parallèle, les sorties d'un modèle dynamique glace-océan, la réanalyse atmosphérique et les observations satellitaires de la couleur de l'océan ont été analysés. Nous avons découvert que les efflorescences pélagiques d'automne dans la baie d'Hudson sont déclenchées lorsque le mélange convectif, forcé par le refroidissement atmosphérique, et la turbulence due au vent étendent la couche mélangée océanique, ventilent la pycnocline, et finalement érodent probablement la nitracline. L'efflorescence d'automne se termine lorsque la mer commence à geler à la fin de l'automne. Le rôle de la dynamique de l'eau douce de surface (provenant à la fois de la fonte des glaces et du ruissellement des rivières) pour le maintien de la stratification de la colonne d'eau rend la réponse du phytoplancton au forçage atmosphérique plus complexe que dans l'océan ouvert. Les observations satellitaires de la couleur de l'océan ont ensuite été appliquées pour évaluer la variabilité spatio-temporelle en termes de rapport carbone-chlorophylle (C_{phy} :[chla]), un indicateur de l'état de photo-acclimatation du phytoplancton. Pour cela, la photo-physiologie a été contrainte par des observations in situ acquises à bord du brise-glace canadien CCGS Amundsen dans la baie de Baffin (GreenEdge Project, 2016) et la baie d'Hudson (BaySys Project, 2018) pendant la transition printempsété. Ces observations inclus le coefficient de rétrodiffusion à 555 nm (b_{bp} (555)), et la concentration en chlorophylle-a ([chla]), ainsi que le rayonnement actif photosynthétique (PAR). Bien que les efflorescences automnales puissent en partie résulter du transport de cellules phytoplanctoniques riches en pigments produits dans le maximum de chlorophylle de subsurface, une augmentation systématique de la C_{phy} du ratio C_{phy}:[chla] dérivés des données satellitaires indiquent que les efflorescences automnales sont potentiellement productives avec une structure de taille du phytoplancton et un état de photo-acclimatation similaires à ceux qui fleurissent en bordure de glace plus tôt en été.

2.1 Introduction

In polar seas, ongoing climatic changes have subjected phytoplankton dynamics to a new configuration of physical forcings that control incoming light, nutrient availability, and water column structure, with impacts on all marine trophic levels (Leu et al., 2011; Wassmann, 2011; Ardyna et al., 2014). Nowadays, the sea-ice retreat is occurring earlier and recovering later (Markus et al., 2009; Stroeve et al., 2011, 2014), lengthening the open water season (Arrigo and van Dijken, 2015). Consequently, annual phytoplankton production rises because more light is available in the upper ocean layer (Bélanger et al., 2013; Arrigo and van Dijken, 2015). In turn, phytoplankton phenology, i.e., the seasonal succession of phytoplankton processes, impacts the carbon pump, pelagic ecosystems, the benthic realm, and valuable fish stocks (Platt et al., 2003; Friedland et al., 2008; Barber et al., 2015). The synchronization between phytoplankton bloom timing and organisms in early life and sensitive developmental stages (eggs or larval) is essential for species survival and recruitment (match/mismatch hypothesis: Cushing, 1990). Satellite observations have suggested that fall bloom occurrence has risen in high northern latitudes during the last decades (Ardyna et al., 2014). In low productive ecosystems like Hudson Bay (Tremblay et al., 2019), the world's most extensive inland sea, an increase of phytoplankton abundance in the fall season can supply extra energy stock for polar species, increasing their overwintering potential.

Field and satellite observations in the middle- and high-northern latitudes have confirmed the importance of fall blooms. For instance, Rho and Whitledge (2007) showed that sediment traps recorded a high flux of organic carbon during the summer-to-fall transition in the Bering Sea. Sigler et al. (2014) reported that large crustacean zooplankton taxa respond to interannual variability in the time interval between spring and fall blooms in the Eastern Bering Sea. In general, short-term physical events, like storms, are assumed to affect the dynamics of fall blooms, as observed over the Nova Scotia Shelf (Greenan et al., 2004) and the sub-polar Japan/East Sea (Kim et al., 2007). Strength of wind-fetch and sea surface freezing delays have intensified phytoplankton blooms triggered by the transport of nutrients into the euphotic zone, as reported by Rho and Whitledge (2007) in the Bering Sea shelf, Fujiwara et al. (2018) in the Chukchi Sea, and Ardyna et al. (2014) and Castro de la Guardia et al. (2019) in even the Arctic Ocean. Although recent studies have sought to understand the dynamics of phytoplankton fall blooms, information is still lacking about processes that trigger and maintain the effective productivity of fall blooms in the north polar seas.

The Hudson Bay System (HBS) drainage basin alone equates to 18% of the total freshwater input of the Arctic Ocean (Déry et al., 2005; Granskog et al., 2011) while melting sea ice supplies twice this freshwater volume during a short melting period throughout the spring-to-summer transition (Mysak et al., 1996). The stratification resulting from this large amount of freshwater produces persistent oligotrophy in the summer (Harvey et al., 1997; Ferland et al., 2011; Lapoussiere et al., 2013; Xi et al., 2013; Tremblay et al., 2019). Ferland et al. (2011) reported low primary production rates in late summer (August and early September) dominated by small-sized phytoplankton adapted to oligotrophic and stratified conditions. In contrast, Xi et al. (2013) measured higher chlorophyll-*a* concentration ([*chla*]) and phytoplankton absorption coefficient in the fall (end of September to early October) compared to summer (July), suggesting an increase in primary productivity later during the open water season in the HBS. Recently, a systematic analysis of satellite-derived [*chla*] suggested that phytoplankton biomass systematically increases during the summer-to-fall transition (Barbedo et al., 2020), but the mechanisms explaining this phenomenon were not examined in detail.

Atmospheric forcing (convection- and wind-driven turbulence) triggers vertical mixing during the fall season, promoting the seeding of the upper-water layer with phytoplankton communities that developed at the subsurface chlorophyll maximum (SCM) during the summer and pumping nutrients in the euphotic zone. SCM phytoplankton is adapted to low light levels (photo-acclimation) with large cells having high intracellular *chla* content (Cullen, 2015; Halsey and Jones, 2015; Marañón, 2015; Westberry et al., 2008; Behrenfeld et al., 2002). Phytoplankton communities with high intracellular chlorophyll-*a* content in an environment of low photosynthetically active radiation (PAR) and excessive turbulence can be saturated quickly in terms of net carbon fixation (low maximum rate of photosynthesis, P_{max} ; Huot et al., 2013) and can result in a satellite overestimation of primary production (Sathyendranath et al., 2020). To gain insights into the physiological state of fall bloom, we investigated how satellite-based approaches can help to address this question.
Phytoplankton community size structure and photo-physiological aspects (i.e., photo-acclimation and photoadaptation) are key aspects for a better understanding of pelagic ecosystems in terms of productivity, food web complexity, and the biological pump (Antoine et al., 2011; Brewin et al., 2014; Sathyendranath et al., 2020). Behrenfeld et al. (2005) used a satellite-derived particle backscattering coefficient (b_{bp}) as a proxy of phytoplankton carbon content (C_{phy}), allowing an estimation of the ratio of phytoplankton carbon to chlorophyll-*a* (C_{phy} :[*chla*]), a proxy of phytoplankton photoacclimation (Behrenfeld et al., 2002). Devred et al. (2011) derived phytoplankton size classes using chlorophyll-specific spectral absorption coefficient in the Canadian east coast and northwest Atlantic. Brewin et al. (2012) examined the chlorophyll-specific backscattering coefficient in relation with small (< 20 μ m) and large (>20 μ m) phytoplankton size classes. In contrast, in Arctic waters where phytoplankton is not the dominant optical component, spectral variations in remote sensing reflectance arise mainly from differences in the bio-optical environment in which specific communities are found (Reynolds and Stramski, 2019). To understand the phytoplankton photoacclimation state and its seasonal evolution, satellite-derived C_{phy} :[*chla*] was estimated with a method that considered the non-algal contribution to b_{bp} (Bellacicco et al., 2019).

Our study focuses on the physical mechanisms responsible for the fall bloom phenomenon as well as potential photo-physiological adaptations of phytoplankton to late summer/fall conditions. Specifically, the objectives were to i) to understand the role of atmospheric forcings and water column structure on fall bloom dynamics, ii) to assess the physiological state of phytoplankton communities blooming in the fall season using satellite-derived optical proxies.

2.2 Materials and methods

To investigate the role of atmospheric and oceanographic processes in triggering and maintaining phytoplankton fall blooms, we employed in synergy the outputs of an ice-ocean dynamic model, climatic reanalysis, the satellite ocean color constellation, and *in situ* bio-optic and radiometry. We discuss the seasonality of atmospheric and oceanographic interplays, water column evolution, and their effects on phytoplankton dynamics in Hudson Bay. In Southern Hudson Bay, inter-annual and seasonal variability of freshwater input results in remarkable shifts in stratification drivers, i.e., salinity and temperature vertical gradients. To better understand the counterpart of atmospheric forcing on the water column and phytoplankton dynamics, we focused on South Hudson Bay, where more pronounced ice-edge and fall blooms were observed ([*chla*] > 2 mg m⁻³), and where riverine input can contribute to the upper-layer stratification during the melting season.

To enlighten phytoplankton dynamics in the fall season, we compared two decades (1998–2018) of ocean color satellite observations with bio-optical conditions collected in situ during a recent Canadian expedition throughout marginal ice zones during the spring-to-summer transition in Hudson Bay (2018), when phytoplankton is expected to bloom. To fill in the lack of information in fall, processes observed and in situ evaluation of ocean color algorithms in spring can support satellite characterizations during summer and fall. We analyzed in detail both satellite-derived [*chla*] and b_{bp} to explore the potential role of photo-acclimation on phytoplankton and its productivity during the fall season.

2.2.1 Ice-ocean model and heat-flux calculations

Vertical profiles of potential temperature and salinity were modeled using version 3.4 of the Nucleus for European Models of the Ocean (NEMO) general circulation model. NEMO is a coupled ice-ocean dynamic model. The experiments used the Arctic and Northern Hemisphere Atlantic configuration run at 1/4° resolution (ANHA4) and 5-day averaged output. The vertical resolution was 50 unevenly spaced levels, with the majority of the resolution in the upper column to capture the mixed layer and thermocline processes. The model inputs for atmospheric fields are taken from the Canadian Meteorological Centre's Global Deterministic Prediction System Re-Forecasts (CGRF; Smith et al., 2014), and the coupled ocean-ice Coordinated Ocean Research Experiments (CORE) bulk formula was used to compute fluxes between the atmosphere and the ocean and to assimilate wind stress into the momentum equations (Large and Yeager, 2004, 2009). River runoff within HBS was provided by calibrated output from the HYdrological Predictions for the Environment (HYPE; Lindström et al., 2010; Gelfan et al., 2017; Andersson et al., 2015). This runoff dataset has not been integrated with observations but included the improvements to the model, such as a better representation of La Grande Rivière

discharge and Nelson River regulation. Outside HBS, the runoff was compiled by Dai and Trenberth (2002), with the addition of Greenland melt by Bamber et al. (2012). Further details on the model setup and evaluation can be found in Ridenour et al. (2019).

Heat fluxes (in W m⁻²), i.e., the difference in short- and long-wave radiation, latent and sensible heat between the atmosphere and the ocean, were computed using the bulk formulas developed by Large and Yeager (2004, 2009). The calculations considered the near-surface atmospheric state (wind, potential temperature, specific humidity, and density), and the ocean state (ocean surface current and temperature). Briefly, sea-surface currents and sea-surface temperature (SST) were calculated from NEMO-ANHA4 model simulations. Atmospheric potential temperature, humidity, wind (10 m), precipitation, short and long-wave radiation were obtained from CGRF, which is assumed suitable to parameterize physical processes of polar seas and has a finer spatial-temporal scale (i.e., 33 km daily) than other current available global reanalysis (Smith et al., 2014).

2.2.2 Satellite ocean color

Values for [*chla*] (in mg m⁻³), particle backscattering coefficient at 443 nm ($b_{bp}(443)$), in m⁻¹), and the diffuse attenuation coefficient at 490 nm ($k_d(490)$, in m⁻¹) were downloaded from the Globcolour Project (http://www.globcolour.info/). Globcolour Level-3 [*chla*] (ESA, 2020) and $b_{bp}(443)$ were estimated using the semi-analytical algorithm of Garver-Siegel-Maritorenna (GSM: Garver and Siegel, 1997; Maritorena et al., 2002). We performed an *in situ* evaluation of the GSM algorithm to ensure the robustness of our choice of for [*chla*] (see Supplementary material). The value for $b_{bp}(555)$ was calculated from $b_{bp}(443)$ using a power law function with a spectral dependency of -1.0337 (Maritorena et al., 2002). The value for $k_d(490)$ was estimated using the quasi-analytical algorithm of Lee et al. (2005). The Globcolour Level-3 (i.e., binned and mapped) merged products have temporal and spatial resolutions of 1 day and 4.63 km, respectively, and cover the period of 1998 to 2018. The merged products improve the spatial-temporal coverage, diminishing gaps due to cloud cover and sea-ice (Maritorena et al., 2010). The binning methodology combines radiometry from ocean color if the sensors are available, which includes: Sea Wide Field-of-view Sensor (SeaWiFS: 1998–2010), Moder-

ate Resolution Imaging Spectroradiometer (MODIS: 2002–2018) aboard the Aqua satellite, Medium-Resolution Imaging Spectrometer (MERIS: 2002–2011), Visible Infrared Imaging Radiometer Suite (VIIRS: 2012–2018), and Ocean and Land Colour Instrument (OLCI:2016–present). Coastal areas with depths shallower than 50 m were removed from analysis to avoid turbidity and bottom effect. Satellite data were restricted to complex water non-scatter dominated and case water-1 (Lee and Hu, 2006) to avoid the influence of non-algal particle backscattering on the estimation of C_{phy} .

2.2.3 Time-series analysis

We evaluated the effect of atmospheric forcing on the water column structure and phytoplankton dynamics in spatial bin areas of 100 × 100 ocean color pixels (approximately 4 km) centered on 84°W 57°N in southern Hudson Bay. Time series of heat flux, wind speed, light level, and [*chla*] were combined with water column profiles. The first optical depth (z_{oC} , in m), the water column layer inside the ocean color satellites range, and the euphotic zone depth (z_{eu} , in m), defined as the depth at which PAR reduces to 1% of the incoming surface value, were estimated using k_d (490), i.e., $z_{eu} = -4.5/k_d$ (490) and $z_{OC} = -1/k_d$ (490), respectively. For that, NEMO simulations were used to produce a high resolution, basin-scale hindcast of ocean vertical structure of potential temperature, salinity, stratification, and mixed layer depth. The mixed layer thickness was calculated based on seawater density (ρ), i.e., the depth of a threshold value of density ($\Delta \rho = 0.01 \ kg \ m^{-3}$) from a near-surface value (de Boyer Montégut et al., 2004). Fluid stratification was quantified using the buoyancy frequency (N^2), known as the Brunt-Vaissala frequency, i.e., the frequency required to break up the stratification (Equation 2.1):

$$N^2 = -\frac{g}{\rho} \frac{\partial p}{\partial z},\tag{2.1}$$

where g is the gravity, ρ is the density, p is the pressure, and z is depth. The heat-flux inversion, i.e., the day of the year when the atmosphere began to cool the ocean, was detected by the first day on which the heat-flux sign was negative between June and November.

To indicate the ice-edge zone, the sea-ice retreat, t_R , was defined as the day at which sea-ice concentration (SIC) is below 10% for at least 24 days (Barbedo et al., 2020). Sea-ice concentration. SIC was

obtained from the National Snow and Ice Data Center (NSIDC), which is based on daily multichannel passive microwave radiometry sensors clustered using the Bootstrap algorithm at 25-km resolution (Comiso, 2000; Comiso et al., 1997).

2.2.4 In situ bio-optics

In situ bio-optical measurements were performed aboard the Canadian Icebreaker NCGC *Amundsen* during the BaySys expedition in Hudson Bay in June 2018 (Ahmed et al., 2021). The sampling was distributed over recently opened waters in western Hudson Bay in the marginal ice zone (MIZ), i.e., the area along the edge of the ice pack that is affected by open ocean processes (Barber et al., 2015), in leads surrounded by landfast ice loading/releasing sediment in the south, and along a transect in the Nelson River plume (Figure 20). The field measurements included in situ particle backscattering, pigment analysis, and in-water radiometry, which are used to support our interpretation of the satellite-derived phytoplankton photoacclimation state described in the next section.

2.2.4.1 Backscattering coefficient

The total spectral backscattering coefficient, $b_b(\lambda)$, is the amount of light scattered by water molecules or suspended particles into the hemisphere from which light has originated. Total $b_b(\lambda)$ can be further divided in terms of additive components of pure water (b_{bw}) and particles (b_{bp}) . The latter is a good proxy of particulate organic carbon (POC) in the open ocean (Stramski et al., 1999). Total $b_b(\lambda)$ was calculated from the volume scattering function (β , in sr⁻¹) measured at a fixed scattering angle (θ_b°) in the backward direction relative to the laser beam using an ECO BB9 (Sea-Bird Scientific). The manufacturer calibrated the instrument before the field campaign. The BB9 operated at nine wavelengths (412, 440, 488, 510, 532, 595, 660, 675, and 715 nm) with $\beta(\theta_b^\circ = 117^\circ)$.

The measurements were performed at 14 stations in Hudson Bay. The data were processed using an open source R package (https://github.com/belasi01/Riops; see also Bélanger et al., 2017) following the manufacturer's protocol (Twardowski et al., 2007). Briefly, the spectral backscattering



Figure 20: Bio-optical stations of the BaySys Expedition, 2018. Distinct light environments were sampled during the spring-to-summer transition in Hudson Bay. Represented are three light attenuation levels in the marginal ice zone: high (cyan triangles), moderate (blue triangles), and low (black triangles); along with Nelson River sediment plume (red squares, inset); phytoplankton bloom under influence of Nelson River plume (green squares, inset); and landfast sea-ice load sediment in southern HB coastal waters (pink circles, Harasyn et al., 2019). Color maps were obtained from the Etopo continental topography (grayscale in meters above sea level; Amante and Eakins, 2009), chlorophyll-*a* concentration ([*chla*], color scale, in mg m^{-3}) for June 2018, obtained from the Globcolour Project.

coefficient was obtained from the measured $\beta(\theta_b^{\circ}, \lambda)$ through integration over the backward hemisphere based on a phase function according to the Mie theory (wavelength-selective scattering) using the relation (Equation 2.2):

$$b_{bp}(\lambda) = 2\pi \chi_p \left| \beta(\theta_b^\circ, \lambda) - \beta_{sw}(\theta_b^\circ, \lambda) \right|$$
(2.2)

where χ_p , a spectrally constant value of 1.1 (Boss and Pegau, 2001), represents the relationship between $\beta(\theta_b^\circ)$ and b_{bp} . The spectral contribution of pure seawater to scattering (β_{sw}) at θ_b° was computed using temperature and salinity at the same time and depth with a CTD sensor (Zhang et al., 2009). The dependence on absorption, *a*, caused by attenuation along with the sensor and light source path was corrected based on simultaneous measurements of total absorption by an absorption and attenuation spectral sensor (ac-s: Sea-Bird Scientific) according to recommendations of Doxaran et al. (2016). Profiles of $b_{bp}(\lambda, z)$ were binned at 0.1-m depth intervals after applying a local polynomial regression smoothing function (Cleveland et al., 1992); $b_{bp}(555)$ was calculated at each depth by fitting a power law function to $b_{bp}(\lambda, z)$. Finally, b_{bp} at 555 nm was selected for further analysis because pigment absorption exhibits weak contribution in this spectral region, as reported by Reynolds et al. (2016).

2.2.4.2 Pigment analysis

Chlorophyll-*a* concentration from discrete samples were measured by the high-performance liquid chromatography (HPLC) technique ([*chla*]_{*HPLC*}, in mg m⁻³). Seawater discrete samples of 1–3 L were collected using Niskin bottles and filtered onto Whatman GF/F filters (25 mm in diameter) under a gentle vacuum (3.98 Hg). The filters were placed immediately in 2-mL cryovials and flash-frozen in liquid nitrogen and then stored at -80° C until analysis. After the cruise, filters were extracted in 100% methanol at -20°C, disrupted by sonication, and clarified later by vacuum filtration through Whatman GF/F filters. Extraction time lasted 2 hours, and HPLC analysis was carried out the same day (Ras et al., 2008; Tran et al., 2013; Robinson et al., 2018). More details on the analytical methods can be found in Matthes et al. (2021) for the BaySys, and Ras et al. (2008) for the GreenEdge data sets. In this study, [*chla*]_{*HPLC*} corresponds to the sum of *chla* and chlorophyllide-*a*.

2.2.4.3 In-water radiometry

Downwelling in-water irradiance profiles, $E_d(z, \lambda)$, were measured by Compact-Optical Profiling System (C-OPS; Hooker et al., 2013) built by Bio-Spherical Instruments Inc. (San Diego, California, USA). C-OPS has 19 bands distributed between the spectral range of 320 to 865 nm measuring the planar downwelling irradiance coupled with auxiliary sensors for water temperature, pressure, pitch, and roll. A similar reference sensor in the ship deck to measure above water surface downwelling irradiance $E_d(0^+, \lambda)$. Above water reference sensor were coupled to the Bioshade to measure the ratio of sun direct to diffuse sky irradiation (E_d^{sun}/E_d^{sky} ; Morrow et al., 2010), which is used for instrument self-shadow correction.

We profiled at least three consecutive downcasts between the sea surface and a variable water depth corresponding to the approximately 1% light level. In-water radiometric measurements were normalized to account for the illumination variations during each cast. Underwater casts trespassing a vertical tilt of 5° were removed from the analysis. In-water radiometry was processed using the R-package COPS available in https://github.com/belasi01/Cops. A detailed discussion about the C-OPS instrument and the processing protocols can be found elsewhere (Mueller et al., 2003; Morrow et al., 2010; Antoine et al., 2013; Hooker et al., 2013; Bélanger et al., 2017).

The daily average of photosynthetic active radiation, (\overline{PAR}) was computed after applying the factor $cos(\theta_s(t))/cos(\theta_{oncast})$, where θ_s is the solar zenith range in the daytime (t) and θ_{oncast} is the solar zenith on cast of the light profile (Reda and Andreas, 2004). Photosynthetic active radiation, *PAR* (in μ mol photons m⁻²s⁻¹), was calculated form trapezoidal integration of $E_d(\lambda, z)$ in the visible spectrum from 400 to 700 nm (Equation 2.3):

$$PAR(z) = \frac{1}{\hbar c} \frac{1}{N} \int_{\lambda=400}^{700nm} \lambda E_d(\lambda, z) \, d\lambda$$
(2.3)

where \hbar is the plank constant (6.623×10⁻³⁴ J s⁻¹), *c* is the constant for the light speed (299,792,458 m s⁻¹), and *N* is the the Avogadro's number (6.022×10²³). $E_d(\lambda, z)$ was measured in μ W m⁻²nm⁻¹. The conversion from mol to μ mol used a factor of 1×10⁶.

The spectral coefficient for diffuse downwelling irradiation attenuation, $k_d(\lambda)$, at a geometric depth, defined as (Equation 2.4):

$$k_d(\lambda, z) = -\frac{1}{E_d(\lambda, z)} \frac{\partial E_d(\lambda, z)}{\partial z}$$
(2.4)

was determined from in-water $E_d(z, \lambda)$ profiles following Mueller et al. (2003). The value for $k_d(\lambda)$ was computed as the local slope of $ln [E_d(z)]$ using a linear regression fit, and assuming a constant k_d within the interval $(z_m - \Delta z) \le z \le (z_m + \Delta z)$ where z_m is the center depth (Equation 2.5):

$$ln[E_d(\lambda, z)] = ln[E_d(\lambda, z_m)] - (z - z_m)k_d(\lambda, z_m)$$
(2.5)

As proposed by Lee et al. (2005), $k_d(z)$ in the euphotic zone may be replaced by the integrated value of k_d from surface to a depth where E_d is reduced to approximately 1% or 10% of its surface value, i.e., k_d value in the layer between $E_d(0^-)$ and 1 or 10% of $E_d(0^-)$. Here, $k_d(E_d 10\%)$ was denominated as k_d because this layer contributes most to the water column photosynthesis and signals measured by remote sensors.

Nelson River and landfast ice introduce considerable quantities of minerogenic particles into Hudson Bay. To reduce the contribution to non-chlorophyllous particles that efficiently backscatter light, our analysis was restricted to the MIZ light environment. Water masses were classified using a cluster analysis applied to $k_d(\lambda)$, which is closely related to inherent optical properties (IOPs) and [*chla*] (Solonenko and Mobley, 2015).

2.2.5 Phytoplankton photo-acclimation proxy

As mentioned in the Introduction, ocean optical properties can be used as proxies to assess phytoplankton photoacclimation or size structure proxies (Huot et al., 2008; Devred et al., 2011; Brewin et al., 2012; Marañón, 2015; Fujiwara et al., 2018; Reynolds and Stramski, 2019). Here, we examined the potential of satellite-derived phytoplankton photo-acclimation proxies to better understand the state of the phytoplankton community characterizing the fall blooms. Our assessment is based on [*chla*] and b_{bp} , which are important proxies for phytoplankton dynamics and pelagic ecosystems. While [*chla*] is a direct proxy for phytoplankton, b_{bp} may be influenced by a wide range of non-chlorophyllous particles such as bacteria, micrograzers, heterotrophic nano-flagellates, ciliates, and viruses; organic particles of detrital origin such as fecal pellets and cell debris (non-living organic detritus derived from the breakdown of micro-organisms); mineral particles of both biogenic (e.g., calcite liths and shells) and terrestrial origins (e.g., clays and sand); bubbles; and plastics (Vaillancourt et al., 2004; Bellacicco et al., 2019). Total b_{bp} , therefore, may be partitioned into two additive components:

$$b_{bp} = b_{bp}^{[chla]} + b_{bp}^k \tag{2.6}$$

where $b_{bp}^{[chla]}$ is the backscattering component that co-varies with phytoplankton biomass and b_{bp}^k , the backscattering background that is due to non-algal particles (NAP) that do not co-vary with phytoplankton biomass.

To support our interpretations of b_{bp} as a phytoplankton proxy, we first needed to estimate b_{bp}^k . Behrenfeld et al. (2005), for example, estimated b_{bp}^k as the intercept of the least-squares regression analysis of the [*chla*] versus b_{bp} relationship. The backscattering background was considered constant over the global ocean and fixed to a value of 0.00035 m⁻¹. More recently, however, Bellacicco et al. (2016) demonstrated that b_{bp}^k was not constant in either space or time scales in the Mediterranean Sea. Similar conclusions were drawn from an extensive analysis of global satellite ocean color data and in situ bio-ARGO data by Bellacicco et al. (2018, 2019), suggesting that b_{bp}^k variability must be considered in order to assess phytoplankton-related backscattering (or carbon content assuming a scaling factor, e.g. Behrenfeld et al., 2005). Therefore, we computed b_{bp}^k at 555 nm on a pixel-to-pixel basis using all daily satellite observations available for the 1998 to 2018 period for each month of open waters (May to October).

Values of b_{bp}^k was calculated as the background value of the relationship between b_{bp} and *chla* by fitting three methods: i) the linear model proposed by Behrenfeld et al. (2005); ii) the model presented by Bellacicco et al. (2019), which was first proposed by Brewin et al. (2012) to account non-linearity

driven by phytoplankton size fractions; and iii) an exponential model that we proposed with an offset to account for b_{bp}^k (Equation 2.7):

$$b_{bp}(555) = a \ [chla]^b + b_{bp}^k(555) \tag{2.7}$$

where *a* and *b* are fitting parameters. The three fitting procedures were first tested on our in situ observations of b_{bp} and $[chla]_{HPLC}$ described above, as well as another data set from the Canadian Arctic (i.e., from the Baffin Bay; results not shown).

Phytoplankton physiological adjustments to environmental conditions (e.g., light, nutrient status, taxonomy, stratification, and grazing) result in changes in the ratio of phytoplankton-carbon biomass $(C_{phy}, \text{ in mg C m}^{-3})$ to [chla] (Geider, 1987; Behrenfeld et al., 2005; Westberry et al., 2008; Sathyendranath et al., 2020). Therefore, assuming that phytoplankton dominates the covarying part of b_{bp} , as proposed by Behrenfeld et al. (2005), we estimated C_{phy} by multiplying $b_{bp}^{[chla]}$ by a fixed scaling factor (SF: 13,000 mg C m⁻²) (Equation 2.8):

$$C_{phy} = b_{bp}^{[chla]} \times SF = \left[b_{bp}(555) - b_{bp}^{k}(555)\right] \times SF$$
(2.8)

2.3 Results

2.3.1 Monthly climatology of chlorophyll-a

Satellite ocean color monthly climatologies (1998–2018) of [*chla*] revealed the seasonal and spatial variability of phytoplankton in the HBS (Figure 21). In May, high [*chla*] (>1 mg m⁻³) in open waters was a manifestation of ice-edge bloom. In June, concentrations remained high in most of the HBS also due to late ice-edge blooms, except in the central HB where oligotrophy was already established. The lowest [*chla*] were observed in August, except in coastal zones influenced by riverine inputs or where strong mixing processes (e.g., tidal mixing) operated year-long (i.e., in Hudson Strait). The trophic conditions revealed by satellite-derived [*chla*] are based on Barbedo et al. (2020) and Perrette et al. (2011) who defined the ice-edge bloom with [*chla*] greater than a threshold of 0.5 mg m⁻³ just after the ice retreat. The term oligotrophy is adopted for low [*chla*], as observed by (Ferland et al., 2011) in

summer in the HBS. Concentrations clearly began to increase again in September almost everywhere and continued to rise in October, including in the central HBS where oligotrophic conditions relaxed ([*chla*] increased from $< 0.2 \text{ mg m}^{-3}$ to $> 0.5 \text{ mg m}^{-3}$). We further examine in the next sections the physical processes potentially involved in explaining the late summer/fall increase in [*chla*] in the southern part of the oligotrophic area.

2.3.2 Atmospheric forcing, [chla], and b_{bv}: Seasonal and interannual variability

Figure 22 shows time-series of [*chla*], $b_{bp}(555)$, wind speed, and heat flux between 2002 and 2009 in the south Hudson Bay (i.e., red box on Figure 21 centered at location 84°W and 57°N). High [*chla*] during the spring-to-summer transition (June–July) was related to ice-edge blooms and, as a consequence, the stratification onset following the ice breakup. A reduction in [*chla*] was abrupt after the ice-edge bloom peak, following a decline in the ocean heating rate until south Hudson Bay reached a surface oligotrophic state (i.e., lowest [*chla*]). Chlorophyll-*a* concentration trends (∂ [*chla*] (∂t)⁻¹) indicated a systematic increase in [*chla*] between summer, with the maximum oligotrophic state, and fall co-occurring with a seasonal process of atmospheric warming ocean decay (i.e., heat flux losing intensity). These trends were obtained by linear fit in the interval of confidence of 99% in 2003 (0.08 mg m⁻³ month⁻¹), 2005 (0.73 mg m⁻³ month⁻¹), 2006 (0.11 mg m⁻³ month⁻¹), 2007 (0.21 mg m⁻³ month⁻¹), 2008 (0.15 mg m⁻³ month⁻¹), and 2009 (0.25 mg m⁻³ month⁻¹). In 2002 and 2004, in contrast, [*chla*] time series remained flat about 0.65±0.26 and 0.48±0.16 mg m⁻³, respectively. In addition to that, a sustained [*chla*] increment during the summer-to-fall transition was observed in 2003, 2005, and 2007, just after the heat-flux inversion (positive to negative), i.e., when the ocean surface begin to cool (heat escaping the ocean).

The time evolution of b_{bp} was distinct from [*chla*]. b_{bp} presented a slight decrease during the springto-summer transition and remained relatively constant in summer. In fall, increases of b_{bp} had small amplitude compared to [*chla*] (e.g. October 12 to 25, 2005 and 2007) or b_{bp} time-series remained almost flat (e.g. 2002, 2003, 2006, 2008, and 2009).



Figure 21: Climatology of chlorophyll-*a* concentration. Satellite ocean color monthly climatology (May, June, July, August, September, and October) of chlorophyll-*a* concentration ([*chla*]: color scale in mg m⁻³) obtained between 1998 and 2018. The study area (red box) centered in 84°W 57°N (red star) in South Hudson Bay where time series of [*chla*], wind speed, heat flux, and water column evolution were extracted in 2005.



Figure 22: South Hudson Bay: phytoplankton dynamic and atmospheric forcing. Time series of chlorophyll-a concentration ([*chla*], mg m⁻³, green circles; 7-day moving average, green line), backscattering coefficient at 555 nm (b_{bp} (555), in m⁻¹, magenta squares, and 7-day moving average, magenta line) from the semi-analytical algorithm (GSM: Garver and Siegel, 1997; Maritorena et al., 2002) of Globcolor project, wind speed (daily, in cyan line, 7-days moving average, blue line) from the Canadian Meteorological Centre's Global Deterministic Prediction System Re-Forecasts (CGRF), and heat flux (gray bars) calculated by bulk formulas (Large and Yeager, 2004) using the NEMO Arctic and Northern Hemisphere Atlantic (ANHA4) with a resolution of 0.25° between 2002 and 2009 in southern Hudson Bay (84°W and 57°N). The sea ice retreat day (t_R) was calculated using sea ice concentration (SIC) from the National Snow and Ice Data Center (NSIDC). Chlorophyll-*a* concentration trends ($\partial [chla](\partial t)^{-1}$) in the 99% interval of confidence were plotted between maximum oligotrophic state in summer and fall (red line).

Wind speed showed high variability, but its signature did not show a clear influence on [*chla*] (Figure 22). This mismatch between wind and [*chla*] were observed when wind components (zonal and meridional) were analyzed (Figure 31). This mismatch is particularly evident when high wind speed events (> 8 m s⁻¹) occurred and heat fluxes were positive. Such events were evident in late summer (August–September) and associated with a relatively low [*chla*] (e.g. 2002, 2003, 2004, and 2005) or followed by an ephemeral incremental increase of [*chla*]. Although strong wind events in summer, during positive heat flux, can result in an increase in [*chla*], as observed in 2003 (around August 13), they can also result in a decrease in [*chla*] (e.g., August 28 and September 27, 2003). For most years analyzed, peaks of wind speed during summer (between August 15 and September 15) were associated with [*chla*] lower than their respective phenological peaks. For example, when high wind speed (exceeding 6 m s⁻¹) was maintained between August 20 and September 12, 2007, [*chla*] remained low (< 0.8 mg m⁻³) relative to the spring and fall blooms (2.0 mg m⁻³).

In summary, wind speed and [*chla*] links in late summer or fall were hard to detect because of the high wind-speed variability, i.e., ranging from 2 m s⁻¹ to above 10 m s⁻¹ during a short time period, and because a large increment in [*chla*] often happened in the presence of moderate wind. However, strong wind events had more impact on [*chla*] when the ocean was cooling (e.g., 2005, 2007). Other factors such as heat fluxes and freshwater inputs have to be considered.

2.3.3 Correlation analysis: chlorophyll versus atmospheric forcings

We extracted correlation coefficients between [*chla*] and wind speed (WS) or heat flux (HF) using a moving average filter with a time window ranging from 1 to 30 days applied to daily time series between 1998 and 2008. For each window range, WS and HF generated a pair of coefficients of correlation with [*chla*]. We segmented time series between pre and fall seasons. The first day of that atmosphere-cooling ocean began (i.e., the day of heat-flux-inversion) defined the fall seasons. As a result, Figure 23 shows a correlation analysis of [*chla*] with atmospheric forcing (WS and HF) on different time scales in southern Hudson Bay. In the spring-to-summer transition period, before the heat-flux inversion, wind speed and heat flux had a weak correlation outside the confidence interval of 95% (p < 0.05). After the heat-flux inversion, [*chla*] and wind speed reached a coefficient of correlation of 0.42 (p < 0.05) while [*chla*] and heat flux reached a high negative coefficient of correlation of -0.71 (p < 0.05) for the moving average filter of the 7-day window. The coefficient of correlation between [*chla*] and wind speed just had the confidence interval of 95% for a filter length of 7 days or longer, which indicated the low impact of high-frequency wind events on the phytoplankton dynamic.

2.3.4 Water column structure evolution

Figure 24 A shows well-marked spring and fall blooms reaching 2 mg m⁻³ separated by an oligotrophic period of [*chla*] below 0.5 mg m⁻³ in 2005. The annual lowest sea surface salinity (< 29.5) and highest stratification ($N^2 \sim 1.5 \times 10^3 \text{ s}^{-1}$) were reached on June 15 (Figure 24 B), as a consequence of freshwater lenses produced by sea-ice melting and riverine input. After that date, there was a transition in the control of vertical stratification (i.e., β to α transition: Carmack and Wassmann, 2006; Carmack et al., 2006) triggered on June 23, associated with the freshwater lens dilution, mixed layer deepening, and pycnocline ventilation. The water column stratification, which was controlled mainly by the salinity gradient becomes controlled by the temperature gradient between July and August (Figure 24 C and D). Pycnocline ventilation was continual with freshwater lens dilution (Figure 24 B and C). On August 10, the mixed layer depth (dashed line) definitively exceeded the first optical depth (z_{OC} , grey line), which was stably positioned around 10 m. The beginning of mixed layer deepening corresponds to the oligotrophic period of 2005 with the lowest [*chla*] observed (< 0.2 mg m⁻³). [*chla*] decreased systematically following the ice-edge bloom dissipation from June 15 to August 18.

The phytoplankton fall bloom was observed as a systematic increase in [*chla*], coinciding with cooling throughout the water column and the heat-flux inversion observed on September 11 (Figure 24 A). The vertical gradients of temperature and salinity remained weak in the upper ocean layer (top 30 m) when the atmosphere-cooling ocean began. The heat-flux inversion also was coincident with the intercept between pycnocline and z_{eu} (Figure 24 A and B). The abrupt increase in [*chla*] coincides with a decreasing trend in wind speed starting on October 5 (Figure 24 A). Although [*chla*] observed during



Figure 23: Response of phytoplankton biomass to atmospheric forcing on a range of time scales. Sensibility analysis to assess the impact of heat flux and wind speed on chlorophyll-a concentration ([*chla*]) using an average filter length ranging its scale from 1 to 30 days in time series between 1998 and 2008 in southern Hudson Bay. The spring-to-summer transition was defined as the period before the heat-flux inversion, and the summer-to-fall transition was the period after heat-flux inversion when the atmospheric cooling ocean began. Coefficients of correlation of [*chla*] in relation to wind speed (WS) and heat flux (HF) with a confidence interval of 95% were marked.

the fall blooms was similar to the spring-to-summer season in ice-edge blooms, the dispersion of daily compared to 7-day averages revealed that the variability of [*chla*] in fall was clearly higher than in the ice-edge blooms (Figure 24 A). Finally, an intensification of fall bloom was marked by another abrupt increase in [*chla*] (> 2 mg m⁻³) after October 13 (Figure 24 A), which was triggered by an intersection between the mixed layer and euphotic depth (Figure 24 B, C, and D), and ceased/collapsed by ocean freezing and sea-ice recovery.

2.3.5 Relationship between chlorophyll-a and particles backscattering coefficient

To gain further insights into the phytoplankton growing in the late summer and fall seasons, we first report the relationship between particle backscattering and chlorophyll-*a* measured in the field in summer. Figure 25A show the relationship between in situ [*chla*]_{*HPLC*} and $b_{bp}(555)$ obtained from field measurements in Hudson Bay in 2018. Stations were grouped in distinct light environments based on $k_d(\lambda)$ with high, moderate, and low light attenuation in marginal-ice zones. Values for [*chla*]_{*HPLC*} ranged from 0.1 to 15 mg m⁻³, $b_{bp}(555)$ from 0.0004 to 0.02 m⁻¹, and $b_{bp}^*(555)$ from 0.0007 to 0.0506 m² (mg chl*a*)⁻¹. These observations were used to test different fitting algorithms to estimate b_{bp}^k , before applying it to satellite ocean color data. As mentioned in Section 2.2.5, we compared the linear fit of Behrenfeld et al. (2005), the nonlinear least-squares algorithm of Bellacicco et al. (2019) and an exponential model (Equation 2.7). The later model performed better with r² of 0.760 (*rms.e* = 0.001, *n* = 37), compared to r² of 0.707 and 0.30 for the Bellacicco et al. (2019) and Behrenfeld et al. (2005) models, respectively. The estimated b_{bp}^k using the exponential model yield values of 0.0023 m⁻¹, which is slightly higher than the value obtained using Bellacicco et al. (2019), and similar to the values obtained with the linear fit. Similar results and conclusions were obtained in the Baffin Bay (results not shown).

The carbon-to-chlorophyll ratio estimated after the application of Equations 2.8 and 2.7, $C_{phy}:[chla]_{HPLC}$, yielded mean a value of 17.31 and maximum value of 120. Figure 25 B shows chlorophyll-specific backscattering at 555 nm ($b_{bp}^*(555)$ in m² (mg chla)⁻¹) as a function of [chla]_{HPLC} in distinct light levels (colored symbols). As reported for high latitudes (Reynolds et al., 2001; Stramska et al.,



Figure 24: Synergy of the sea-ice model, wind speed reanalysis, and ocean color satellites in South Hudson Bay, 2005. Influence of atmospheric forcing and water column structure on phytoplankton phenology in southern Hudson Bay at 84°W and 57°N in 2005: (A) time series of [*chla*] from Globcolor Project (GSM: Garver and Siegel, 1997; Maritorena et al., 2002) in log scale (daily, green squares, and 7-day moving average, green line), heat flux (HF: grey bars) and wind speed (daily, cyan line, and 7-day moving average, blue line) taken from the Canadian Meteorological Centre's Global Deterministic Prediction System Re-Forecasts (CGRF; Smith et al., 2014). Profiles in the color scale of (B) Brunt-Vaissala frequency (N^2), (C) salinity, and (D) temperature modeled from the Nucleus for European Models of the Ocean (NEMO). The important layer for phytoplankton dynamics are marked on vertical profiles: satellite-derived first optical depth (z_{OC} , white line) and euphotic zone depth (z_{eu} , purple line); mixed layer depth (MLD, black traced line); and pycnocline (N^2_{max} , black line).

2003; Wang et al., 2005; Zhuang et al., 2020), we observed an inverse relation between $b_{bp}^*(555)$ and $[chla]_{HPLC}$.

2.3.6 Satellite-derived phytoplankton photoacclimation proxy

Besides, [*chla*] (Figure 21), ocean color satellite monthly climatologies revealed the seasonal and spatial variability of particles backscattering in the HBS, which is assumed to respond to both phytoplankton and non-algal particle concentrations. The monthly climatology of $b_{bp}(555)$ (Figure 26) shows the highest values (> 0.002 m⁻¹) near the coast, simultaneously with the seasonal peak of river runoff and ice melting between May and June. The b_{bp} was maximum in May (mean ± standard deviation: $0.0025 \pm 0.0005 \text{ m}^{-1}$, n = 12312) and June ($0.0022 \pm 0.0006 \text{ m}^{-1}$, n = 60957), decreased in July ($0.0019 \pm 0.0006 \text{ m}^{-1}$, n = 69238), and remaining constant in August ($0.0016 \pm 0.0005 \text{ m}^{-1}$, n = 62450).

Similar to Bellacicco et al. (2020), b_{bp}^k (555) was estimated by applying Equation 2.7 to all satellite daily observations available for a given month between 1998 and 2018, and for a given 4.5-km resolution pixel. The spatially resolved b_{bp}^k (555) monthly maps are shown in Figure 27 and statistics for the whole HB in boxplot in Figure 38. The Seasonal minimum coincided with fall blooms in September (0.0004±0.0004 m⁻¹, *n* = 70839) and October (0.0002±0.0003 m⁻¹, *n* = 62442), and ice-edge blooms in May (0.0004±0.0005 m⁻¹, *n* = 12304). Seasonal low contribution of NAP to total backscattering (b_{bp}^k : b_{bp}) also occurred in May (14.6%) and October (13.8%). b_{bp}^k (555) reached the seasonal peak after the ice-edge bloom season in July (0.0006±0.0007 m⁻¹, *n* = 69238), simultaneous with its peak of NAP contribution to total backscattering (b_{bp}^k : b_{bp} of aproximately 36.2%).

Monthly phytoplankton carbon, C_{phy} , was estimated by subtracting b_{bp}^k (Figure 27) from b_{bp} (Figure 26) and multiplying by a scaling factor of 13,000 mg C m⁻² (Equation 2.8) (Behrenfeld et al., 2005; Bellacicco et al., 2020). The seasonal patterns in C_{phy} (Figure 28) slightly differ from [*chla*] (Figure 21) and b_{bp} (Figure 26). In general, C_{phy} was higher than 27.9 mg C m⁻³ in May and 21.1 mg C m⁻³ in June during the ice-edge bloom, then decreased to reach a minimum in August (<12.4 mg C



Figure 25: Chlorophyll-*a* concentration, light backscattering coefficient and photosynthetic active radiation interplay in the Eastern Canadian Arctic. Scatter plots of in situ coincident chlorophyll-*a* concentration ([*chla*]_{*HPLC*}, in mg m⁻³) measured using high-performance liquid chromatography (HPLC) and particulate backscattering coefficients ($b_{bp}(555)$, in m⁻¹) by ECO BB9 in Hudson Bay, 2018 (A). Distinct light environments in the marginal ice zone (MIZ) were grouped based on light attenuation, $k_d(\lambda)$, (high, cyan triangles; moderate, blue triangles; and low, black triangles). The b_{bp} -*chla* relations were fitted using models proposed by Behrenfeld et al. (2005; dotted line), Bellacicco et al. (2019; dashed line), and an exponential equation with offset (this study, black line) to account the non-algal background backscattering (b_{bp}^k). (B) chlorophyll-specific backscattering ($b_{bp}^*(555)$, in m² (mg chla)⁻¹) as a function of [*chla*]_{*HPLC*}, and daily average photosynthetic active radiation ($\overline{PAR}(z)$, in color scale) in Hudson Bay (squares).



Figure 26: Climatology of total backscattering coefficients. Satellite ocean color monthly climatology (May, June, July, August, September, and October) of the total particle backscattering coefficient at 555 nm, $b_{bp}(555)$, obtained between 1998 and 2018.



Figure 27: Climatology of non-algal backscattering coefficients. Satellite ocean color monthly climatology (May, June, July, August, September, and October) of the non-algal particle backscattering coefficient at 555 nm (b_{bp}^k (555), in m⁻¹) obtained between 1998 and 2018, estimated from relationship between satellite-derived b_{bp} (555) and [*chla*].

m⁻³). During the summer months, C_{phy} remained high in the southern HBS and in the coastal waters of Hudson Strait. An overall increase in C_{phy} was observed in September (15.7 ±5.9 mg C m⁻³, n = 70841), and during fall blooms in October (18.3 ± 5.9 mg C m⁻³, n = 62450; Figure 38).

The seasonal variability of [chla] and C_{phy} resulted in considerable seasonal variability in the C_{phy} : [chla] ratio (Figure 29). Here, we present the seasonal evolution of this parameter, which is known to reflect phytoplankton light acclimation (photoacclimation), nutrient availability, and temperature (Geider, 1987; Geider et al., 1997; Sathyendranath et al., 2009; Jakobsen and Markager, 2016). In May, the phytoplankton found in the marginal ice zone presented high concentration of carbon (C_{phy} : $27.2 \pm 7.9 \text{ mg C m}^{-3}$, n = 12312) and chlorophyll-a ([chla]: $1.13 \pm 0.44 \text{ mg m}^{-3}$, n = 12312). [chla] higher than 2 mg m⁻³ dominated the open water regions near the coasts, with maximum C_{phy} (> 20 mg C m^{-3}) observed in polynyas, i.e., in the Northwest Hudson Bay and the south of Belcher Islands. C_{phy} :[chla] were particularly low along the ice edge in the northwest polynya. C_{phy} :[chla] increased systematically offshore from May to June. High C_{phy} :[chla] (> 40) occurred coincidentally to maximum annual solar flux (summer solstice) and remained high in oligotrophic regions in the central HBS until August. Relatively low Cphy:[chla] values are found in eastern HB and in coastal waters of the Hudson Strait where high [chla] was also evident (Figure 21). From August to October, C_{phy}:[chla] tends to decrease everywhere in the HBS, except in some coastal zones (e.g., Ungava Bay). The seasonal minimum was reached in October $(22.0 \pm 7.2, n = 62450)$ with values lower than those observed during the spring bloom in May (26.5 ± 9.7 , n = 12312). At this time of the year, the phytoplankton contribution to backscattering $(b_{phy}:b_{bp})$ was the largest (approximately 86%).

2.4 Discussion

2.4.1 Phytoplankton fall bloom onset

How is the phytoplankton fall bloom phenomenon triggered and maintained in Hudson Bay? The synergy of the ocean color satellite, sea-ice dynamic model, climatic reanalysis, and in situ bio-optic profiles underscores the influence of atmospheric forcing and water-column evolution on phytoplank-ton dynamics.



Figure 28: Climatology of phytoplankton carbon. Satellite ocean color monthly climatology (May, June, July, August, September, and October) of the total phytoplankton carbon (C_{phy} , in mg C m⁻³) obtained between 1998 and 2018 in Hudson Bay.



Figure 29: Climatology of ratio phytoplankton carbon to chlorophyll. Satellite ocean color monthly climatology (May, June, July, August, September, and October) of ratio phytoplankton carbon to chlorophyll-*a* concentration (C_{phy} : [*Chla*]) obtained between 1998 and 2018. C_{phy} was computed using the backscattering coefficient of non-algal particles (NAP) at 555 nm b_{bp}^k (555) spatially resolved at pixel scale. b_{bp}^k (555) were estimated by the Bellacicco et al. (2019) method using satellite-derived b_{bp} (555) and [*chla*] calculated from the semi-analytical algorithm (GSM: Garver and Siegel, 1997; Maritorena et al., 2002) of the Globcolor Project merged daily 4 km products.

2.4.1.1 Role of freshwater

As observed in Figure 24, analogous to other years presented in Figures 32 to 37, the seasonal evolution of the water column follows these stages: 1) freshwater lens dilution during summer; 2) vertical displacement between mixed layer and pycnocline; 3) mixed layer deepening and pycnocline ventilation; 4) a transition between a β (haline) to α (thermal) stratification; 5) euphotic depth reaching the pycnocline and, subsequently, the depth of the mixed layer.

Climatic maps of [*chla*] and C_{phy} , and C_{phy} :[*chla*] (Figs. 21, 28 and 29), revealed that the ice-edge blooms in the spring-to-summer and the rise in phytoplankton in the summer-to-fall transitions were productive features interrupted by a relatively severe oligotrophy. This oligotrophic period was defined by a high seasonal C_{phy} :[*chla*] in regions of [*chla*] persistence below 0.5 mg m⁻³, which occupied more than 50% of the bay. Ice-edge and fall blooms are, by comparison, very distinct in terms of water column structure, stratification, and heat flux. In spring, the freshwater lens produced the highest annual stratification near the sea surface, while mixed layer deepening and pycnocline ventilation affected the whole euphotic layer in fall.

As presented in Figure 24, the annual maximum of stratification coincided with the seasonal peak of riverine input and ice melting in June and July (Prinsenberg, 1984). According to Déry et al. (2005), riverine inflow can exceed 4 km³ day⁻¹ in midsummer. In the upper layer, freshwater lenses (salinity < 30) produced strong stratification, which held both the mixed layer and pycnocline close to the surface layer (approximately 10 m) (Stewart and Lockhart, 2005; Granskog et al., 2011). After the seasonal peaks of ice-melting and continental drainage (Prinsenberg, 1984; Déry et al., 2005), the dilution of freshwater lenses triggered a continuous process of pycnocline ventilation and mixed-layer expansion until sea surface freezing at the end of autumn (Figure 24). Meanwhile, after the peak of heat flux (atmospheric warming ocean) and sea-ice retreat, the vertical stratification, previously controlled by salinity gradients, was then switched by a temperature gradient, i.e., it switched from β to α stratification (Carmack and Wassmann, 2006; Carmack et al., 2006). As discussed by Carmack and Wassmann

(2006) and Carmack et al. (2006), phytoplankton production and vertical distribution of chlorophyll in thermal-stratified (α stratification) polar seas is more sensitive to mixing and convection than salinity-stratified (β stratification) shelves dominated by freshwater.

The pre-fall-bloom stage occurred when the euphotic zone became shallower until it found the maximum stratification layer, which was getting deeper responding to pycnocline ventilation, and [*chla*] had risen from 0.4 to 0.9 mg m⁻³ between 11 and 19 September 2005, the beginning of heat-flux inversion period. Then, a massive increase in [*chla*] was triggered when mixed layer deepening reached z_{eu} . When this stage was reached, the euphotic layer and whole phytoplankton productivity layer became confined to the mixed layer, characterized by weak stratification and homogeneous profiles of salinity and temperature. Similar to observations reported by Fujiwara et al. (2018) in the Chukchi shelf, wind-driven and convective turbulence intensified the erosion of water column structure in south Hudson Bay. Subsequently, the fall bloom development, defined by a significant increase in [*chla*], followed a homogenization of the whole productive layer (Figure 24 and 32 to 37).

In south Hudson Bay, NEMO modeling revealed high interannual variability of freshwater input with years of low (2006, 2007, and 2008; Figures 35, 36, and 37) and high (2002 and 2004; Figure 32 and 34) surface salinity. As a result, the response of phytoplankton to atmospheric forcing will depend on freshwater inputs, which vary from year to year. Riverine input can increase the stocks of nutrients and remineralization in the whole bay. However, freshwater counteracts brine rejection by blocking the upward flux of nutrients from the deep-nutrient pool in winter (Eastwood et al., 2020). Phytoplankton can promptly assimilate nutrients from river restringing production in coastal areas and river plumes in summer (Jacquemot et al., 2021; Kuzyk et al., 2010). Indeed, the interannual variability of complex interplays of nutrient inventories, atmospheric-heating ocean, and wind-driven turbulence throughout summer are pre-conditions for the phytoplankton dynamics in the fall season. For example, years of predominant low upper-layer stratification (e.g., 2006) can allow nutrient replenishment in the euphotic layer sustaining an increase of chlorophyll throughout the summer but weakening an eventual fall bloom triggered by convection due to prior depletion of the subsurface nutrient pool. On the other hand, strong-stratification counteracts the vertical transport of nutrients from below the euphotic zone

and reinforces the oligotrophy. SCM responds directly to the water column structure in Hudson Bay as discussed by Ferland et al. (2011), Estrada et al. (2012), Sibert et al. (2010, 2011) and Lapoussiere et al. (2013). In summer, it can restrict phytoplankton production in the sub-surface chlorophyll-*a* maximum causing a nutricline deepening at levels below the range of convective-driven turbulence, which will dampen the fall bloom process (e.g., 2002 and 2004).

2.4.1.2 Role of winds and heat fluxes

Turbulent mixing is key to understanding the bloom onset. As reported by Falkowski and Oliver (2007), the climate-driven processes that influence turbulent mixing in the ocean seem to have strongly influenced the diversity and relative abundance of the major eukaryotic phytoplankton taxa in the geological (Phanerozoic Eon) and the contemporary ocean (Anthropocene). Sources of turbulence in the upper layer occur over a wide range of spatial and temporal scales and result in a non-homogeneous turbulence vertical distribution in the mixed layer. As detailed by Franks (2015), turbulence in the ocean is a result of energy dissipation through the following processes: wind, waves, Langmuir circulation, and convectively-driven turbulence. Both wind-driven and convection-driven (heat fluxes) processes were examined for fall bloom onset in HB (Figure 23 and 31). The convection impacts uniformly and strongly the mixed layer defining the seasonal pycnocline. Otherwise, wind-driven turbulence is likely dominant in the upper layer, decays with depth and its dissipation occurs in a short time scale (hours or less). Wind-driven turbulence can impact negatively phytoplankton production in the upper layer, especially in the first optical depth, (Behrenfeld, 2010; Taylor and Ferrari, 2011; Fischer et al., 2014; Franks, 2015). In polar seas, an increase in annual phytoplankton production, in part, is assumed to be caused by storm events that drive turbulence in the upper ocean layer (Ardyna et al., 2013; Fujiwara et al., 2018). However, a direct link between storms and fall blooms is not a general consensus as pointed out by Sigler et al. (2014). In Hudson Bay, sea-surface wind events only have a direct impact on [chla] after heat-flux inversion, i.e., when the atmosphere began to cool the upper-ocean layer (Figure 22). However, the increase in [chla] after the HF inversion is not systematic and probably depends on the nature of the stratification (α versus β stratification), i.e., the presence of freshwater in the upper ocean.

As discussed by Kim et al. (2007) in the Japan/East Sea and Olita et al. (2014) in the Mediterranean Sea, the phytoplankton response takes some time to assimilate a new supply of nutrients introduced into the upper ocean layer. However, lagged correlations between wind speed and [chla] were not statistically significant. Otherwise, convective-driven turbulence has a homogeneous effect on the whole mixed layer that determines its seasonal depth. As reported by Ferland et al. (2011) in summer (August and September), the depths of the nutricline and sub-superficial chlorophyll-a maximum depths are very close to the euphotic zone depth in Hudson Bay. Therefore, convective-driven turbulence results in the mixed layer deepening and pycnocline ventilation, potentially releasing nutrients and phytoplankton communities from the SCM into the upper euphotic layer. The freshwater input and sea-ice melting impact the resilience of the water column structure against wind-driven turbulence because freshwater shields the upper-layer structure, and the absence of convection dampens the bloom development, as observed in situ during the summer-to-autumn transition on the northern Chukchi Sea (Nishino et al., 2015). Although nutrient resupply by Ekman pumping is an important factor in increasing phytoplankton production, excessive turbulence and mixing can have a negative effect. As demonstrated by Franks (2015), wind-driven turbulence strongly affects the upper layer but loses efficiency with depth. In addition to that, the restructuring of stratification in response to the wind-driven turbulence is a much faster process than the restructuring in response to convection (Franks, 2015).

The negligible impact on [*chla*] in response to persistent strong winds and high-frequency wind events (Figure 22), coastal upwelling (Enriquez and Friehe, 1995) forced by winds parallel to coastal line orientation (Supplementary material: Figure 31) and in the ice-edge (Dumont et al., 2010), or in the absence of convection prior to heat-flux inversion (Figure 23), supported the idea that fall blooms are triggered when convective-driven turbulence began to erode stratification. Specifically, wind-driven mixing alone can be more effective in limiting the phytoplankton production in the first optical depth than promoting by nutrient transport via Ekman pumping. As presented in the section Ice-Ocean model and heat flux calculations (Material and Methods), the wind has a direct effect on heat flux. Although wind speed is key to understanding how atmospheric forcing impacts phytoplankton dynamics, our results highlight the importance of atmospheric cooling of the surface ocean on stratification. We found that the water column stratification resisted wind-driven turbulence events until the atmosphere began effectively to cool the ocean, producing a systematic increase of [*chla*].

2.4.2 Phytoplankton photoacclimation

As mentioned in the Methods, phytoplankton physiological adjustments to environmental conditions result in changes in the ratio of phytoplankton-carbon biomass (C_{phy}) to [*chla*]. We estimated C_{phy} from satellite-derived particles backscattering after considering the non-algal backscattering background. We first discuss this backscattering background, followed by a discussion on the use of C_{phy} :[*chla*] as a proxy to investigate the seasonal evolution of phytoplankton photoacclimation, and how it informs the productivity of fall blooms.

2.4.2.1 Contribution of non-algal particles to total backscattering

All matter in the ocean scatters light, whether water molecules, sea-salt ions, or particles (Zhang et al., 2020). Natural aquatic assemblages have a variable pool of particle size, shape, and composition (organic/inorganic), which limit our ability to correctly interpret ocean color satellite observation of b_{bp} in terms of phytoplankton photo-physiologic aspects (Koestner et al., 2020; Organelli et al., 2018). Uncertainties on the use of b_{bp} to infer about phytoplankton community composition came from the intricate effect of non-algal particles (NAP), composed of organic detritus (e.g., heterotrophic organisms, fecal pellets, and cell debris) and inorganic sediments (e.g., clays, sand, calcite, and liths). For example, inorganic particles generally dominated the backscatter of assemblages because of the high refractive index of minerogenic particles, compared with organic-dominated assemblages (Koestner et al., 2020; Reynolds et al., 2016; Effler et al., 2013). Optically complex waters exhibit diverse particle types where phytoplankton and NAP represent varying proportions of the suspended particle pool, subject to potentially large and independent variations (Reynolds and Stramski, 2019). In order to get more insights about phytoplankton-related backscattering, we assessed from satellite ocean color data the NAP contribution on a pixel basis using an approach similar to that proposed by Bellacicco et al. (2018, 2020). The satellite-derived b_{bp}^k is the contribution of NAP to b_{bp} that does not covary with [chla]. Based on field observations, b_{hn}^k was calculated using an exponential equation with offset (Figure 25) reached better performance than the non-linear model proposed by Bellacicco et al. (2019) or the linear model of Behrenfeld et al. (2005). More importantly, we showed that b_{bp}^k varies in space and time (Figure 27,39, and 38) with the highest values obtained after the ice-edge bloom (in June or July) (excluding the nearshore coastal waters). This result may reflect the production of non-algal particles such as micrograzers, bacteria, viruses, cell debris, and fecal pellets during post-bloom conditions, reaching a contribution to b_{bp} of about 35%. The contribution of NAP, however, is relatively low compared to the global ocean, but similar to that reported in the productive waters of the North Atlantic (Bellacicco et al., 2018). At the ice edge in May, for example, we observed low b_{bp}^k : b_{bp} (Figure 38) and high [*chla*], which could involve two processes: i) ice-algae and sympagic communities are fast-sinking aggregates that quickly removed NAP from the pelagic to the benthic realm (Lannuzel et al., 2020; Trudnowska et al., 2021); ii) early ice retreat results on a faint manifestation of under-ice blooms and massive ice-edge blooms (Barbedo et al., 2020).

2.4.2.2 Satellite-derived C_{phy}:[chla] proxy

Provided that a satellite climatology successfully described the seasonality of b_{bp}^k and b_{bp} in HBS, C_{phy} :[chla] appeared as a robust proxy to investigate the seasonal evolution phytoplankton community size structure and photo-physiology in the summer-to-fall transition. However, we recognized that the conversion of b_{bp} to phytoplankton carbon may be controversial since is not possible to isolate the backscattering signal from phytoplankton cells alone (nor phytoplankton carbon from POC) from bulk measurements in the natural environment (Sathyendranath et al., 2009). Therefore, C_{phy} includes the contribution of all particles that co-vary with [chla]. Absolute values of C_{phy} :[chla] reported here (Figure 29) in spring and fall seasons, or in coastal waters, is in the lower range compared to the literature in the open ocean (Bellacicco et al., 2016; Sathyendranath et al., 2009), but similar to the range (10 to 60) reported for coastal waters of the North Baltic Sea (same latitude as the HB) (Jakobsen and Markager, 2016). A phytoplankton population composed of smaller cells backscatters more light than the one composed of larger cells, for an equal amount of chlorophyll present (Vaillancourt et al., 2004; Reynolds et al., 2016; Koestner et al., 2020). Low values of C_{phy}:[chla] probably indicate the presence of larger cells with low backscattering efficiency and high chlorophyll-a content that are typically found in low light environments and/or nutrient-replenished (mesotrophic or eutrophic) environments (Devred et al., 2006; Barbieux et al., 2018).

2.4.2.3 C_{phy}:[chla] seasonal variability

As exposed in Figure 29, the highest seasonal values of $C_{phy}:[chla]$ were associated with oligotrophy in the summer. Therefore, satellite ocean color observations highlighted the photo-acclimation strategy of phytoplankton communities to deal with the high summer irradiance and nutrient depletion in the upper layer of the HBS. Satellite observations and vertical profiles acquired in the spring-tosummer transition help us to improve our understanding of phytoplankton dynamics. In situ empirical relation of $b_{bp}(555)$, [chla] and PAR in distinct light attenuation environments of MIZ revealed that phytoplankton communities in the upper layer at high PAR levels had a relatively low intracellular pigment content and small size structure, consequently, high $b_{bp}^*(555)$ and $C_{phy}:[chla]$ (Figure 25). As reported by Westberry et al. (2008), for example, the upper layer phytoplankton community generally have low pigment content and small size structure cells to better deal with relatively high PAR, poor nutrient, and high wind-driven turbulence. On the other hand, the phytoplankton community around the SCM is photo-acclimatized to a balance between low PAR, relative high nutrient, high stratification, and low turbulence which result in relatively large cells and high chlorophyll-a intracellular content, i.e., relatively low $b_{bn}^*(555)$ and $C_{phy}:[chla]$ (Brewin et al., 2012; Barbieux et al., 2018).

During the fall season, a decrease of C_{phy} :[*chla*] and null stratification in the productive layer may indicate an advection/seeding of SCM communities to the first optical depth. Otherwise, climatology depicted photoacclimation as a seasonal process synchronized with solar elevation and nutrients in Hudson Bay. For example, low C_{phy} :[*chla*] in ice-edge bloom is likely due to high nutrient availability in a shallow mixed layer under the maximum seasonal light incoming in May and June. In summer, high C_{phy} :[*chla*] indicated the presence of small phytoplankton cells with relatively low intracellular chlorophyll pigments in oligotrophic domains under high PAR (Figure 21 and 28). Although very distinct water columns structure involve ice-edge and fall blooms, in general, similar and relatively low C_{phy} :[*chla*] in domains of severe oligotrophy during summer. Phytoplankton photoacclimation, size structure, and community were similar in ice-edge and fall blooms, (Figure 21, 28, and 29). In addition to that, a seasonal increment of C_{phy} together with [*chla*] (Figures 21 and 28), a decrease of b_{pp}^k (Figure 27) and its relative contribution to b_{pp} (Figures 39 and 38) support the hypothesis of a productive fall bloom.

2.5 Conclusions

The present study achieved a synergy between hydrodynamic modeling, climate reanalysis, oceancolor imagery, and in situ observations to better understand essential aspects of the phytoplankton dynamics, with special attention dedicated to the fall bloom phenomenon. Atmospheric cooling of the ocean and wind-driven turbulence can facilitate the transport of nutrients by mixed-layer deepening and pycnocline ventilation after the heat-flux inversion when the atmospheric cooling of the ocean began. However, the interplay of phytoplankton and atmospheric forcing is not straightforward in a region where both haline and thermal processes affect water-column stratification.

Satellite-based optical proxies revealed that phytoplankton communities with low carbon-to-chlorophyll ratio observed at the surface in the fall may be advected from the subsurface chlorophyll-*a* maximum to the depth visible by space-borne sensors. However, the significant increase in phytoplankton-related carbon concentration (while non-algal backscattering remained constant) indicated that these fall blooms are potentially productive. To quantify the relative importance of fall blooms in the Arctic and sub-arctic seas, the carbon-to-chlorophyll ratio can improve the parameterization of the phytoplankton primary production from satellite or coupled biogeochemical models (Sathyendranath et al., 2020; IOCCG, 2015).

The persistence of fall blooms can enhance the carbon pump and mitigate Arctic warming by removing greenhouse gases (carbon dioxide). However, the biochemical capability of the Arctic and sub-Arctic seas to assimilate high content of organic matter discharged by rivers and produced in situ by phyto-plankton blooms in this rapidly changing Arctic scenario remains an open topic.

2.6 Data Accessibility Statement

In situ backscattering coefficient and chlorophyll-*a* concentration in this research are made available through the BaySys data repository (open access).

2.7 Acknowledgments

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Additional information: http://umanitoba.ca/faculties/environment/departments/ceos/ research/BaySys.html.

2.8 Funding information

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2.9 Supplemental material

2.9.1 Evaluation of chlorophyll-a concentration ocean color satellite algorithms

We evaluated the semi-analytical model GSM (Garver and Siegel, 1997; Maritorena et al., 2002) and the empirical band-ratio algorithm recently proposed for the Arctic Ocean inflow and outflow ecoregions by Lewis and Arrigo (2020) (AOReg.emp). Since remote sensing can only estimate the surface concentration, we computed the chlorophyll-*a* concentration "seen" by a satellite sensor ([*chla*]_{*sat*}), using discrete samples analysed by HPLC (Morel and Berthon, 1989). [*chla*]_{*sat*} is a depth-weighted average for the "penetration depth" (z_{pd}), defined as the first optical depth: $z_{pd} = 1/kd(443)$) (Morel and Berthon, 1989):

$$[chla]_{sat} = \frac{\int_0^{z_{pd}} chla(z) e^{-2k_d z} dz}{\int_0^{z_{pd}} e^{-2k_d z} dz}$$
(2.9)

where chla(z) was optically weighted using z and $k_d(443)$ (i.e., $f(chla(z)_{HPLC}, k_d(443)))$).

A total of 13 stations from Hudson Bay where both HPLC and C-OPS data were available were used. Figure 30 shows that GSM (r^2 : 0.566, RMSD_{log} 0.290, bias_{log}: -0.097) reached similar performance of AOReg.emp (r^2 : 0.409, RMSD_{log} 0.305, bias_{log}: 0.083). These results indicate that both algorithms were slightly biased, but GSM was less scattered than the empirical algorithm. The GSM is more robust in coastal waters (pink symbols) compared to the empirical algorithm that produces very high [*chla*]. Knowing the case-2 nature of the HB, GSM was chosen for this study.

2.9.2 Wind direction effect on chlorophyll-*a* concentration

Coastal line orientation is a determinant for water column enrichment forced wind-driven coastal upwelling. The variability of wind directional components can define coastal areas under wind-driven coastal upwelling (Enriquez and Friehe, 1995). In addition to that, the orientation of sea-ice edges (Dumont et al., 2010) can also have similar effect during the sea-ice recovery at the end of the fallwinter transition. However, as illustrated in Figure 31, relations between time series of [*chla*], zonal (*u*), and meridional (*v*) wind components were difficult to assess in south Hudson Bay centered at $84^{\circ}W$ 57°N.


Figure 30: In situ evaluation of satellite-derived chlorophyll-*a* concentration algorithms. Evaluation of chlorophyll-*a* concentration ([*chla*]_{sat}, in mg m⁻³) derived from remote sensing reflectance (R_{rs} , in m⁻¹) using (A) the semi-analytical algorithm (GSM: Maritorena et al., 2002) and (B) the band ratio Arctic Ocean algorithm dedicated to inflow and outflow ecoregions (OCReg.emp: Lewis and Arrigo, 2020). R_{rs} was in-water derived from C-OPS profiles (Mueller et al., 2003). We simulated [*chla*]_{sat} using coefficient for light attenuation at 443 nm k_d (443) and profiles of HPLC pigments, similar proposed by Morel and Berthon (1989).

2.9.3 Water column structure evolution in the south Hudson Bay

Figures 32, 33, 34, 35, 36, and 37 show the water column structure evolution of potential temperature, salinity, stratification, and mixed layer depth, first optical depth, and euphotic zone, time-series of [*chla*], wind speed and heat flux between 2002 and 2008 (except for 2005) in the South Hudson Bay centered at 84°W 57°N.

2.9.4 Seasonal phytoplankton photo-acclimation

Nonparametric one-way analysis of variance and multi-statistic tests (MatLab functions: *anova1.m* and *multcompare.m*) of $b_{bp}(\lambda)$ and [*chla*] indicated that phytoplankton communities and bio-optics characteristics are significant are distinct between each months with a confidence interval of 95% (P < 0.05). Figure 38 show satellite-derived monthly climatologies of [*chla*], C_{phy} , C_{phy} :[*chla*] ratio, $b_{bp}(555)$, $b_{bp}^k(555)$; and $b_{bp}^k(555)$: $b_{bp}(555)$ ratio obtained from 1998 to 2018 in the Hudson Bay System. The Figure 39 shows monthly maps of satellite-derived climatology of $b_{bp}^k(555)$: $b_{bp}(555)$ ratio.



Figure 31: South Hudson Bay: phytoplankton dynamic and wind components. Time series of chlorophyll-a concentration ([*chla*]: mg m⁻³, green circles, and 7 days moving average in green line) from the semi-analytical algorithm (GSM: Garver and Siegel, 1997; Maritorena et al., 2002) of Globcolor project, wind u-component (daily in light blue line and 7 days moving average in blue line) and wind v-component (daily in light orange line and 7 days moving average in orange line) from the Canadian Meteorological Centre's Global Deterministic Prediction System Re-Forecasts (CGRF) between 2002 and 2009 in the south Hudson Bay (84°W and 57°N). Chlorophyll-a concentration trends ($\partial Chla(\partial t)^{-1}$) in the interval of confidence of 99% were plotted between maximum oligotrophic state in summer and fall (red line).



Figure 32: Atmosphere, ocean and phytoplankton, 2002. Influence of atmospheric forcing and water column structure on phytoplankton phenology: (A) time series of [*chla*] from Globcolor Project (GSM: Garver and Siegel, 1997; Maritorena et al., 2002) in log scale (daily in green squares, and 7-days moving average in green line), heat flux (HF: grey bars) and wind speed (daily in cyan line, and 7-days moving average in blue line) taken from the Canadian Meteorological Centre's Global Deterministic Prediction System Re-Forecasts (CGRF; Smith et al., 2014). Profiles in the color scale of (B) Brunt-Vaissala frequency (N^2), (C) salinity, and (D) temperature modeled using the Nucleus for European Models of the Ocean (NEMO). The vertical profiles had important layers for phytoplankton dynamics marked: satellite-derived first optical depth (z_{OC} : white line) and euphotic depth (z_{eu} : purple line); mixed layer depth (MLD: black traced line); and pycnocline (N_{max}^2 : black line).



Figure 33: Synergy of the sea-ice model, wind speed reanalysis, and ocean color satellites in south Hudson Bay, 2003. Influence of atmospheric forcing and water column structure on phytoplankton phenology: (A) time series of [*chla*] from Globcolor Project (GSM: Garver and Siegel, 1997; Maritorena et al., 2002) in log scale (daily in green squares, and 7-days moving average in green line), heat flux (HF: grey bars) and wind speed (daily in cyan line, and 7-days moving average in blue line) taken from the Canadian Meteorological Centre's Global Deterministic Prediction System Re-Forecasts (CGRF; Smith et al., 2014). Profiles in the color scale of (B) Brunt-Vaissala frequency (N^2), (C) salinity, and (D) temperature modeled using the Nucleus for European Models of the Ocean (NEMO). The vertical profiles had important layers for phytoplankton dynamics marked: satellite-derived first optical depth (z_{OC} : white line) and euphotic depth (z_{eu} : purple line); mixed layer depth (MLD: black traced line); and pycnocline (N_{max}^2 : black line).



Figure 34: Synergy of the sea-ice model, wind speed reanalysis, and ocean color satellites in South Hudson Bay, 2004. Influence of atmospheric forcing and water column structure on phytoplankton phenology: (A) time series of [*chla*] from Globcolor Project (GSM: Garver and Siegel, 1997; Maritorena et al., 2002) in log scale (daily in green squares, and 7-days moving average in green line), heat flux (HF: grey bars) and wind speed (daily in cyan line, and 7-days moving average in blue line) taken from the Canadian Meteorological Centre's Global Deterministic Prediction System Re-Forecasts (CGRF; Smith et al., 2014). Profiles in the color scale of (B) Brunt-Vaissala frequency (N^2), (C) salinity, and (D) temperature modeled using the Nucleus for European Models of the Ocean (NEMO). The vertical profiles had important layers for phytoplankton dynamics marked: satellite-derived first optical depth (z_{OC} : white line) and euphotic depth (z_{eu} : purple line); mixed layer depth (MLD: black traced line); and pycnocline (N_{max}^2 : black line).



Figure 35: Synergy of the sea-ice model, wind speed reanalysis, and ocean color satellites in South Hudson Bay, 2006. Influence of atmospheric forcing and water column structure on phytoplankton phenology: (A) time series of [*chla*] from Globcolor Project (GSM: Garver and Siegel, 1997; Maritorena et al., 2002) in log scale (daily in green squares, and 7-days moving average in green line), heat flux (HF: grey bars) and wind speed (daily in cyan line, and 7-days moving average in blue line) taken from the Canadian Meteorological Centre's Global Deterministic Prediction System Re-Forecasts (CGRF; Smith et al., 2014). Profiles in the color scale of (B) Brunt-Vaissala frequency (N^2), (C) salinity, and (D) temperature modeled using the Nucleus for European Models of the Ocean (NEMO). The vertical profiles had important layer for phytoplankton dynamics marked: satellite-derived first optical depth (z_{OC} : white line) and euphotic depth (z_{eu} : purple line); mixed layer depth (MLD: black traced line); and pycnocline (N_{max}^2 : black line).



Figure 36: Synergy of the sea-ice model, wind speed reanalysis, and ocean color satellites in South Hudson Bay, 2007. Influence of atmospheric forcing and water column structure on phytoplankton phenology: (A) time series of [*chla*] from Globcolor Project (GSM: Garver and Siegel, 1997; Maritorena et al., 2002) in log scale (daily in green squares, and 7-days movel average in green line), heat flux (HF: grey bars) and wind speed (daily in cyan line, and 7-days movel average in blue line) taken from the Canadian Meteorological Centre's Global Deterministic Prediction System Re-Forecasts (CGRF; Smith et al., 2014). Profiles in color scale of (B) Brunt-Vaissala frequency (N^2), (C) salinity, and (D) temperature modeled using the Nucleus for European Models of the Ocean (NEMO). The vertical profiles had important layer for phytoplankton dynamics marked: satellite-derived first optical depth (z_{oC} : white line) and euphotic depth (z_{eu} : purple line); mixed layer depth (MLD: black traced line); and pycnocline (N_{max}^2 : black line).



Figure 37: Synergy of the sea-ice model, wind speed reanalysis, and ocean color satellites in South Hudson Bay, 2008. Influence of atmospheric forcing and water column structure on phytoplankton phenology: (A) time series of [*chla*] from Globcolor Project (GSM: Garver and Siegel, 1997; Maritorena et al., 2002) in log scale (daily in green squares, and 7-days moving average in green line), heat flux (HF: grey bars) and wind speed (daily in cyan line, and 7-days moving average in blue line) taken from the Canadian Meteorological Centre's Global Deterministic Prediction System Re-Forecasts (CGRF; Smith et al., 2014). Profiles in the color scale of (B) Brunt-Vaissala frequency (N^2), (C) salinity, and (D) temperature modeled using the Nucleus for European Models of the Ocean (NEMO). The vertical profiles had important layers for phytoplankton dynamics marked: satellite-derived first optical depth (z_{OC} : white line) and euphotic depth (z_{eu} : purple line); mixed layer depth (MLD: black traced line); and pycnocline (N_{max}^2 : black line).



Figure 38: Seasonal influence of bio-optical properties in the Hudson Bay. Boxplots of satellite ocean color monthly climatology (May, June, July, August, September, and October) of (A) chlorophyll-a concentration ([*chla*]), (D) backscattering coefficient at 555 nm $(b_{bp}(55))$, (c) non-algal particle background contribution to backscattering at 555 nm $(b_{bp}^k(555))$, (d) relative contribution of NAP background to particle backscattering coefficient $(b_{bp}^k(555)/b_{bp}(555))$, in %), (E) phytoplankton carbon (C_{phy}), and (F) ratio phytoplankton carbon to chlorophyll (C_{phy} :[*chla*]) obtained between 1998 and 2018. Satellite-derived products were calculated using the semianalytical algorithm (GSM: Garver and Siegel, 1997; Maritorena et al., 2002) of the Globcolor Project merged daily 4 km products. The central red line marks are respective median, black ashes are averages, the edges of the blue boxes are the 25th and 75th percentiles, and the whiskers extend to the most extreme data points between $\pm 0.26\sigma$ considering a normal distribution.



Figure 39: Seasonal influence of non-algal particles on light backscattering coefficient. Satellite ocean color monthly climatology (May, June, July, August, September, and October) relative contribution of NAP to particle backscattering coefficient $(b_{bp}^k(555)/b_{bp}(555))$, in %) obtained between 1998 and 2018. $b_{bp}^k(555)$ were estimated using satellite-derived $b_{bp}(555)$ and [*chla*] calculated from the semi-analytical algorithm (GSM: Garver and Siegel, 1997; Maritorena et al., 2002) of the Globcolor Project merged daily 4 km products.

3

Sensitivity analysis of satellite-derived phytoplankton primary production in the eastern Canadian Arctic

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Abstract

Satellite ocean color radiometry (OCR) is a suitable tool for the systematic observation of phytoplankton production in open waters, even in harsh environments and ice-infested seas. In arctic and sub-arctic seas, global OCR algorithms for net phytoplankton primary production (NPP) may be biased due to polar communities adapted to low solar declination, the persistence of sub-surface chlorophyll-a maximum (SCM), under-ice production, and the presence of terrigenous optically active constituents. To understand how the interplays between oceanographic processes, marine bio-optics, phytoplankton dynamic, and photo-physiology impact the performance of satellite NPP assessment, we performed a sensitivity analysis of the Takuvik-UQAR satellite-based PP model using an in situ data set from Hudson Bay (BaySys, 2018), and Baffin Bay (Green Edge, 2016). To resolve phenological stages throughout marginal-ice zones, NPP models required an additional parametrization of the vertical distribution of chlorophyll at the early stages of SCM development, which represented a decrease from 0.53 to 0.23 g C m⁻² day⁻¹ (in RMSD, i.e., root mean squared difference between model and reference). Seasonal and regional variability of phytoplankton absorption $(a_{\phi}^*(\lambda))$, driven by different phytoplankton communities, had a minor effect on NPP accuracy. In contrast, to resolve photo-acclimation NPP, models must rely on accurate estimations for the photosynthetic parameters light saturation (E_k) and chlorophyll-*a* normalized maximum production rate (P_{max}^B) . We proposed a conciliation of carbon and chlorophyll production-production approaches using an E_k model that depends on the chlorophyll-specific backscattering coefficient at 555 nm (b_{bp}^* (555)) and the daily average of photosynthetic usable radiation, proxies of photo-physiology, intra-cellular pigment content, and size structure. P_{max}^{B} yields the largest uncertainties on NPP (RMSD between 0.45 to 0.75 g C $m^{-2} day^{-1}$) in marginal-ice zones. On the other hand, salinity explains 81% of P_{max}^{B} variability where sediments from continental drainage caused the re-mineralization of nutrients, e.g., river plumes and land-fast sea ice melting, which can compensate for errors of satellite derived-NPP associated with optically-complex waters in coastal waters.

Résumé

La radiométrie satellitaire de la couleur de l'océan (OCR) est un outil approprié pour l'observation systématique de la production phytoplanctonique dans les eaux libres, même dans les environnements difficiles d'accès et les mers infestées de glace. Dans les mers arctiques et subarctiques, les algorithmes OCR globaux pour la production primaire nette de phytoplancton (NPP) peuvent être biaisés en raison des communautés polaires adaptées à un faible éclairement solaire, à la persistance d'un maximum de chlorophylle-a (SCM) sous la surface, de la production primaire sous la glace et de la présence de constituants optiquement actifs d'origine terrigène. Pour comprendre comment les interactions entre les processus océanographiques, la bio-optique marine, la dynamique du phytoplancton et la photo-physiologie influent sur la performance de l'évaluation de la NPP par satellite, nous avons effectué une analyse de sensibilité du modèle Takuvik-UQAR concu pour estimer la NPP dans les mers arctiques. L'évaluation est réalisée à partir d'un ensemble de données in situ provenant de la baie d'Hudson (BaySys, 2018) et de la baie de Baffin (Green Edge, 2016). Pour résoudre les états trophiques changeants dans les zones de glace marginale, les modèles de PPN ont nécessité une paramétrisation supplémentaire de la distribution verticale de la chlorophylle dédiée aux premiers stades de développement des SCM, ce qui a représenté un gain de performance de 0.53 à 0.23 g C m⁻² jour⁻¹ (c'est-à-dire la différence quadratique moyenne (RMSD) entre le modèle et la référence) . La variabilité saisonnière et régionale de l'absorption phytoplanctonique due à une communauté phytoplanctonique différente a un effet mineur sur l'estimation de la PPN. Pour résoudre le problème de la photo-acclimatation, les modèles de PPN doivent aujuster les paramètres photosynthétiques que sont la saturation en lumière (E_k) et le taux de production maximal normalisé par la concentration chlorophylle-a (P^B_{max}) . Nous proposons une conciliation des approches de production de carbone et de chlorophylle à l'aide d'un modèle de E_k qui ingère le coefficient de rétrodiffusion spécifique de la chlorophylle à 555 nm $(b_{hn}^*(555))$ et le rayonnement photosynthétique utilisable moyen quotidien, proxies de la photo-physiologie, du contenu en pigments intracellulaires et de la structure de taille. P_{max}^{B} s'est avéré donner les plus grandes incertitudes sur la NPP (RMSD entre 0,45 et 0,75 g C m⁻² jour⁻¹), mais aucune relation n'a été trouvée entre P_{max}^{B} et les variables environnementales. D'autre part, une relation linéaire inverse entre la salinité et la P^B_{max} a été observée ($r^2=0.81$), probablement provoqué par les apports continentaux ou la re-minéralisation des nutriments, par exemple, les panaches fluviaux et la fonte rapide de la glace de mer, qui peut compenser les erreurs de la PPN dérivée par satellite associées aux eaux optiquement complexes dans les eaux côtières.

3.1 Introduction

Arctic air temperature warming and sea-ice loss are the most prominent manifestations of climatic changes in the last decades on Earth's system (Lannuzel et al., 2020). The pan-Arctic air temperature rising rate is two-fold that observed on the global scale. The velocity and severity of trends are compared to abrupt changes during the last glacial period, in the Dansgaard–Oeschger events 120,000–11,000 years ago (Jansen et al., 2020). Global climate, teleconnections, and regional processes like sea-ice albedo feedback, remobilization of permafrost organic carbon (Bader, 2014), and atmospheric vertical lapse-rate feedback (Pithan and Mauritsen, 2014) amplify Arctic warming driving dramatic and unprecedented changes in north-polar seas (Ardyna and Arrigo, 2020; IOCCG, 2015; Arrigo, 2013; Wassmann, 2011). Global ocean phytoplankton production ranged between 38.8 to 42.1 Gt Carbon per year between 1998 and 2018 (Kulk et al., 2020). Although climatic fluctuations and seasurface warming have driven a decline in ocean production over the past century (Boyce et al., 2010), recent trends obtained from satellites in the Arctic Ocean reported an increasing trend of 21.5% in chlorophyll-*a* concentration ([*chla*]) and 56.5% in integrated-annual production between 1998 and 2018 (Lewis and Arrigo, 2020).

Arctic primary production (PP) raised 20% for each drop of 10^6 km^2 of sea-ice coverage between 2003 and 2007 (Arrigo and van Dijken, 2015). Arctic sea-ice declined ~ $2.0 \times 10^6 \text{ km}^2$ during the satellite era between 1979 and 2017 (Brennan et al., 2020) at a rate of -4.57% per decade (Comiso et al., 2017). The timing of the Arctic-wide melt season has been anticipated at a rate of 5 days per decade since 1979 (Stroeve et al., 2014). Sea ice is melting earlier, freezing later, and the open-water season is extending (Ardyna and Arrigo, 2020). A decrease in sea-ice thickness, snow-layer depth, timing shifts of melt, and drainage onsets allow more light to penetrate into the ice-pack and reach the upper ocean layer (Babin, 2020; Tedesco et al., 2019; Horvat et al., 2017; Leu et al., 2015). When sea-ice retreats, the sea surface releases stocked heat, producing water vapor, clouds, and fog, reducing the incoming light in ice-edge zones (Bélanger et al., 2013). Besides, the continuum water-column heating during the open-water season forces a convey of water vapor to the atmosphere (Laliberté et al., 2021). However, the lengthening of the open water season has augmented the annual light incoming into the Arctic pelagic ecosystems (Ardyna and Arrigo, 2020; Arrigo et al., 2020; Lewis and Arrigo, 2020; Stroeve et al., 2020; Horvat et al., 2017).

The main processes controlling the recent arisen of phytoplankton production in Arctic Ocean are nutrients input from continental drainage (Terhaar et al., 2021; Arrigo et al., 2020), sea-ice losses allowing an increasing of light incoming in the upper ocean layer (Ardyna and Arrigo, 2020; Arrigo et al., 2020; Lewis and Arrigo, 2020; Stroeve et al., 2020; Horvat et al., 2017). However, the assessment of total phytoplankton production relies on how ocean color satellites can resolve the interplays between ecosystem and photo-physiology in the wide range of light environments of north polar seas (IOCCG, 2015).

Pan-Arctic net primary production (NPP) can only be assessed from satellite observations or ocean modeling (Babin et al., 2015). However, global standard ocean color algorithms on which satellitederived NPP rely, and even general Arctic-adapted ones, can fail to estimate bio-optical properties with acceptable accuracy in the Arctic and adjacent polar seas (Lee et al., 2015). This can be explained by the presence of colored dissolved organic matter (CDOM) and non-algal particles (NAP) that are often dominant in north polar seas, which can lead to an overestimation of phytoplankton biomass (i.e, chlorophyll-*a* concentration, [*chla*]) (IOCCG, 2015; Hirawake et al., 2012). For example, the significant CDOM absorption in the blue bands can lead up to a five-fold overestimating of [*chla*] in coastal waters influenced by large river input, as in the southeastern Beaufort Sea (Ben Mustapha et al., 2012).

Besides [*chla*] and bio-optical properties of the water column, NPP estimation from space need assumptions on phytoplankton photosynthetic efficiency to harvest light and fixed the carbon dioxide, which depends on species, size structure, and photoacclimation. Ocean processes that control light, nutrients, stratification, and grazing force phytoplankton communities to adjust their physiology, species composition, and structure. In turn, the dynamic of phytoplankton influences ecological links, the biological carbon pump, and ecosystem functioning, and consequently, branches the climatic change impact on all life in polar seas. Phytoplankton strategies of photo-physiological acclimation to environmental conditions challenge satellite-ocean color algorithms (Lin et al., 2016). To photoacclimate to environmental conditions, phytoplankton communities adjust the carbon-to-chlorophyll ratio (Bellacicco et al., 2020; Behrenfeld et al., 2005), spectral absorption through pigments production (Brunelle et al., 2012; Matsuoka et al., 2011, 2007; Bricaud et al., 1998), size and taxonomic structure (Hirata and Suzuki, 2017; Lacour et al., 2017; Devred et al., 2016; Uitz et al., 2008; Claustre et al., 2005). As a result, photosynthetic parameters such as the light saturation index and the maximum photosynthetic production will vary (Bouman et al., 2017; Richardson et al., 2016; Huot et al., 2013; Arrigo et al., 1998), as well as their vertical distribution (Bouman et al., 2020; Moeller et al., 2019; Ardyna et al., 2013).

In north polar seas, extreme conditions such as low solar elevations, sea-ice, low temperature, the predominance of optical complex waters, and abrupt trophic transitions (e.g., marginal-ice zones, summer oligotrophic set up with the development of sub-surface chlorophyll-*a* maximum (SCM), and fall blooms) produce unique phytoplankton photosynthetic parameters, bio-optics, and a very dynamic photo-physiology (IOCCG, 2015). Therefore, the performance of satellite NPP models rely on regional tuning, dynamic adjustment to the bio-optical complexity of marine environments, and resolving photophysiology in north polar seas (Lombard et al., 2019; Lewis et al., 2019; Graff and Behrenfeld, 2018; Demidov et al., 2017; Lacour et al., 2017; Babin et al., 2015; IOCCG, 2015; Lee et al., 2015).

There is a wide range of ocean color remote sensing NPP models applied to the Arctic Ocean (Babin et al., 2015; Lee et al., 2015). For instance, the models are often grouped as depth-resolved model (DIM), vertically generalized production model (VGPM: Behrenfeld and Falkowski 1997), wavelength-resolved model (WIM: Morel 1991; Platt and Sathyendranath 1988), and carbon-based productivity model (CbPM: Behrenfeld et al. 2005). However, they ingest similar parameters to resolve phyto-plankton carbon production such as satellite-derived [*chla*], photosynthetic active radiation (PAR), and production versus irradiance (P–E) curve parameters (Babin et al., 2015). Lee et al. (2015) evaluated the performance of more than 30 NPP models applied to the Arctic waters. They showed that models tuned for the Arctic region performed slightly better than other models. Among the tested model, the WIM model of Bélanger et al. (2013), based on the formulation proposed by Platt et al. (1980), provided relatively good performance. This model has been further developed and improved

over recent years at UQAR-Takuvik and was recently used to study north polar primary productivity (Mayot et al., 2020; Vernet et al., 2021). Here we used this model together with recent *in situ* observations to evaluate its sensitivity to the parameterization and to improve its performance in the Canadian Arctic.

To do so, we performed a sensitivity analysis of the UQAR-Takuvik NPP model to parametrizations based on recent bio-optical observations from the Nelson River plume (Jacquemot et al., 2021; Smith et al., 2017; Sergeant, 1973), the Kivalliq polynya in northwestern Hudson Bay (Bruneau et al., 2021; Landy et al., 2017), and marginal-ice zones (MIZ) in the Hudson Bay (Matthes et al., 2021; Barbedo et al., 2020) and the Baffin Bay (Randelhoff et al., 2019; Oziel et al., 2019). These regions were sampled during the spring-to-summer transition (June) and encompass a wide range of key marine ecosystems found in the eastern Canadian Arctic. The specific objectives of the study were three-fold: I) to assess the performance of parameterizations of chlorophyll-*a* vertical distribution, photosynthetic production vs. irradiance curves, and light profiles using in situ bio-optics and radiometry; II) to tune a satellite-derived phytoplankton production model to MIZ in the Canadian eastern Arctic (ECA), and III) understand how interplays of environmental conditions and phytoplankton photo-physiology impact NPP satellite retrievals.

In the following sections, we first present the field methods (section 3.2.1) including phytoplanktonrelated parameters (pigments, taxonomy, and size structure) and the in-water radiometry. The NPP model formulation, parameters, and evaluation metrics are presented in section 3.2.2. Section 3.3 presents the sensitivity analysis methodology in more detail, which includes a reference simulation and a series of perturbed simulations to assess the impact of each parameter on the NPP estimations. The results are presented in three subsections starting with a description of the distinct light environments contemplated in the BaySys 2018 and GreenEdge 2016 oceanographic expeditions (section 3.4.1), followed by the results of the sensitivity analysis (section 3.4.2), phytoplankton community structure and taxon (section 3.4.3). Finally, we discussed how uncertainties are propagated on NPP satellite assessments (sections 3.5.1), how interplays of oceanographic processes, phytoplankton taxonomy, photo-physiology, and vertical distribution influence satellite-derived primary production (sections 3.5.2 and 3.5.3).

3.2 Material and methods

3.2.1 Field observations

In situ data used to perform the sensitivity analysis came from two major oceanographic expeditions carried on the Canadian icebreaker *CCG Amundsen* in Hudson Bay System (BaySys project: June 2018) and Baffin Bay (GreenEdge project: June 2016). The sampling locations are presented in Figure 40.

3.2.1.1 Phytoplankton characterization

The NPP model relies on phytoplankton abundance as quantified using the chlorophyll-*a* pigment concentration, optical properties, and photosynthesis efficiency. Here we present the chemical, optical, physiological, and biological properties of phytoplankton obtained from the field observations.

3.2.1.2 Taxonomy

Phytoplankton taxonomic analyses were conducted with seawater samples collected in Niskin bottles near the surface (5 m) and targeting the sub-surface chlorophyll maximum depth. Samples were fixed with Lugol's acid iodine solution and stored in the dark at room temperature until analysis. Phytoplankton cells were enumerated and identified to species level using inverted microscope model Nikon Eclipse TS100, and abundances for each taxon were expressed as a number of cells per liter of seawater (Utermohl, 1958; Lund et al., 1958). Phytoplankton was further categorized into major taxonomic groups and total individual abundance was calculated. These groups are Diatoms (*Bacillariophyceae*),Dinoflagellates (*Dinophyceae*),Coccolithophores (*Prymnesiophyceae*), Phaeocystis, Cryptomonads (*Cryptophyceae*), Chrysophytes (*Chrysophyceae*), Prasinophytes (*Prasinophyceae*), and Chlorophytes (*Chlorophyceae*).



Figure 40: Bio-optical stations of BaySys Expedition (2018) and GreenEdge Expedition in Baffin Bay (2016). Sampling locations from GreenEdge and BaySys expeditions overlaid on bathymetry. Chlorophyll-*a* concentration in the first week of June was obtained from (GSM: Garver and Siegel 1997; Maritorena et al. 2002) algorithm of Globcolour Project. The symbols and colors of the station indicate the light environment as derived from in-water radiometry described in section 3.2.1.3

3.2.1.2.1 Pigment analysis Chlorophyll-*a* concentration and accessory pigments assemblage were measured from discrete samples by the High-Performance Liquid Chromatography (HPLC) technique. In Hudson Bay, we collected water samples at the optical depths of 100% (i.e., sea surface, n. 33), 30% (13.8±10.2 m, n. 32), 15% (15.2±3.2 m, n. 17), 5% (36.1±7.8 m, n. 17), 1%, and 0.2% (52.0±10.6 m, n. 12). In Baffin Bay, each station have 10 samples collected at depths regular spaced from surface to 120 m. A volume of seawater (1–3 L) was collected using a Niskin bottle and filtered onto Whatman GF/F filters (25 mm in diameter) under a gentle vacuum (~ 3.98 Hg). The filters were put immediately in 2 mL cryovials, flash-frozen in liquid nitrogen, and then stored at -80°C until analysis. More details on the analytic methods can be found in Matthes et al. (2021) for the BaySys, and in Ras et al. (2008) for the GreenEdge data sets, respectively. Briefly, the filters were extracted in 100% methanol at -20°C, disrupted by sonication, and clarified later. Extraction time lasted 2 hours and HPLC analysis was carried out the same day (Ras et al., 2008; Tran et al., 2013; Robinson et al., 2018). In this study, [*chla*]_{HPLC} corresponds to the sum of chlorophyll-*a*, divinyl-chlorophyll-*a*, and chlorophyllide-*a*.

3.2.1.2.2 Light absorption spectra The phytoplankton spectral light absorption coefficient $(a_{\phi}(\lambda), \text{ in m}^{-1})$ was calculated by the sum of chemotaxonomic pigment (i.e., chlorophylls and caratenoids) specific spectrum $(a_{\phi,i}^*, \text{ in m}^2 \text{ mg}^{-1})$ obtained in Clementson and Wojtasiewicz (2019) weighted by their respective concentrations $(C_i, \text{ in mg m}^{-3})$ (Equation 3.1):

$$a_{\phi}(\lambda) = \Sigma C_i a_{\phi,i}^*(\lambda) \tag{3.1}$$

3.2.1.2.3 Phytoplankton community size structure To compute the phytoplankton community size structure, we used the accessory pigments: fucoxanthin (Fuco), peridinin (Peri), 19'-hexanoylyfucoxantin (Hex), 19'-butanoyloxyfococanthin (But), alloxanthin (Allo), total chlorophyll*b* (TChlb: sum of monovinyl, and divinyl forms), and zeaxanthin (Zea). As proposed by Vidussi et al. (2001) to investigate the effect of physical processes on algae dynamics in the Mediterranean Sea and applied by several authors in the Arctic (e.g., Huot et al. 2013; Reynolds and Stramski 2019). Phytoplankton community size structure was clustered into three size classes: micro-plankton (D >20 μ m), nano-plankton (D: $2 - 20 \ \mu$ m), and pico-plankton (D <2 μ m), where D indicates the cell diameter. Size structure was calculated using seven accessory pigments and weighting coefficients to represent average ratios between the concentrations of chlorophyll-*a* and each diagnostic pigment from HPLC analysis:

$$f_{micro} = (1.41 \ Fuco + 1.41 \ Peri) / \Sigma DP$$
 (3.2)

$$f_{nano} = (0.6 Allo + 0.35 But + 1.27 Hex) / \Sigma DP$$
(3.3)

$$f_{pico} = (0.86 zea + 1.01 TChlb) / \Sigma DP$$
(3.4)

where ΣDP is the sum of the weighted concentration of all seven diagnostic pigments:

$$\Sigma DP = 1.41 \ Fuco + 1.41 \ Peri + 0.60 \ Allo + 0.35 \ But + 1.27 \ Hex + 0.86 \ Zea + 1.01 \ TChlb$$
 (3.5)

3.2.1.2.4 Phytoplankton production vs. irradiance (P-E) curves Photosynthesis versus irradiance (P-E curves) parameter was determined based on fixation rates of carbon isotope 14 (¹⁴C). The method of Babin et al. (1994) was adopted for both cruises. Matthes et al. (2021) described the method for the BaySys cruise in detail. Briefly, six water samples were taken using Niskin bottles at the optical depths of 100%, 30%, 15%, 5%, 1%, and 0.2%. Each sample was sub-sampled into 12 clear cultures flasks of 50 ml (i.e., 6 in duplicate for each light level) and one opaque flask. Culture flasks were inoculated with inorganic ¹⁴C in the form of NaH¹⁴CO₃, which concentration ranged between 0.2 and 1.0 μ C mL⁻¹ depending on the phenological stage and the incubation period-length. In an incubation chamber (Babin et al., 1994), flasks were exposed to irradiance levels decreasing from 860 to 0 mumol photons $m^{-2} s^{-1}$ at -1.6°C during 2–4 hours. The protocol allows the determination of one P-E curve per depth sampled (Huot et al., 2013; Babin et al., 1994). Photosynthetic parameters include the phytoplankton light saturation index (E_k in μ mol photons m⁻² s⁻¹) and the maximum production rate normalized by $[chla]_{HPLC}$ (P^B_{max} in g C g Chla⁻¹ h⁻¹) estimated from P–E curves fitted into the original equation of Platt et al. (1980) (see section 3.2.2 below). A total of 101 and 185 P-E curves were obtained for the BaySys and GreenEdge expeditions, respectively. The photoinhibition parameter for phytoplankton production (β^B) was not accounted for because values were close to 0 for phytoplankton in the water column in Hudson Bay (Matthes et al., 2021) and the Baffin Bay.

3.2.1.3 In water radiometry

The downwelling in-water irradiance $(E_d(z, \lambda) \text{ in } \mu \text{W m}^{-2} \text{ nm}^{-1})$ and upwelling in water radiance $(L_u(z, \lambda) \text{ in } \mu \text{W m}^{-2} \text{ nm}^{-1} \text{ sr}^{-1})$ were measured by Compact-Optical Profiling System (C-OPS: Hooker et al. 2013) built by Bio-Spherical Instruments Inc. (San Diego, California, USA). C-OPS has 19 bands distributed between the spectral range of 320 to 865 nm measuring the planar downwelling irradiance and upwelling radiance coupled with auxiliary sensors for water temperature, pressure, pitch, and roll. A reference sensor measured above-water surface downwelling irradiance $E_d(0^+, \lambda)$ from the ship deck. Above water reference sensor were coupled to the Bioshade facility to measure the ratio of sun direct to diffuse sky irradiation $(E_{d sun}/E_{d sky})$ (Morrow et al., 2010). which is used to correct the subsurface $L_u(z, \lambda)$ from instrument self-shadow (Zibordi and Ferrari, 1995).

We profiled consecutive downcasts (at least 3 profiles) between the sea surface and a variable water depth corresponding to the level of 1% of light in relation to the surface from the Amundsen's front deck. In some GreenEdge stations, C-OPS was deployed from a barge (~12 m), avoiding the ice-breaker shadow, and other large ship perturbation, for example, additional turbulence in the mixed layer. In-water quantities (\Re) were normalized to account for the instantaneous illumination variations during each cast using simultaneous above downwelling irradiance (Equation 3.6):

$$\Re(z,\lambda,t_0) = \Re(z,\lambda,t) \frac{E_d(0^+,\lambda,t_0)}{E_d(0^+,\lambda,t)},$$
(3.6)

where $\Re(z, \lambda, t_0)$ identifies the radiometric parameters as they would have been recorded at all depths z at the same time t_0 of the start of acquisitions. Underwater casts trespassing a vertical tilt of 5° were removed from the analysis. $L_u(z, \lambda)$ was corrected for in-water optical instrument self-shading using the model developed by Gordon and Ding (1992) as implemented following Zibordi and Ferrari (1995). In-water radiometry was processed using a Matlab script based on the R-package COPS available in https://github.com/belasi01/Cops. A detailed discussion about the C-OPS instrument and the processing protocols can be found elsewhere (Bélanger et al., 2017; Antoine et al., 2013; Hooker et al.,

2013; Morrow et al., 2010; Mueller et al., 2003). The apparent optical properties (AOPs) relevant for this study are the remote sensing reflectance, $R_{rs}(\lambda)$ and the diffuse attenuation coefficient $k_d(\lambda)$ as detailed below.

3.2.1.3.1 Remote sensing reflectance To obtain $R_{rs}(\lambda)$ from in-water radiometry, the justbelow surface-upwelling radiance $(L_u(0^-, \lambda))$ must be extrapolated from a sub-surface layer using a linear fit of $\ln[L_u([z \ 0^-], \lambda)]$ (Mueller et al., 2003). However, light fluctuations caused by surface waves, the so-called lens effect or wave-focusing effect (Zaneveld et al., 2001), difficult the extrapolation of $L_u(z, \lambda)$ to $L_u(0^-, \lambda)$. The linear decay of $ln[L_u([z \ 0^-], \lambda)]$ can be poorly constrained or even unacceptable when a very thin layer is determined or, on the other hand, a thick layer is unfitted by an eventual non-homogeneity between upper- and near-surface in-water layers. We implemented an automatic procedure to select the ideal layer to extrapolate $L_u(0^-, \lambda)$. It is based on the stable relation between in-water $(E_d(0^-, \lambda))$ and above-water irradiances $(E_d(0^+, \lambda))$, which is less affected by surface lens effect. Considering that, $E_d(z, \lambda)$ just-below (at null depth $z = 0^-$) and -above the sea surface $(z = 0^+)$ simultaneously measured must respect the Equation 3.7:

$$E_d(0^-, \lambda) \sim 0.97 \ E_d(0^+, \lambda)$$
 (3.7)

where, the constant 0.97 accounts for the air-sea transmittance and Fresnel reflectance for profiles under solar elevations above 30° (Mueller et al., 2003), and low-to-moderate wind speed, which were the atmospheric-ocean state of all stations analyzed (Lukovich et al., 2021). $E_d(0^-, \lambda)$ was obtained from linear fits of $\ln[E_d([z_i \ 0^-], \lambda)]$ using variable vertical layer lengths (z_i) between 0.1 and 5 m ranging in an interval of 0.1 m for each band. The extrapolation-interval appropriateness was determined if $E_d(0^-, \lambda)$ derived from in water profile of length z_i and $E_d(0^+, \lambda)$ measured above-water in the ship deck satisfied the Equation 3.7 within 5% (Hooker et al., 2013) and r² of 0.99 (Bélanger et al., 2017; Antoine et al., 2013), $L_u(0^-, \lambda)$ was extrapolated from this layer using a linear-fit for $\ln[L_u([z \ 0^-], \lambda)]$. Otherwise, we excluded the profile from the analysis.

After having identified the subsurface layer that best reproduced the Equation 3.7. The water-leaving

radiance, $L_w(0^+, \lambda)$ was derived from $L_u(0^-, \lambda)$ using the air-sea interface relation in the Equation 3.8:

$$L_w(0^+, \lambda) = 0.54 \ L_u(0^-, \lambda) \tag{3.8}$$

where the constant 0.54 accounts for the partial reflection and transmission of the upwelled radiance through the sea surface (Mueller et al., 2003). In summary, this method is similar to the one initially proposed by Antoine et al. (2013) and modified by Bélanger et al. (2017) (see also section 3.7.1 in the supplementary material that compares the methods).

Finally, for each station, $R_{rs}(\lambda)$ was calculated from the average of distinct profiles using the $L_u(0^+, \lambda)$ to $E_d(0^+, \lambda)$ ratio (Equation 3.9):

$$R_{rs}(\lambda) = L_w(0^+, \lambda) / E_d(0^+, \lambda)$$
(3.9)

 $R_{rs}(\lambda)$ were used to classify the stations into the case-1 and case-2 water type scheme developed by Lee and Hu (2006) based on the remote sensing reflectance spectral ratios 412 to 443 and 555 to 490 nm. In addition to case-1 water type, the method distinguish Case-2 waters into two categories for turbid or CDOM-dominated waters (Supplemental Material, Section 3.7.2).

3.2.1.3.2 Diffuse light attenuation and optical classification The coefficient for diffuse attenuation of spectral downwelling irradiance $(k_d(\lambda))$ at a geometric depth is defined as:

$$k_d(z,\lambda) = -\frac{1}{E_d(z,\lambda)} \frac{\partial E_d(z,\lambda)}{\partial z}$$
(3.10)

As proposed by Mueller et al. (2003), $k_d(\lambda)$ was computed as the local slope of $\ln [E_d(z, \lambda)]$ versus depth using a linear regression fit, and assuming a constant $k_d(z, \lambda)$ within the interval of depths $(z_m - \Delta z) \le z \le (z_m + \Delta z)$ where z_m is the central depth (Equation 3.11):

$$\ln[E_d(z,\lambda)] = \ln[E_d(z_m,\lambda)] - (z - z_m) k_d(z_m,\lambda)$$
(3.11)

In this study, $k_d(\lambda)$ referred to as the depth-integrated value of $k_d(\lambda)$ for the surface layer spanning for the very surface (0⁻) to the depth where E_d is reduced to 10% of its surface value ($E_d(0^-)$). This layer contributes most to the water column photosynthesis and signals measured by remote sensors (Lee et al., 2005).

 $k_d(\lambda)$ was used to classify the 54 stations into PAR attenuation classes. This was done using a k-means cluster analysis, which takes into account the spectral shape and the magnitude of $k_d(\lambda)$ (Antoine et al., 2013; Solonenko and Mobley, 2015). Figures 41-A and B show $R_{rs}(\lambda)$ and $k_d(\lambda)$ grouped according to the attenuation magnitude and shape. Six optical classes were obtained, which are briefly presented here.

- **Marginal-ice zone** (**MIZ**) (high, moderate, and low light attenuation): In the MIZ, three levels of attenuation can be distinguished: high (black), moderate (blue), and low (cyan) light attenuation). These stations were profiled in a wide range of sea-ice conditions ranging from fully covered by sea-ice (small-leads open by the icebreaker), natural leads (scale of 1 km), ice edges, and open-water. Sea ice was in distinct thermodynamic stages such as melt ponds, sea ice fractured, broken, and re-freezed in winter;
- **Nelson River sediment plume:** This class includes four shallow and extremely turbid waters stations (red) influenced by sediment re-suspension due to wind mixing and tidal cycles;
- **Nelson river phytoplankton bloom:** Two stations with eutrophic conditions were observed just outside the Nelson river plumes (green). The ecological importance of these stations was highlighted by the presence of hundreds of Belugas (*Delphinapterus leuca*);
- **Southern HB coastal waters:** Stations profiled in natural leads surrounded by sea-ice load sediment (Harasyn et al., 2019), and in the open water region under the influence of the Nelson River plume. The particle backscattering coefficient is high in southern HB (pink) because the Nelson River plume and landfast ice release minerogenic particles and nutrients, the last intensifying the phytoplankton production.

3.2.1.3.3 Photosynthetic usable radiation (PUR) The PP model used in this study is based on photosynthetic usable radiation (PUR) rather than photosynthetic active radiation (PAR) to account for the spectral absorption of phytoplankton. It is similar to PAR (about 35% lower; Huot et al. 2013), except that PUR is weighted by the phytoplankton normalized absorption spectra and represents the subset of PAR that is readily absorbed by phytoplankton, as described by Morel (1978). Therefore, PUR varies as a function of spectral PAR and $a_{\phi}(\lambda)$ normalized by its peak in blue spectrum at 443 nm ($a_{\phi}(443)$).

The instantaneous photosynthetic usable radiation (PUR(z,t): in μ mol photons m⁻² s⁻¹) was computed from scalar irradiance ($E_o(z, \lambda, t_0)$). To estimate $E_o(z, \lambda, t)$, $E_d(z, \lambda, t)$ was divided by the meancosine of downwelling irradiance ($\overline{\mu}_o$) (Morel, 1991). For that, we applied the approximated expression $\overline{\mu}_o \sim (a_t + b_{bt})/k_d$ (Sathyendranath et al., 1989) using either measured or modeled values for $a_t(\lambda)$, $b_{bt}(\lambda)$, and $k_d(\lambda)$. When apply to remote sensing data, those parameters can be derived from R_{rs} using quasi-analytical algorithms (QAA: Lee et al. 2005. PUR(z,t) was calculated in the daylight period (i.e., θ_s above the horizon) in the visible spectrum from 400 to 700 nm by trapezoidal integration, after applying the factor $cos(\theta_s(t))/cos(\theta_s(t_0))$, where θ_s is the solar zenith range in the daytime (t). $\theta_s(t_0)$ is the solar zenith at the start time of light profile acquisitions, t_0 , of the cast (Reda and Andreas, 2004) (Equation 3.12):

$$PUR(z,t) = \left[\frac{\cos\theta_s(t)}{\cos\theta_s(t_0)}\right] \frac{1}{\hbar c} \frac{1}{N} \lambda \int_{400}^{700} \frac{a_\phi(\lambda)}{a_\phi(443)} E_o(\lambda, z, t) \quad d\lambda$$

$$= \left[\frac{\cos\theta_s(t)}{\cos\theta_s(t_0)}\right] \frac{1}{\hbar c} \frac{1}{N} \lambda \int_{400}^{700} \frac{a_\phi(\lambda)}{a_\phi(443)} \frac{E_d(\lambda, z, t)}{\overline{\mu}_o(\lambda)} \quad d\lambda$$
(3.12)

where \hbar is the plank constant (6.623×10⁻³⁴ J s⁻¹), *c* is the constant for the light speed (2.998×10⁸ m s⁻¹), and *N* is the Avogadro number (6.022×10²³). The conversion from mol to μ mol was applied (1×10⁶). In the NPP analysis below, $E_d(\lambda, z, t)$ was either measured using the C-OPS, or modeled from surface irradiance and k_d using the Equation 3.13:

$$E_d(\lambda, z, t) = E_d(\lambda, 0^-, t) e^{-k_d(\lambda)z}$$
(3.13)

3.2.2 Net primary production (NPP) modeling

3.2.2.1 Model formulation and parameters

The primary production model of UQAR-Takuvik (Bélanger et al., 2013) used in this study is based on the model of Platt et al. (1980). It describes the mass of organic carbon photosynthetically fixed per unit water volume occurring locally at a depth *z* and time instant *t* (PP(z, t), mg C m⁻³ s⁻¹) as presented in the Equation 3.14:

$$PP(z,t) = P^{B}_{max}(z) \ chla(z)(1 - e^{-PUR(z,t)/E_{k}(z)})$$
(3.14)

NPP model inputs can be summarized as follow:

chla(*z*): a vertical profile of chlorophyll-*a*, which can be measured or modeled (in mg Chla m^{-3});

 $E_k(z)$: a vertical profile of light saturation index (in mol photons m⁻² s⁻¹);

 $P^B_{max}(z)$: a vertical profile of normalized maximum production rate (in g C [g Chla m⁻³]⁻¹ h⁻¹);

- PUR(z, t) a vertical profile of photosynthetic usable radiation (in mol photons m⁻² s⁻¹), which is calculated using eq. 3.12 that requires itself the following inputs:
 - $E_o(\lambda, z, t)$: a vertical profile of scalar irradiance (in mol photons m⁻² s⁻¹), which can be measured directly from E_d profiles or calculated from surface irradiance spectra with a diffuse attenuation coefficient ($k_d(\lambda)$) using eq. 3.13, and an average cosine coefficient ($\overline{\mu}_o(\lambda)$);
 - $a_{\phi}(\lambda, z)$: a phytoplankton absorption spectra (in m⁻¹), which can vary as a function of [*chla*] (e.g., Bricaud et al., 1998; Matsuoka et al., 2011);

Obviously, obtaining vertical profiles of all these input parameters from space is impossible. Some of these parameters can be derived directly from the spectral remote sensing reflectance (e.g., surface *chla*, k_d). At the same time, others have to rely on *in situ* measurements or empirical relationships involving environmental variables (e.g., sea surface temperature, mixed layer depth). The sensitivity analysis presented in section 3.2.2 consists in testing different approaches to assessing the inputs of the NPP model (eq. 3.14).

3.2.2.2 Model skill and statistics for error analysis

Satellite-derived production model skill was assessed using root-mean-square difference (RMSD) between a given model configuration (NPP_{mod}) and a reference value of NPP based on *in situ* observations (NPP_{ref}; see section 3.3.1 for details):

$$\mathbf{RMSD} = \left(\frac{1}{N} \sum_{i=1}^{N} \left(\mathbf{NPP}_{mod, i} - \mathbf{NPP}_{ref, i}\right)^2\right)^{1/2}$$
(3.15)

where N is the number of observations. Generally, the smaller the RMSD, the better model performs. To measures how well mean and variability are modeled, we applied the bias (B) and unbiased root mean square error (URMSD, often refereed to as centred RMSD) as shown in the respective Equations 3.16 and 3.17):

$$bias = \overline{NPP}_{mod} - \overline{NPP}_{ref}$$
(3.16)

$$\text{URMSD} = \left(\frac{1}{N} \sum_{i=1}^{N} \left[(\text{NPP}_{mod, i} - \overline{\text{NPP}}_{mod}) - (\text{NPP}_{ref, i} - \overline{\text{NPP}}_{ref}) \right]^2 \right)^{1/2}$$
(3.17)

The σ_{ref} and σ_{mod} are standard deviation of reference and model, respectively (Equations 3.18 and 3.19):

$$\sigma_{ref} = \left[N^{-1} \sum_{i=1}^{N} (\text{NPP}_{ref, i} - \overline{\text{NPP}}_{ref})^2 \right]^{1/2}$$
(3.18)

$$\sigma_{mod} = \left[N^{-1} \sum_{i=1}^{N} (\text{NPP}_{mod, i} - \overline{\text{NPP}}_{mod})^2 \right]^{1/2}$$
(3.19)

To evaluate the agreement between the variability of NPP_{ref} and NPP_{mod} , the linear coefficient of correlation (*r*) is defined as:

$$r = \frac{1}{\sigma_{ref} \sigma_{mod}} \frac{1}{N} \sum_{i=1}^{N} \left[(\text{NPP}_{mod, i} - \overline{\text{NPP}}_{mod}) \times (\text{NPP}_{ref, i} - \overline{\text{NPP}}_{ref}) \right]$$
(3.20)

where *r* tends to 1 as the strength of variability approaches to agreement and -1 for a inverse relation between model and reference. However, as *r* is normalized by σ_{mod} and σ_{mod} , it does not contain information about the difference of amplitude between model and reference. To complement *r*, the normalized standard deviation σ_* indicates how the amplitude of model variability's is related to reference, calculated as $\sigma_* = \sigma_{mod}/\sigma_{ref}$. Similar performed by Jolliff et al. (2009), our sensitivity analysis compared NPP_{ref} and NPP_{mod} plotting these statistical parameters (bias, URMSD, *r*, and σ_{ref} , and σ_{mod}) in the target and Taylor diagrams.

To measure how well the modeling can predict the *in situ* reference compared to simplistically using the average observations as a predictor, the Nash–Sutcliffe model efficiency index (ME) was computed as presented below:

$$ME = 1 - \left[\frac{(NPP_{mod, i} - NPP_{ref, i})^2}{(NPP_{ref, i} - \overline{NPP}_{ref})^2}\right]$$
(3.21)

where the range of *ME* lies between 1.0 (perfect fit) and $-\infty$. If ME < 0, the mean value of the observations would have been a better predictor than the model estimate.

3.3 Sensitivity analysis

To quantify the impact of the parameters on the performance of satellite-derived NPP, the model (Equation 3.14) was run using measured and modeled inputs. *In situ* data described in Section 3.2.1 were first used as inputs to the NPP model to produce a reference estimation (NPP_{ref}). In the sensitivity analysis, the reference simulation was perturbed by exchanging only one model input at a time, while conserving the measured values for the other variables (NPP_{mod}). For calculate NPP_{ref} and NPP_{mod}, *PUR*(*z*, *t*) was estimated from on cast *in situ*, $E_d(\lambda, z, t_0)$, for each station with *t* ranging from 0 to 24 using the equation 3.12. While the inputs P_{max}^B , chla(z), and $E_k(z)$ were assumed constant during the day. These values of the perturbed input used in NPP_{mod} were obtained from published empirical models or algorithms applied to spectral remote sensing reflectance. We performed a total of 23 perturbations using the parametrizations listed in Section 3.3.2, which included the approaches to resolve profiles of chlorophyll-*a* (Section 3.3.2.1), light (Section 3.3.2.2), E_k (Section 3.3.2.3), and P_{max}^B (Section 3.3.2.4).

3.3.1 Reference simulation

The reference of daily depth-integrated net primary production (NPP_{ref}) was obtained for each station using input values from *in situ* measurements (N = 12 for BaySys and 11 for GreenEdge). PP(z, t) was computed using Equation 3.14 at a depth interval, Δz , of 0.1 m from surface to 2 optical depths and a time step of 10 minutes. PP(z, t) was integrated over depth and time to obtain NPP_{ref} in mg C m⁻² day⁻¹. As mentioned above, input variables included vertical profiles of $E_d(z, \lambda)$, discrete *in situ* samples of [*chla*]_{HPLC}, E_k , P_{max}^B , and $a_{\phi}^*(\lambda)$. Discrete values were linearly-interpolated within the productivity layer with Δz of 0.1 m as needed for NPP(z, t) calculation. To compute PUR(z, t), an estimation of $\overline{\mu}_o$ was needed to assess the scalar irradiance, which was obtained by calculating $(a_t + b_b)/k_d$ with R_{rs} -derived k_d and inherent optical properties, i.e., total light absorption (a_t) and backscattering (b_b) coefficients, both estimated using the QAA v5 algorithm (Lee et al., 2005).

3.3.2 Perturbed simulations

3.3.2.1 Phytoplankton chlorophyll-a

Chlorophyll-*a* concentration is one of the most important variable in satellite-derived NPP models. We tested five different methods, as presented in Table 4. From a remote sensing perspective, only surface concentration can be estimated. The concentration "seen" by a satellite sensor ([*chla*]_{sat}) comes from the upper part of the euphotic zone and can be calculated from the discrete samples using a weighted mean from the so-called "penetration depth" (z_{pd} , i.e., the first optical depth: $z_{pd} = 1/kd(443)$):

$$[chla]_{sat} = \frac{\int_0^{z_{pd}} chla(z) e^{-2k_d z} dz}{\int_0^{z_{pd}} e^{-2k_d z} dz}$$
(3.22)

where *chla*(*z*) was optically weighted using *z* and k_d (443), an approach similar to Morel and Berthon (1989) who used the attenuation coefficient for PAR irradiance (k_d^{PAR}), and to Lewis and Arrigo (2020) who used k_d (490).

The first simulation (or run C1; Table 4) uses [*chla*]_{sat} simulated from *in situ* data using eq. 3.22 and assumes a vertically homogeneous water column. This run allows quantifying the error when assuming



Figure 41: Remote sensing reflectance and light attenuation. R_{rs} (A) and k_d (B) spectra grouped into six optical classes based on $k_d(\lambda)$, including three sub-classes for the marginalice zones (MIZ): low (cyan triangle), moderate (blue triangle) and high (black triangle). Landfast ice domain (pink circles) and Nelson river plume waters (red and green squares).

Table 4: chlorophyll-*a* concentration inputs dedicated to sensitivity analysis of satellitederived phytoplankton production

| Run | Input | Vertical profile | Model | Reference |
|-----|--|------------------|--|---|
| C1 | [chla] _{sat} | homogeneous | Equation 3.22 with <i>in situ</i> $[chla]_{HPLC}$ and $k_d(443)$ | Morel and Berthon (1989) |
| C2 | $[chla]_{GSM}$ | homogeneous | Semi-analytic | Garver and Siegel; Maritorena et al. |
| C3 | [chla] _{AOR.emp} | homogeneous | Band ratio ¹ AOR.emp | Lewis and Arrigo (2020) |
| C4 | [<i>chla</i>] _{sat} , region, phe- nology | non-homogeneous | empirical | Ardyna et al. (2013) |
| C5 | [chla] _{surface} | non-homogeneous | empirical (Figure 42) | This study |

¹ Ocean color band ratio (*R*) and specific ocean color sensor (*i*) coefficients ($a_i, b_i, c_i,...$);

a homogeneous [*chla*] profile for a theoretically perfect retrieval of [*chla*]_{*sat*} from space. To quantify the errors associated with satellite retrievals of surface [*chla*], two commonly used ocean color (OC) algorithms were tested. Run C2 is based on the semi-analytical algorithm of Garver-Siegel-Maritorena (GSM: Garver and Siegel 1997; Maritorena et al. 2002) that has been used to assess pan-arctic NPP in Bélanger et al. (2013), and C3 used the recent Arctic Ocean regional empirical (AOR.emp) band ratio algorithm of Lewis and Arrigo (2020).

Satellite sensors can not measure directly the contribution of deep subsurface chlorophyll maximum to primary production as the water-leaving radiance only emerged from the first optical depth (Morel and Berthon, 1989). As mentioned above, the runs C1, C2, and C3 assume a homogeneous chlorophyll profile equal to satellite measurements as applied by Bélanger et al. (2013). Two approaches were tested to quantify the impact of non-homogenous chla(z) profiles: 1) we tested the model of Ardyna et al. (2013) in which chla(z) is determined by an empirical model fitted using trophic predictors, i.e., the surface chlorophyll-*a*, the region (Hudson Bay or Baffin Bay), and the seasonal variability along pre-bloom versus post-bloom conditions (run C4); and 2) a regional model for MIZ based on the observations made during BaySys and Greenedge (run C5). The latter is further described below.

Following Morel and Berthon (1989), we normalised $chla(z)_{HPLC}$ by the chlorophyll-*a* concentration as "seen" from satellite ([*chla*]_{*sat*} in Equation 3.22), and depth by euphotic zone depth (z/z_{eu}), where $z_{eu} = 4.6/kd(443)$. We restrict our analysis to the light level above the layer of two euphotic depths, i.e., inside the productive layer. Next the shape of chla(z):[*chla*]_{*sat*} in relation to z/z_{eu} was fitted for MIZ light environments (Figure 41) using the shifted-Gaussian model (Equation 3.23):

$$chla(z) = chla_{sat} \left[c_M + e^{-\left[\frac{z/z_{eu}-z_M}{\Delta z}\right]^2} \right]$$
(3.23)

where c_M represents a peak at light level z_M with amplitude Δz . In light environments of MIZ ECA, c_M , z_M , and Δz were 1.07, 0.3, and 1.11. As illustrated in Figure 42-A, this model reached a good performance of $r_{95\%}^2$: 0.94, $N_{samples}$: 154, and RMSD: 0.98, where $r_{95\%}^2$ is the coefficient to linear determination obtained in an interval of confidence of 95%. Nevertheless, some stations presented SCM that is not captured by the average model.

In the run C5, we applied $[chla]_{sat}$ (same as C1) as input in the shifted-Gaussian model (the red curve of Figure 42-A, Equation 3.23) to yield the chla(z) profiles.

3.3.2.2 Light profiles

The spectral NPP model relies on photosynthetic usable radiation (PUR) modeled using eqs. 3.12. Four simulations were performed to test the sensitivity of the satellite-based NPP model to PUR parametrization. For all of them, we use the measured surface irradiance just below the sea surface, $E_d(0^-, t)$, with the C-OPS were used and $\overline{\mu}_d$ from an approximation based on θ_{sun} , k_d and IOPs R_{rs} -derived using the QAA v5 model (Lee et al., 2016, 2005):

- **L0:** $R_{rs}(\lambda)$ and $k_d(\lambda)$ were in-water derived from the C-OPS (Section 3.2.1.3) to simulate the best possible performance of an satellite estimation of PUR(z);
- L1: $k_d(\lambda)$ was retrieved from the C-OPS $R_{rs}(\lambda)$ using the QAA v5 (Lee et al., 2016). Then eq 3.13 was used to calculate $E_d(z, t)$ as input to eqs. 3.12. This is the same method as in Bélanger et al. (2013);
- L2: the sensitivity to phytoplankton spectral light absorption was performed using the empirical model of $a_{\phi}(\lambda, z)$ proposed by Matsuoka et al. (2011) for springtime. The measured profile of $[chla]_{HPLC}$ was used as input in the model. The spectral irradiance and $\overline{\mu}_d$ are modeled as in the reference simulations;
- L3: as in L2, but for the parameterization for the fall season of Matsuoka et al. (2007).

3.3.2.3 Light saturation index, E_k

 E_k varies as a function of nutrient supply, light history, temperature, and day-length (Harrison and Platt, 1986; Sakshaug and Slagstad, 1991; Huot et al., 2013). Variation in E_k in the water column could be predicted using empirical models relating E_k with the mean daily PUR at a given depth $(\overline{PUR(z)})$, the geometric depth (z), the geometric depth normalized by euphotic depth (z/z_{eu}), or the


Figure 42: Chlorophyll-a profiles modeled for marginal-ice zones in the Canadian eastern Arctic. Discrete profiles in log-scale of *in situ* chlorophyll-a concentration measured by HPLC ([*chla*]_{*HPLC*} in mg m⁻³) and respective shifted-Gaussian model (red line) obtained in MIZ in June in Hudson Bay (2018) and Baffin Bay (2016). (B) boxplot of chlorophyll-*a* concentrations simulation of "as seen by" satellite acquisitions ([*chla*]_{*sat*} in mg m⁻³) calculated from profiles of [*chla*]_{*HPLC*} and k_d (Equation 3.22) in all ECA light environments (Symbols represent light environments clustered from $k_d(\lambda)$ shapes as shown in Figure 41).

chlorophyll-specific backscattering coefficient (b_{bp}^*) (Table 5). In our sensitivity analysis, five distinct schemes were tested:

- E1: Arrigo and coll. (Arrigo and Sullivan, 1994; Arrigo, 1994; Arrigo et al., 2008) modeled the vertical variation of E_k as a function of $\overline{PUR(z)}$, using a logistic function taking as input E_k^{max} , i.e., the maximum observed value for E_k (see Eqs. 13 and 14 in Arrigo et al., 2008). A value for E_k^{max} of 80 μ mol photons m⁻² s⁻¹, A of 2.2, and B of 0.336 were used, as adopted by Bélanger et al. (2013) and corresponding to value reported for the Southern Ocean by Arrigo et al. (2008).
- E2: Same as E1, but for low light-adapted ice-algae (Arrigo and Sullivan, 1994) using a E_k^{max} of 18 μ mol photons m⁻² s⁻¹, a value of 2 for the parameter *A*, and *B* as a exponential function of E_k^{max} (Table 5).
- E3: Same as E1, but for an E_k^{max} of 25.7 μ mol photons m⁻² s⁻¹ and a value of 2.2 and 0.336 for the parameter *A* and *B*, respectively. Ardyna et al. (2013) derived this parametrization in the Beaufort Sea with the data set presented by Huot et al. (2013).
- **E4:** Huot et al. (2013) fitted a log-linear function between $\overline{PUR(z)}$ to a data set from the southeastern Beaufort Sea ($E_k = 11.2 + 9.73 \log_{10}(\overline{PUR})$).
- E5: Using the same data set as in E3, Huot et al. (2013) observed a decrease in E_k as a function of depth ($E_k = 69 \times 10^{-0.011z}$).
- E6: To account for the variability of light attenuation, we proposed the relationship $E_k = 36.1 exp(-0.69z/z_{eu})$, where z_{eu} is the depth at which the light intensity is 1% of surface irradiance (Figure 43-C).
- E7: The last model predicted E_k from *in situ* observations of b_{bp}^* from BaySys and Greenedge. b_{bp}^* can be estimated from satellite ocean color measurements and is known to be a proxy for phytoplankton photoacclimation and community size structure (Behrenfeld et al., 2005).

Figure 43 illustrates how E_k models fit ours *in situ* observations in the MIZ of the eastern Canadian Arctic. We tested the logistic equation proposed initially by Arrigo and Sullivan (1994) ($r_{95\%}^2$: 0.49, n: 130 RMSD: 8.6) fitted using the daily average PUR (\overline{PUR}) as the predictor (Figure 43-A). E_k was also fitted with an exponential as a function of geometric depth ($r_{95\%}^2$: 0.43, n: 125 RMSD: 8.7; Figure 43B), which performed better than using light-level normalized depth ($r_{95\%}^2$: 0.35, n: 125,

RMSD: 9.1; Figure 43C). Finally, we found a relationship between E_k and the chlorophyll-specific backscattering coefficient at 555 nm (b_{bp}^* (555): in m² (mg Chla)⁻¹). The relationship provided the best performance overall ($r_{95\%}^2$: 0.49, n: 114, RMSD: 8.7), however, it was poorly constrained when turbid waters with high values of b_{bp}^* were included (Figure 43D).

We tested these parametrizations in the sensitivity analysis, but only the one providing the best results was retained. As mentioned above, **E7** combines the E_k versus b_{bp}^* for the upper water column (0 $\rightarrow z_{pd}$) and the logistic model for the deeper ($z_{pd} \rightarrow z_{eu}$).

3.3.2.4 Maximum photosynthetic production rate

Together with *chla*, P_{max}^{B} is one of the most important photosynthetic parameters that will drive the rate of carbon fixation in the water column. Five runs were performed:

- **P1:** This run assumed vertically homogeneous P_{max}^B fixed at 2.00 g C (g *chla*)⁻¹ h⁻¹ as adopted by Bélanger et al. (2013) following the published values of Harrison and Platt (1986).
- **P2:** Same as **P1**, but for the average value reported by Huot et al. (2013) of 3.16 g C (g *chla*)⁻¹ h⁻¹
- **P3:** $P^B_{max}(z)$ is modeled using an exponential function of depth proposed by Huot et al. (2013) for the Beaufort Sea (their eq. 4).
- **P4:** Same as **P3**, but using model parameter published by Bouman et al. (2017) for the north polar seas.
- **P5:** P_{max}^B observations in the Hudson Bay and the Baffin Bay did not show any clear relationship with depth, water type, or temperature. As a result, this run assumes vertically homogeneous P_{max}^B fixed at 1.82 g C (g *chla*)⁻¹ h⁻¹ although regional differences were notice between the HB and BB where P_{max}^B values of 1.43 and 2.04 g C (g *chla*)⁻¹ h⁻¹ were observed respectively.



Figure 43: Dependence of phytoplankton light saturation index to environmental conditions. Phytoplankton light saturation index (E_k) as a function of environmental conditions in Hudson Bay, and Baffin Bay. The panels depicted E_k (y-axe) as a function of (A) mean daily PUR (\overline{PUR}) using a logistic (red curve) and a log-linear (dashed black) functions, (B) *z* fitted with an exponential function, (C) light-level normalized depth (z/z_{eu}), and (D) chlorophyllspecific backscattering coefficient (b_{bp}^* : in m² (mg Chl)⁻¹). The equations were empirically fitted using a non-linear least square with a robust bi-square regression trust-region algorithm in MatLab. To compare relationships between E_k and \overline{PUR} obtained in MIZ ECA light environments(A), we plotted the logistic function obtained by Arrigo and Sullivan (1994) for ice-algae (AR94: magenta dashed line) and by Arrigo et al. (2008) in polar seas (AR08: red dashed line), and Ardyna et al. (2013) in the Beaufort Sea (ARD13: green dashed line).

| Run | Equation ¹ | Reference |
|----------------|---|--|
| $E_k(z)$ funct | tion of daily average photosynthetic usable radiation in | the photoperiod (\overline{PUR}) |
| E1,E2,E3 | $E_k = E_k^{max} / \left(1 + A e^{-B \overline{PUR}(z)} \right)$, where | Arrigo and Sullivan (1994); Arrigo et al. (2008); Ardyna et al. (2013) |
| E1 | E_{k}^{max} =18, A=1.7, and B=0.12 | Arrigo and Sullivan (1994) |
| E2 | E_k^{max} =80, A=2, and B = $e^{1.089-2.12 \log_{10}(E_k^{max})}$ | Arrigo et al. (2008) |
| E3 | E_k^{max} =25.7, A=2.2, and B=0.336 | Ardyna et al. (2013) |
| E4 | $E_k(z) = A + B \log_{10}(\overline{PUR}(z))$, where A=11.2 and | Huot et al. (2013) |
| | <i>B</i> =9.73 | |
| E_k function | n of depth | |
| E5 | $E_k(z) = A \ 10^{B \ z}$ | Huot et al. (2013) |
| E_k parame | trizations proposed to marginal-ice zone in Eastern Car | nadian Arctic |
| E6 | $E_k(z) = A \ e^{[B \ z/z_{eu}]}$ | this study |
| E7 | $E_k(z \rightarrow z_{pd}) = A e^{\left[B \ b_{bp}^*(555)\right]}$ and same as E1 but | This study |
| | fitted to MIZ EAC (i.e., E_k^{max} =29.8, A=1.2, and | |
| | $B=0.03$) for $z = z_{pd} \rightarrow z_{eu}$ | |

Table 5: parameterization of the photosynthesis light saturation.

¹ A and B are empirical parameters.

3.3.3 Satellite-like simulations

Three distinct configurations of the UQAR-Takuvik satellite NPP model were also included in the sensitivity analysis. The first two have already been applied to investigate phytoplankton dynamics in the Arctic Ocean (Bélanger et al., 2013; Ardyna et al., 2013), while the third one is based on the regional parametrization emerging from this study. Briefly:

- **Be13:** To assess the impact of cloudiness on Arctic production, Bélanger et al. (2013) applied homogeneous *chla*(*z*) from the GSM algorithm (**C2**), the Lee et al. (2016, 2005) models for light attenuation (**L1**), the spring Arctic $a_{\phi}^*(\lambda)$ model of Matsuoka et al. (2011) (**L2**), E_k model proposed by Arrigo et al. (2008) for the southern ocean (**E1**), and a constant P_{max}^B value of 2.00 g C (g chla)⁻¹ h⁻¹ for Arctic waters (Harrison and Platt, 1986) (**P1**);
- Ar13: To understand the impact of sub-surface chlorophyll-*a* maximum on Arctic production, Ardyna et al. (2013) selected a configuration similar to **Be13** but for chla(z) was parameterized using climatology profiles, region, and season (C4), and E_k modeled using the Beaufort sea parameterization (E3);
- **Ba22:** We proposed a regional parametrization that best fitted the MIZ stations of Hudson and Baffin bays, i.e., *chla*(*z*) as in **C5** (Figure 42), $a_{\phi}^*(\lambda)$ as in (**L2**), E_k as in (**E7**) (Table 5 and Figure 43-A and D), and P_{max}^B at 1.43 g C (g *chla*)⁻¹ h⁻¹ in Hudson Bay and 2.04 g C (g *chla*)⁻¹ h⁻¹ in Baffin Bay (**P5**).

3.4 Results

3.4.1 Environmental conditions, biomass, production rates, and water optical properties

To provide the context of the study, we first presented the environmental conditions, biomass, production rates, and water optical properties of the eastern Canadian Arctic observed in June, a season that has been under-sampled despite the fact that surface irradiance is at its peak (Laliberté et al., 2021). Figure 44 shows, as an example, a panorama of sea-ice, ocean, and atmosphere states for six stations in Hudson Bay. The Figure 41 showed that open water, MIZ and natural leads sampled had relatively low attenuation in the blue compared to red and NIR bands, and relatively low R_{rs} in green relative to the blue spectrum. Southern HB stations had higher R_{rs} due to suspended particles resulting in significant water-leaving radiance in the NIR compared to the blue bands. This water is dominated by high scattering due to the freshwater influence and sediment transported by landfast ice. The station in the Nelson River plume had high attenuation in both UV and NIR bands and high R_{rs} at the green because of the high concentration of suspended sediment and phytoplankton.

We analyzed a total of 330 discrete samples of $[chla]_{HPLC}$ collected in 16 stations in HB and 28 stations in BB. $[chla]_{HPLC}$ presented a normal distribution (Kolmogorov-Smirnov test, p = 0.01; not shown) with $[chla]_{HPLC}$ of 1.14 ± 0.99 mg m⁻³ ranging from 0.05 to 4.29 mg m⁻³ in Hudson Bay and 0.54 ± 0.51 mg m⁻³ ranging from 0.01 to 12.84 mg m⁻³ in Baffin Bay. A total of 32 profiles out of 44 had a sub-surface chlorophyll maximum (2.74 ± 2.53 mg m⁻³ at 26.00 ± 19.94 m) detected below the z_{pd} (Fig. 42). Conversely, upper layer held the highest $[chla]_{HPLC}$ (0.43 ± 0.95 mg m⁻³ at 2.83 ± 12.51 m) within z_{pd} in 12 profiles. z_{pd} extended up to 4.88 ± 3.25 m in HB, and 8.67 ± 2.39 m in BB.

Mean concentration in the euphotic zone ($[chla]_{eu}$) ranged between 0.07 to 23.10 mg m⁻³ in HB and 0.24 to 5.36 mg m⁻³ in BB. The value was lower in the first penetration depth with $[chla]_{sat}$ ranging from 0.12 to 3.40 mg m⁻³ and 0.14 to 2.53 mg m⁻³ in HB and BB, respectively. Diffuse attenuation was also larger and more variably in HB ($k_d(443) = 0.09$ to 4.91 m⁻¹) compared to BB (0.07 to 0.24 m⁻¹). The relations between $[chla]_{eu}$ versus $[chla]_{sat}$ or versus $k_d(443)$ indicated that upper layer k_d ($r_{95\%}^2$: 0.38, r_{adj}^2 : 0.36, RMSD: 0.26) was a more robust statistical-predictor for the average chlorophyll within euphotic layer than $[chla]_{sat}$ ($r_{95\%}^2$: 0.21, r_{adj}^2 : 0.19, RMSD: 0.26). As exposed in Figure 42-B, the trophic stages in the upper layer agreed with light environment categories. For example, the average of $[chla]_{sat}$ increased in relation to the attenuation level of each light environment, i.e., 0.4 ± 0.30 , 0.96 ± 0.30 , and 1.96 ± 1.06 mg m⁻³, respectively, for low, moderate, and high light attenuation clusters.

In eastern Arctic Canadian, daily depth-integrated NPP ranged from 0.02 to 1.40 g C m⁻² d⁻¹ in June. In Hudson Bay and Baffin Bay, the average daily integrated production was 0.37 ± 0.39 and 0.56 ± 0.57 g C m⁻² d⁻¹, respectively. The stations H11, H18, H25, and G204, classified as high light attenuation in MIZ were the most productive (0.99±0.60 g C m⁻² d⁻¹). The highest production occurred at stations H18 in the northwest Hudson Bay polynya (1.33 g C m⁻² d⁻¹) and G204 (1.40 g C m⁻² d⁻¹) in the central part of south Baffin Bay (68.7°N and 59.3°W). In moderate attenuation in the MIZ stations (H22B, H36, H38, G107, G310, G707, G713, and G719), the NPP was 0.57 ± 0.55 g C m⁻² d⁻¹. In low attenuation stations (H15, H16, H44, G321, G603, G605, G608, and G618), lower NPP was observed with 0.27 ± 0.17 g C m⁻² d⁻¹. In South HB coastal waters characterized by higher turbidity (stations H32, H34, and H46), the production was low ($0.26\pm.15$ g C m⁻² d⁻¹). At station H46, for example, a newly formed natural small lead surrounded by landfast sea-ice, the production was as low as 0.09 g C m⁻² d⁻¹. The lowest NPP was observed in the Nelson River plume within shallow and extremely turbid waters, where production was only 0.03 ± 0.02 g C m⁻² d⁻¹ in stations BN1 and BN5. However, the production rates rose fourfold (0.12 g C m⁻² d⁻¹) when the sediment plume just began to be settled at station BN6 just outside the turbid plume.

3.4.2 Sensitivity analysis

Table 6 and Figure 45 present the results of sensitivity analysis of satellite-based NPP models to their parametrizations in MIZ. Following the approach of Jolliff et al. (2009) and Lee et al. (2015), we evaluate the performance of each run using the target and Taylor diagrams in Figure 45. In the target diagram (Figure 45-A), bias/ σ_{ref} (y-axis) and URMSD/ σ_{ref} (x-axis) show how each run modeled the NPP_{ref} regarding systematic difference and variability, respectively. Note, we normalized bias and URMSD by σ_{ref} , and adopted the sign of [$\sigma_{mod} - \sigma_{ref}$] (hereafter referred as ±URMSD/ σ_{ref}). The nearest to the center indicated better performance of NPP_{mod} compared to NPP_{ref}.

3.4.2.1 Sensitivity to chlorophyll-*a*

All chla(z) performed well to account the variability of NPP_{ref} (i.e. R>0.80). However, spreads in target and Taylor diagram (Figure 45) demonstrated high discrepancy among chla(z) models. Homo-



Figure 44: Light environments: Distinct domains sampled during the spring-summer transition during the expeditions Green Edge 2016 and BaySys 2018: Marginal-ice zone with relatively (A) high, (B) moderate, and (C) low light attenuation, (D) Nelson River sediment plume, (E) Nelson River plume with phytoplankton bloom (F) leads in landfast ice load sediments.



Figure 45: Target and Taylor diagram: PP in Eastern Canadian Arctic. (A) Target and (B) Taylor diagrams for the individual models and sensitivity analysis of phytoplankton production parametrizations in relation to reference PP, as presented on Table 6.

| Model | Pertubation | RMSD | \pm URMSD/ σ_{ref} | bias/ σ_{ref} | r | ME | Reference |
|-----------------------|--|------|-----------------------------|----------------------|------|-------|----------------------------|
| Sensitivi | ity to chlorophyll-a | | | | | | |
| C1 | Homogeneous profile equal [chla] _{sat} | 0.19 | -0.31 | -0.05 | 0.91 | 0.89 | Bélanger et al. (2013) |
| C2 | Homogeneous equal R_{rs} -derived [<i>chla</i>] _{<i>GSM</i>} | 0.41 | 0.68 | -0.05 | 0.85 | 0.52 | Maritorena et al. (2002) |
| C3 | Homogeneous equal R_{rs} -derived [<i>chla</i>] _{AOR.emp} | 0.26 | 0.43 | -0.04 | 0.87 | 0.81 | Lewis and Arrigo (2020) |
| C4 | Climatology: north polar seas | 0.53 | 0.66 | 0.58 | 0.80 | 0.20 | Ardyna et al. (2013) |
| C5 | Climatology: MIZ ECA | 0.23 | -0.37 | -0.10 | 0.88 | 0.84 | this study |
| Sensitivi | ity to light profiles $(PUR(z))$ | | | | | | |
| L0 | In-water derived $k_d(\lambda)$ | 0.11 | 0.15 | 0.10 | 0.95 | 0.97 | Mueller et al. (2003) |
| L1 | Above-water derived $k_d(\lambda)$ using QAA v5 | 0.26 | -0.39 | -0.19 | 0.89 | 0.80 | Bélanger et al. (2013) |
| L2 | $a_{\phi}(\lambda)$: Spring Arctic Ocean | 0.27 | 0.37 | 0.27 | 0.95 | 0.78 | Matsuoka et al. (2011) |
| L3 | $a_{\phi}(\lambda)$: Fall Arctic Ocean | 0.24 | 0.32 | 0.23 | 0.95 | 0.83 | Matsuoka et al. (2007) |
| Sensitivi | ity to E_k | | | | | | |
| E1 | Logistic function of \overline{PUR} for ice algae | 0.18 | 0.24 | 0.17 | 0.95 | 0.91 | Arrigo and Sullivan (1994) |
| E2 | Logistic function of \overline{PUR} for Southern Ocean | 0.39 | -0.49 | -0.43 | 0.90 | 0.55 | Arrigo et al. (2008) |
| E3 | Logistic function of \overline{PUR} for Beaufort Sea | 0.22 | -0.32 | -0.17 | 0.91 | 0.87 | Ardyna et al. (2013) |
| E4 | Log-linear function of \overline{PUR} for Beaufort Sea | 0.17 | -0.28 | -0.01 | 0.92 | 0.92 | Huot et al. (2013) |
| E5 | Exponential function of depth for Beaufort Sea | 0.34 | -0.44 | -0.35 | 0.90 | 0.67 | Huot et al. (2013) |
| E6 | Exponential function of z/z_{eu} | 0.13 | 0.22 | 0.04 | 0.94 | 0.95 | this study |
| E7 | $f_5(b_{bp}^*, [0^- z_{pd}])$ and $f_1(PUR, [z_{pd} z_{eu}])$ | 0.11 | 0.18 | 0.02 | 0.94 | 0.97 | this study |
| Sensitivi | ity to P^B_{max} | | | | | | |
| P1 | P^B_{max} : average in Arctic Ocean | 0.47 | -0.74 | 0.27 | 0.63 | 0.35 | Bélanger et al. (2013) |
| P2 | P^B_{max} : average in Beaufort Sea | 0.79 | 0.85 | 1.00 | 0.63 | -0.81 | Huot et al. (2013) |
| P3 | $P^{B}_{\underline{m}ax}(z)$: Exponential function of depth for north polar seas | 0.46 | -0.75 | -0.14 | 0.64 | 0.40 | Huot et al. (2013) |
| P4 | $P^B_{max}(z)$: Exponential function of depth for north polar seas | 0.48 | -0.73 | 0.33 | 0.64 | 0.33 | Bouman et al. (2017) |
| P5 | P^{B}_{max} : average in MIZ ECA | 0.45 | -0.74 | 0.16 | 0.63 | 0.40 | this study |
| Satellite | models | | | | | | |
| Model | ¹ $PUR(k_d, a_{\phi}^*)$ chla $E_k P_{max}^B$ | | | | | | |
| Be13 | QAA v5, M11 C2 E2 P1 | 0.41 | -0.64 | 0.21 | 0.72 | 0.53 | Bélanger et al. (2013) |
| Ar13 | QAA v5, M11 C4 E2 P1 | 0.94 | -1.10 | 1.10 | 0.05 | -1.50 | Ardyna et al. (2013) |
| Ba22 | QAA v5, M11 C5 E7 P5 | 0.48 | -0.79 | 0.15 | 0.59 | 0.33 | this study |
| ¹ PUR calc | culated ingesting the $a_{\phi}(\lambda)$ model of Matsuoka et al. (2011) (M11); | | | | | | |
| | the intervalue of the matrix of the interval of the matrix C and C | | | | | | |

²AR98: E_k parameterization proposed by Arrigo et al. (1998).

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geneous profiles of chl*a* equal to $[chla]_{sat}$ calculated from *in situ* HPLC (**C1**) reached the best performance with RMSD of 0.19 g C m⁻² day⁻¹ but, as expected, underestimated NPP with URMSD/ σ_{ref} at -0.31 and bias/ σ_{ref} at -0.05. For comparison, R_{rs} -derived band ratio AOR.emp (Lewis and Arrigo, 2020) and GSM (Maritorena et al., 2002) algorithms produced similar bias of the NPP (-0.04 and -0.05), but larger variability (URMSD/ σ_{ref} = 0.43 and 0.68). AOR.emp showed a high model efficiency index (ME: 0.81) compared to GSM (ME at 0.52).

The runs that account for vertical variability of the biomass (*chla*(*z*)) did not result in much greater performance. The run C5 using the mean *chla*(*z*) observed in the MIZ (Figure 42) resulted in high *r* of 0.88, ME of 0.84, RMSD at 0.23 g C m⁻² day⁻¹ and a normalized bias of -0.10, which better than the performance of the Ardyna et al. (2013) model (**C4**). The later yield poor ME of 0.20, a RMSD of 0.53 m⁻² day⁻¹, a normalized bias of +0.58, and a large variability with URMSD/ σ_{ref} at 0.66, which was similar the performance of **C2** for [*chla*]_{*GSM*}.

3.4.2.2 Sensitivity to light profiles, *PUR*(*z*)

As observed in the Figure 45 and Table 6, satellite-derived light profiles estimated by k_d and $\overline{\mu}_o$ resulted in an RMSD of 0.11 g C m⁻² day⁻¹. As **L0** represents the error associated to an ideal satellite retrieval of k_d , light attenuation produces a systematic overestimation of NPP (±URMSD/ σ_{ref} : 0.10) and NPP variability (bias/ σ_{ref} : 0.15). Although both **L0** and **L1** were efficient to resolve light profiles (ME>0.80), QAA v5 R_{rs} -derived k_d (**L1**) increased RMSD to 0.26 g C m⁻² day⁻¹, and underestimated NPP variability (URMSD/ σ_{ref} -0.39), and systematically underestimated NPP (bias/ σ_{ref} at -0.19). In terms of *r*, both **L0** (R: 0.95) and **L1** (R: 0.89) shown that satellite-derived k_d well represented the variability of NPP_{ref}.

PUR maybe also affected by the spectral shape of the phytoplankton absorption coefficient. The $a_{\phi}^*(\lambda)$ model proposed by Matsuoka et al. (2011) for Arctic spring time (**L2**) and by Matsuoka et al. (2007) for the fall seasons (**L3**) generated RMSD at 0.27 and 0.24 g C m⁻² day⁻¹, respectively, overestimated the variability (URMSD/ σ_{ref} at 0.37 and 0.32), and resulted in systematic overestimation (bias/ σ_{ref})

at 0.27 and 0.23). Independent of the choice of $a_{\phi}^*(\lambda)$ model (L2 or L3), *r* remains at 0.95, indicating low sensitivity of satellite-derived NPP to regional and seasonal algal absorption variability. The model proposed for fall (Matsuoka et al., 2007) reached a better performance than spring values reported for the high Arctic (Matsuoka et al., 2011). These results should be interpreted with caution because the true $a_{phy}(\lambda)$ was not used here but estimated from HPLC pigments.

Figure 46 shows the performance of remote sensing algorithms to estimate PUR profiles compared to in-water reference irradiance profiles. Based on 54 stations analyzed, the coefficient of determination (r^2) of modeled versus the reference instantaneous PUR reached 0.87 (Figure 46-A), which is slightly higher than for the daily integrated PUR (r^2 :0.74, Figure 46-B). Maximum PUR at noon reached $3.1 \times 10^3 \mu$ photons m⁻² s⁻¹. Here, the photo-period integration only accounted for the solar zenith variations, however, variability of cloud coverage, sea-ice, and in-water bio-optical properties may effectively change the radiative balance during a given day (Bélanger et al., 2013; Laliberté et al., 2016).

Figure 46-C shows the vertical variability of the difference between modeled and measured PUR. An underestimation of PUR is found between 5 and 15 m where high variability of [*chla*], out of the range of ocean color satellites, was also observed. In contrast, the difference between modeled and reference PUR profiles was minimum in low light levels below 25 m, and in the surface layer above 5 m. Because of satellite-derived k_d is very-well constrained to the layer in which the light attenuated by 10% in relation to $E_d(0^-)$ (Lee et al., 2005), while model of vertical light distribution results in low error propagation in total production at low light levels (Figure 46).

3.4.2.3 Sensitivity to E_k

All E_k models tested yield high correlation between NPP_{ref} and NPP_{mod} the daily variability of phytoplankton production (r > 0.90). The models that predict E_k from \overline{PUR} (E1, E2, E3, and E4) were close to NPP_{ref} with a RMSD ranging from 0.17 (E4) to 0.39 g C m⁻² day⁻¹ (E2) (Figure 45 and Table 6). Among the \overline{PUR} -based models, the log-linear function proposed by Huot et al. (2013) to Beaufort Sea reached the best efficiency (ME: 0.92) with a RMSD at 0.17 g C m⁻² day⁻¹ and slightly negative bias (-0.1), but underestimate the NPP_{ref} variability (URMSD/ σ_{ref} at -0.28). In contrast, the Arrigo et al. (2008) model for the Southern Ocean (E2) reached the largest errors and the poorest statistics (RMSD at 0.39 g C m⁻² day⁻¹, URMSD/ σ_{ref} : -0.49, bias/ σ_{ref} : -0.43, ME: 0.55). The depth-dependent model proposed by Huot et al. (2013) in Beaufort Sea (E5) had the lowest ME (0.67) resulting in high RMSD (0.34 g C m⁻² day⁻¹).

The best E_k model was the one proposed in this study (E7) based on assembled model using b_{bp}^* within the satellite penetration depth (z_{pd}) , and a regional logistic model as a function of \overline{PUR} below z_{pd} . When compared to all model perturbations analyzed (C, L, E, and P), E7 reached the best performance, as seen in the target and Taylor diagrams (the white star in Fig. 45).

3.4.2.4 Sensitivity to P_{max}^B

The results revealed that the P_{max}^B parameter has the largest impact on satellite NPP retrievals. For example, the use of average values obtained in the Beaufort Sea (**P2**) depreciated RMSD to 0.79 g C m⁻² day⁻¹, overestimated NPP variability with ±URMSD/ σ_{ref} at 0.85 and increased the systematic overestimation (bias/ σ_{ref} at 1.00), which were the highest errors among all model perturbations. **P1**, **P3**, **P4** and **P5** highly underestimated PP variability to an URMSD/ σ_{ref} ranging from -0.74 to -0.73. All P_{max}^B models represented ~64% of NPP_{ref} variability with *r* ranging from 0.63 to 0.64. The exponential function of depth (**P3**) proposed by Huot et al. (2013) resulted the lowest RMSD (0.46 g C m⁻² day⁻¹), less expressive systematic error (bias/ σ_{ref} : -0.14), and the best efficiency (ME: 0.40) among P_{max}^B models. However, **P3** highly underestimated NPP_{ref} variability (URMSD/ σ_{ref} at -0.75).

In Arctic, $P_{max}^B B$ ranges from 0.3 to 7.0 mg C [mg Chl⁻¹ hour⁻¹] acconting to regional, seasonal, and inter-species variability Babin et al. (2015). For example, polar diatoms, P_{max}^B range between 0.2 and 2.46 g C [g *chla*]⁻¹ hour⁻¹] (Schuback et al., 2017). Bouman et al. (2017) reported seasonal variability of P_{max}^B ranging between 1.86 ± 0.91 in spring, 1.93 ± 1.29 in Summer, 2.10 ± 1.12 in Autumn and 1.15 ± 0.76 mg C [mg Chl⁻¹ hour⁻¹] in Winter. In summer of eastern Canadian Arctic, Schuback et al. (2017) observed P_{max}^B ranging from 3.2 to 4.1 mg C [mg Chl⁻¹ hour⁻¹ in the western Hudson Bay, and 1.8 to 7.6 in Baffin Bay.

Figure 47 shows the relation between P_{max}^B and salinity (*S*) in distinct light environments. In MIZ, the values of P_{max}^B was 1.65±0.80, 0.92±0.59, and 1.39±0.53 g C (g *chla*)⁻¹ h⁻¹ for high, moderate, and low attenuation light environments, respectively. In MIZ, no relationship was found between salinity and P_{max}^B , except a weak correlation for the moderate attenuation (r^2 : 0.41). On the other hand, in southern Hudson Bay, where the salinity ranged from 28.4 to 31.8, a strong linear relationship with P_{max}^B was found (r^2 : 0.81).

3.4.3 Phytoplankton community structure

Phytoplankton community structure may explain the regional difference in terms of photosynthetic parameters. As illustrated in Figure 48, our analysis of the taxonomy composition and quantitative vertical distribution revealed that similar communities are found in the surface and SCM. The taxonomy composition, in an interval of confidence of 99.9%, showed that surface and sub-surface phytoplankton communities were more coupled in Hudson Bay, according to a coefficient of correlation of 0.95 than in Baffin Bay with a coefficient of correlation of 0.87. In Hudson Bay, the community are dominated by diatoms (*Bacillariophyceae* with chloroplast and empty frustules), flagellates (undetermined, i.e., *Flagellate ssp.* with diameter ranging from 2 to 20 μ m), coccolithophorids (*Prymnesiophyceae*), and ciliates. In Baffin Bay, Coccolithophorids (*Prymnesiophyceae*) was dominant 71.93% follow by flagellate 9.28%, and diatoms (*Bacillariophyceae* 1.00% (Figure 48).

Figure 49 shows the fractional contribution of each pigment-derived size class to the total. In Hudson Bay, micro-plankton monopolized by $81.32\pm11.82\%$, while nano-plankton and pico-plankton represent only $5.54\pm5.16\%$ and $13.12\pm9.78\%$, respectively. In the Baffin Bay, micro-plankton remained the dominant size class ($57.12\pm18.07\%$), however, nano-plankton ($17.49\pm10.15\%$) and pico-plankton ($23.39\pm17.68\%$) are significant.

3.5 Discussion

How does satellite-derived phytoplankton production perform in the MIZ conditions in the eastern Canadian Arctic in summer? Can regional tuning improve performance in ECA-MIZ? How do interplays of oceanographic processes and phytoplankton photo-physiology (size structure and photo-acclimation) impact NPP satellite retrievals? To address these questions, we ranked the NPP satellite inputs and compared the performance of recent satellite models dedicated to pan-Arctic in Section 3.5.1. Our analysis contemplated distinct phonological stages in MIZ as discussed in Section 3.5.2. The sensitivity of satellite production models is discussed in regard to the regional variability between the Baffin Bay and the Hudson Bay, environmental drivers, phytoplankton photoacclimation, timing, and development of phytoplankton vertical distribution (Section 3.5.3).

3.5.1 Propagation of uncertainties on phytoplankton NPP assessment

The sensitivity analysis (Fig. 45 and Tab.6) allowed us to rank the parameters for satellite-derived NPP assessment (Eq. 3.14) in terms of importance. The first, P_{max}^B modeling appeared as the main source of uncertainties as it yields the largest RMSD. Second, NPP assessments are also sensitive to the absolute value of surface *chla* and to a lesser extent to the parametrization of *chla*(*z*). In contrast, the sensitivity to E_k and to PUR(z) modeling is significantly smaller.

The simplification of the productive-water column as a homogeneous k_d layer was the lowest source of uncertainties for satellite NPP assessment (Fig. 46). However, errors emerged from ocean-color algorithms uncertainties, for example, the QAA to derive k_d from R_{rs} (Fig. 45 and Tab.6). The uncertainty propagated from satellite-derived k_d and $a_{\phi}^*(\lambda)$ modeling produced similar RMSD on NPP. However, they have an opposite effect, $a_{\phi}^*(\lambda)$ produced an NPP overestimation while R_{rs} -derived k_d yield an underestimation of NPP.

As a consequence, satellite-derived NPP was poor-sensitivity to the role of distinct phytoplankton communities on the spectral shape of light absorption, i.e., low sensitive to $a_{\phi}^*(\lambda)$ model and inde-

pendent of phytoplankton communities origin, e.g., Hudson Bay, Baffin Bay, spring-, or fall-Arctic Ocean, (Table 6 and Figure 45). One reason explaining why $a_{\phi}^*(\lambda)$ led to an overestimation of NPP, is the fact that models do not account for the photo-protective non-photochemical quenching (NQP) in case of light in excess, or packaging effect, both common in Arctic phytoplankton communities (IOCCG, 2015). NQP protects photosynthetic machinery against insolation by the fluorescence emission (high fluorescence quantum yield) and heat dissipation, which result in less light assimilated in the photosynthesis compared to the yield of PUR. Pigment packaging, i.e., intact-pigmented cells absolving less light than a solution of the same pigments, results in relative flattening of the blue and red absorption peaks (less-spectral selective) in measured $a_{\phi}^*(\lambda)$ compared to in vivo (Morel and Bricaud, 1981).

Regional tuning improved the prediction of *chla* in two ways: i) the dedicated Arctic regional bandratio algorithm AOR.emp (Lewis and Arrigo, 2020) allowed better performance of NPP assessment compared to the global semi-analytical algorithm GSM (Garver and Siegel, 1997; Maritorena et al., 2002); and ii) the *chla*(*z*) climatic model dedicated to MIZ (Fig. 42) improved the result compare to the parametrization proposed by Ardyna et al. (2013). In ECA, the trophic transition from productive MIZ to summer oligotrophy resulted in complex phytoplankton vertical distribution (Figure 42) and photo-physiology (Figure 43) in the MIZ. Barbedo et al. (2022) based on satellite ocean-color $b_{bp}^*(555)$, a proxy for C_{phy} :[*chla*], showed that oligotrophy and high light incoming in summer lead a remarkable increase on C_{phy} :[*chla*] in Hudson Bay (see chapter 2). Even that, the ratio C_{phy} :[*chla*] could be assumed constant to estimate annual phytoplankton production in the Arctic Ocean, as applied by Lewis and Arrigo (2020). E_k modelling reached great performance because the assimilation \overline{PUR} and b_{bp}^* accounted photo-physiology in ECA-MIZ (Fig. 43).

If regional tuning improved the NPP results for individual sensitivity assessment of *chla*(*z*), *PUR*(*z*), P_B^{max} and E_k , why our regional model (Be22) does not perform better than the parameterization of Bélanger et al. (2013) (**Be13**)? As shown in Tab. 6, **Be13** satellite model simulation reached better performance than **Be22** in most statistic metrics (RMSD: 0.26 g C m⁻² day⁻¹, URMSD/ σ_{ref} : -0.39, *r*: 0.72, and ME: 0.53), except for the bias/ σ_{ref} (0.21 versus 0.15 for **Be22**). The **Be22** configuration

selected **C5** for *chla*(*z*) (RMSD:0.23 g C m⁻² day⁻¹) and **E7** for E_k (RMSD: 0.11 g C m⁻² day⁻¹) and **P5** for P_{max}^B (RMSD: 0.45 g C m⁻² day⁻¹)), whose performed better that the other models. Their effect of overestimation on NPP, URMSD/ σ_{ref} at 0.32 (**C5**) and 0.18 (**E7**), respectively, can not counteract the underestimation NPP forced by P_{max}^B (URMSD/ σ_{ref} : -0.74). Even that, the simplification of homogeneous vertical chlorophyll structure could lead an underestimation on NPP, as observed in **C1** (URMSD/ σ_{ref} : -0.31). According Ben Mustapha et al. (2012), GSM tends to overestimated [*chla*] in the range of [*chla*]_{sat} observed in ECA-MIZ (0.1–4.0 mg m³) because the high blue light absorption of CDOM and NAP. Therefore, the model **C2** results on NPP overestimation (URMSD/ σ_{ref} : 0.68), which counteract the error driven by denying the occurrence of SCM.

3.5.2 Phenological states and taxonomy in marginal ice zones

Understanding how natural assembles respond to environmental conditions is essential to improve satellite ocean color and models dedicated to the phytoplankton dynamic of north polar seas (Lacour et al., 2017; Devred et al., 2016; Behrenfeld et al., 2002). A taxon is more apt to thrive the ecological competition for resources and to overlap predating when occupies its respective fundamental niche, i.e., the specific conjuncture of environmental conditions required for success in nature (Oziel et al., 2020; Gafar and Schulz, 2018). In MIZ, the sea-ice-seasonal melting triggers a succession of changes in the drivers of algae dynamics. In this shifting environment, polar micro-algae must acclimate to overwhelm ecological succession (Behrenfeld et al., 2017; Lacour et al., 2017; Palmer et al., 2013). Here we discuss our results in terms of the phytoplankton community observed in the MIZ in early summer.

The dominance of diatoms and the presence of empty frustules produced by intense grazing indicated a stage of post-boom-peak (Figure 48). Our results agree with observations of Lee et al. (2019) in the Chukchi Sea and the East Siberian Sea, where pelagic diatoms dominated blooms beneath the sea-ice zone, while small phytoflagellates (e.g., prymnesiophytes, prasinophytes, dinoflagellates, and crypto-phytes) indicated post-bloom period. The BaySys expedition was the first to widely sample Hudson Bay in the spring-to-summer transition. The complex phytoplankton vertical structure profiled in the

Hudson Bay (Figure 42) can be attributed to a transitional tropic stage from marginal-ice zone blooms to pre-summer oligotrophy. According to (Matthes et al., 2021), blooms were likely past their peak, however, our results showed that diatoms mainly controlled production. This contrast with the small cells that prevailed in summer (Ferland et al., 2011) and in early fall (Lapoussiere et al., 2013).

As reported by Schuback et al. (2017) for the western Hudson Bay, Baffin Bay, Labrador Sea, and Canadian Arctic Archipelago, inorganic nitrogen is an environmental predictor of P_{max}^B . Salinity was successfully applied by Tremblay et al. (2008) as a proxy of seasonal nutrients draw-down on the Beaufort Shelf influenced by the Mackenzie River. However, our results showed that salinity was just a relevant environmental predictor for phytoplankton maximum production, where the freshwater source is mainly continental. For example, salinity explained 88% of P_{max}^B variability in the southern Hudson Bay light environment (Figure 47), where nutrient remineralization was sustained by river plumes (Jacquemot et al., 2021), and landfast sea-ice transporting and releasing sediment (Harasyn et al., 2019). In the Chukchi and Beaufort Seas, Palmer et al. (2013) reported low variation in P_{max}^B despite vastly range of nutrient and light conditions, except in rich-nitrate sites (>10 μ mol kg⁻¹). We observed that in MIZ light environments of Hudson Bay and Baffin Bay, freshwater from sea-ice melting contributed to an increase in stratification without significant input of nutrients that resulting in a poor relationship between salinity and P_{max}^B in MIZ (Figure 47).

Hudson Bay has a semi-enclosed cyclonic circulation and high freshwater input, which result in the low influence of Arctic Water intrusion and long-time water resilience in the bay. In coastal areas, where river plumes are constrained, phytoplankton production prompt assimilates the nutrient-inventory (Kuzyk et al., 2010). The Nelson River plume plays a local role in primary production as inorganic nitrogen is readily consumed in the neritic (e.g., 2–5 m deep) inner-estuarine transition zone (Bergeron and Tremblay, 2014). As reported by Jacquemot et al. (2021), in the Baysys 2018 expedition, [NO₂+NO₃] decrease downstream in the Nelson River Plume from 0.44 to 0.03 μ mol L⁻¹, and silica [Si(OH)₄] from 38.52 to 1.21 μ mol L⁻¹. On the other hand, in offshore, freshwater intensifies salinity gradients, forcing insulation between the upper-layer and the deep-nutrient pool, which set up a deficit of nitrate, nitrite ([NO₂+NO₃]<0.5 μ mol L⁻¹), and silicate in the euphotic zone (Tremblay)

et al., 2019; Ferland et al., 2011).

The Baffin Bay is an Arctic out-shelf with cyclonic circulation. Its nutrient inventory is controlled by a balance between Arctic Waters (warm and salty) throughout the Lancaster and Jones Sounds from the Canadian Arctic Archipelago, and the Naires strait, while the Western Greenland current transport Atlantic Water (S>35.5 and T>-1.0°C) transformed by runoff and cooling in the David Strait (Joli et al., 2021; Burgers et al., 2020; Bergeron and Tremblay, 2014; Coote and Jones, 1982). On the other hand, the riverine input is about 713 km³ year⁻¹ (Kuzyk et al., 2010) in the Hudson bay, which equates to 12% of the total Pan-Arctic runoff (St-Laurent et al., 2011). The contrasting of Arctic Water and freshwater influence results in a low ratio of Si:N in the Baffin Bay compared to Hudson Bay which, in turn, differentiated their phytoplankton taxonomy (Bergeron and Tremblay, 2014; Vidussi et al., 2001). As reported by Lafond et al. (2019), the dominance of taxon with a calcareous exoskeleton (i.e., coccoliths) in relation to Diatoms results in scarce silica environments in the Baffin Bay compared to Hudson Bay. As discussed by Vidussi et al. (2001), exogenous nitrates are principally used by large phytoplankton (micro-phytoplankton) which mainly contribute to new production, while regenerate forms of nitrogen (ammonium and urea) are the likely source for small phytoplankton. Our results indicated that the dominance of Diatoms, composed of siliceous frustules, and flagellates supported by nitrogen recycling in Hudson Bay, in relation to low Si:N ratio in Baffin Bay, which a heterogeneity of taxon dominated by Coccolithophorids, which calcium carbonate liths are less dependent of silicon availability (figure 48).

3.5.3 Interplays of phytoplankton photo-physiology, community size structure, and production vs. irradiance (P-E) curves

Phytoplankton photo-acclimation affects both E_k and P_{max}^B , however, these parameters are related to distinct photosynthetic processes. E_k has a direct impact on the relationship between fluorescence emission and instantaneous PAR (O'Malley et al., 2014; Behrenfeld et al., 2009) in the photosynthetic reaction center II, while P_{max}^B is largely defined by the capacity of the Calvin cycle reactions (O'Malley et al., 2014).

As observed by Babin et al. (1996) in the northeast tropical Atlantic, the low nitrogen concentration in the upper layer and nutricline deepening, force a reduction of E_k steepness with depth. Our analysis showed, although E_k decrease with geometric depth (z) or optical depth (z/z_{eu}), these models only explained 43% and 37% of E_k variability, respectively (Figure 43-B and C). Jackson et al. (2017) showed that C_{phy} :[*chla*] is a highly-variable property that responds to E_k and daily irradiance in the mixed layer. (Palmer et al., 2013) demonstrated the potential light incoming to predicted both E_k and C_{phy} :*chla*. Our study showed, for the first time, that $b_{bp}^*(555)$, a satellite ocean color proxy of C_{phy} :[*chla*], allowed superior performance to model E_k even in optically-complex waters. Satellite ocean color algorithms are able to estimate $b_{bp}^*(555)$ using R_{rs} -based semi-analytical models (Lewis and Arrigo, 2020), however, the range of ocean-color satellite is restrict to the first optical depth. In this way, to calculate E_k , we assembled $b_{bp}^*(555)$ based model in the first optical depth (as estimated by satellite-derived $1/k_d$), and \overline{PUR} based on the deeper light levels.

Our results show that the Hudson Bay, where diatoms and large-cells (< 10 μ m) dominated, had lower P_{max}^{B} (1.43 g C g chla⁻¹ h⁻¹ in a total of 101 samples) than the Baffin Bay (2.04 g C g chla⁻¹ h⁻¹ in a total of 185 samples), where small cell sizes like dinoflagellates, and small flagellate, and picoeukaryotes dominated. As observed by Schuback et al. (2017) in the sub-Arctic seas (Labrador sea, Hudson Bay, Baffin Bay, and the CanadianArctic Archipelago), low irradiance levels below the mixed layer lead to an increase in pigment packaging and intra-cellular chlorophyll content which, in turn, decreases P_{max}^{B} (i.e., the chlorophyll normalized maximum production). P_{max}^{B} can increase in communities predominantly composed of large cells, as observed by Huot et al. (2013) in the Beaufort Sea and Claustre et al. (2005) in the North Atlantic Ocean. We speculate that the predominance of stabilized sub-surface chlorophyll maximum and low-light incoming in the Baffin Bay compared to Hudson Bay determined the photo-acclimation in terms of P_{max}^{B} , which overwhelmed the community-size structure influence on P_{max}^{B} presumed by Huot et al. (2013) and Claustre et al. (2005).

In MIZ, P_{max}^B error strongly affects satellite-derived PP (Figure 45 and Table 6). Even that, some efforts to fit P_{max}^B have been reported, for example, based on phytoplankton functional groups (Ver-

net et al., 2021; Gafar et al., 2019; Hirata and Suzuki, 2017; Richardson et al., 2016; Claustre et al., 2005), size structure (Richardson et al., 2016), light incoming (Palmer et al., 2011), and the historical of mixture, light, and nutrients (Graff and Behrenfeld, 2018; Behrenfeld et al., 2008, 2002). In north polar seas, P_{max}^B remained poorly constrained (Lacour et al., 2017, 2015). We could not find a predictor that performed better than P_{max}^B average value, except in southern Hudson Bay. There we found a relation between salinity and P_{max}^B (Figure 47). This result revealed a potential for the use of sea-hydrodynamic models to predict profiles of salinity and P_{max}^B . This synergy between ocean color algorithms and hydrodynamic models can improve satellite NPP estimations.

3.6 Conclusions

Our sensitivity analysis covered a wide range of phytoplankton assembles, and key light environments in the Canadian Eastern Arctic. In MIZ, distinct phenological stages were contemplated from underice blooms, and ice-edge blooms, to summer oligotrophy. The Canadian Eastern Arctic is seasonally covered by sea ice, sea-ice break-up occurs concomitant to the seasonal peak of light incoming and nutrient availability, producing its most productive feature. However, MIZ is very dynamic because of the effect of a wide branch of environmental processes that directly affect algae dynamics. To improve the performance of satellite-derived phytoplankton production, we suggest increasing the model sensitivity to phytoplankton photo-physiology. For that, satellite models should account for the phenological stages of MIZ because of the effect of distinct photo-physiology and vertical distribution (SCM) on phytoplankton production. In this way, we present some advances to assess pelagic production, for example, the E_k model based on photo-acclimation and community structure using the proxy b_{bp}^* (555), a parametrization of the vertical distribution of chlorophyll-*a* dedicated to ECA MIZ. Our sensitivity analysis allowed a better understanding of how oceanographic processes and phytoplankton photo-physiology affect satellite NPP models. Finally, for future pan-Arctic production assessments, how to predict P_{max}^{B} , and the feasibility of satellite ocean color models extrapolation under-ice in MIZ.

3.7 Supplemental material

3.7.1 Retrieval of $R_{rs}(\lambda)$ using autonomous selection of the $L_u(0^-, \lambda)$ extrapolation layer

To evaluate the performance of in water R_{rs} -derived, we analysed the error ($\varepsilon_{\%}$) between two distinct methods (*A* and *B*) similar to Bélanger et al. (2013); Gordon and Ding (1992) (Equation 3.24):

$$\varepsilon_{\%} = 100 \left(\frac{R_{rs}^B(\lambda) - R_{rs}^A(\lambda)}{R_{rs}^A(\lambda)} \right)$$
(3.24)

The Figure 50 shows performance of $R_{rs}(\lambda)$ in-water derived using autonomous selection of the depth for $L_u(0^-, \lambda)$ extrapolation in the upper ocean layer in relation the algorithm evaluated by Bélanger et al. (2017). The box plot of relative percentual error ($\varepsilon_{\%}$: Equation 3.24) shows the autonomous selection of ideal depth to fit the extrapolation of $L_u(0^-, \lambda)$ to $L_u(0^+, \lambda)$ across the sea-air surface reached good performance because relatively low percentual error (i.e. $\varepsilon_{\%} \sim 0\%$) in the visible spectrum (400 to 700 nm), less human interactions to achieve $R_r s(\lambda)$, and ensures that L_u extrapolation is done in a layer in conform to the relation between in- and above-water downwelling irradiance ($E_d(0^-, \lambda)$ and ($E_d(0^+, \lambda)$).

3.7.2 Optically complex waters classification

We applied the case-1/-2 water classification scheme developed by Lee and Hu (2006) based on the remote sensing reflectance spectral ratios 412 to 443 (RR_{12} : $R_{rs}(412)/R_{rs}(443)$) and 555 to 490 nm (RR_{53} : $R_{rs}(555)/R_{rs}(490)$). 412, 443, 490, and 555 are the center wavelengths (in nm) of Sea-viewing Wide Field-of-View Sensor (SeaWiFS) bands 1, 2, 3, and 5, respectively. The follow empirical polynomial function (Equation 3.25) represents the Case-1 water monotonic relation presupposed to RR_{12} and RR_{53} :

$$RR_{12}^{CS1} = 0.9351 + 0.113/RR_{53} - 0.0217/(RR_{53})^2 + 0.003/(RR_{53})^3$$
(3.25)

where the superscript *CS* 1 represents Case-1. RR_{12} indicates the relative abundance of CDOM per [*chla*]. RR_{53} referred as a measurement of [*chla*], and $R_{rs}(555)$ as particle backscattering (Lee and Hu, 2006). Case-1 waters hold a monotonic relation between $R_{rs}(555)$ and RR_{53} (Equation 3.26):

$$R_{rs}(555) = 0.0006 + 0.0027 RR_{53} - 0.0004 (RR_{53})^2 - 0.0002 (R_{53})^3$$
(3.26)

The relations between RR_{12} and RR_{53} provide guidance on CDOM absorption in relation to [*chla*], while, RR_{53} and $R_{rs}(555)$ represent a monotonic relation of particle backscattering with [*chla*]. According Lee and Hu (2006), case-1 waters are bound in the monotonic Equations 3.25 and 3.26, allowing ±10% deviation of RR_{12} and ±50% desviation of $R_{rs}(555)$.

Figure 51-A and B show that case-2 water was predominant in the Baffin Bay and Hudson Bay. Figure 51-A points that [*CDOM*] and [*chla*] did not co-variate in large part of MIZ, Nelson river, and sediment-rich waters. The MIZ stations classified like case-2 waters (Figure 51-A) had RR_{12} ratio ($R_{rs}(412)/R_{rs}(443)$) smaller than RR_{12}^{CS1} , which indicates the relatively high CDOM compared to [*chla*]. Notably, $k_d(\lambda)$ magnitude (high, moderate, or low) did not reflect the case-1 or 2 water classification because the clusters classified like MIZ have components in both water case-1 and 2. The Figure 51-B shows that b_{bp} had a strictly relation to [*chla*] in MIZ stations. Nelson river station had relatively high $R_{rs}(555)$ (> 0.008 sr⁻¹) and mismatch with the band ratio $R_{rs}(555)/R_{rs}(490)$, which shows that Nelson river plume did not have a monotonic relation between [*chla*] and b_{bp} .



Figure 46: Light assimilation: (A) Instantaneous and (B) daily integrated Photosynthetic Usable Radiation (PUR) in the euphotic zone form in water profiles in relation to simulated from above water radiometry. (C) Boxplot of difference (ΔPUR) between instantaneous PUR measured in the water profiles and simulated from above water radiometry. The central red mark indicates the median, and the bottom and top edges of the blue boxes indicate the 25th and 75th percentiles, whiskers extend to the most extreme data points not considered outliers.



Figure 47: Salinity vs. maxima phytoplankton production in eastern Canadian Arctic. Photoacclimation relationships of maxima phytoplanktonic production normalized by chlorophyll-a concentration $(P_{max}^{B} \text{ in g C} (\text{g } chla)^{-1} \text{ day}^{-1})$ vs. salinity (*S* in PSU). P_{max}^{B} Average values and standard deviation $(\mu \pm \sigma)$ were shown for distinct light environments. *S* explains 81% of P_{max}^{B} variability in southern Hudson Bay and 41% in marginal-ice zone light environment with moderate light attenuation, but in high and low light attenuation *S* and P_{max}^{B} linear relations were not constrained.



Figure 48: Phytoplankton taxonomy in HB and BB. Variation in the relative abundance of phytoplankton groups at the surface (A and C) and at subsurface chlorophyll-*a* maximum (B and C) in the Hudson Bay System and the Baffin bay, respectively. The coefficient of correlation of the taxonomy composition between surface and SCM assembles is 0.95 with 99% of confidence in the Hudson Bay System.



Figure 49: Phytoplankton size structure community in spring-to-summer transition in eastern Canadian Arctic. The pigment-derived fractional contribution to [*Chla*] of three phytoplankton size classes in the sea surface layer: microplankton (>20 μ m), nanoplankton (2–20 μ m), and picoplankton (<2 μ m).



Figure 50: Remote sensing reflectance autonomous depth for sea-air extrapolation of upwelling radiance. Box plot of relative percentual error ($\varepsilon_{\%}$: Equation 5) between $R_r s(\lambda)$ inwater derived by Bélanger et al. (2017) algorithm and the implementation of the autonomous selection of the depth for $L_u(0^-, \lambda)$) extrapolation in the upper ocean layer during the Spring-Summer transition in the Hudson Bay 2018, and the Baffin Bay 2016.



Figure 51: Classification of optical water cases: (A) $R_{rs}(412)/R_{rs}(443)$ and (B) $R_{rs}(555)$ as a function of $R_{rs}(555)/R_{rs}(490)$. (A) The solid line corresponds to Equation 8 and the dashed curves shed curves to $\pm 10\%$, which stations inside these thresholds were included in case water-1. Symbols with the filled color indicated the stations that [*chla*] has a monotonic relation with particle backscattering (Equation 9). (B) The solid line corresponds to Equation 9 and the dashed curves to $\pm 50\%$. Symbols with filled color show stations classified as case water-1 (Equation 8).

Future Perspectives

4.1 Toward a satellite-derived phytoplankton production model extrapolated to underice.

Phytoplankton phenology in the polar region can be largely influenced by sea-ice thermodynamic stages at the end of the winter and in spring. Melt, pond, and drainage onsets, for example, are good indicators of the light transmission through the ice, which is a key component controlling the phytoplankton bloom initiation. The timing of physical processes is the center to understand the phytoplankton phenology. Events preceding a phytoplankton bloom, if well characterized can supply important information for quantifying, understanding, and predicting impacts on phytoplankton dynamics.

Ponds increase light transmission throughout the ice-pack (Arrigo et al., 2014; Frey et al., 2011) triggering the under-ice production season. Therefore, pond fraction and time of onset can control the balance between under-ice and pelagic production throughout the marginal-ice zones. This balance depends on timing in relation to the seasonal cycle of photosynthetic active radiation ($PAR(0^+)$) and nutrient availability. For example, in the case of the late melting season, the sea-ice transition to open waters will occur simultaneously to the seasonal peak of $PAR(0^+)$. In other scenarios, a long melting duration under low $PAR(0^+)$ cannot be efficient to deplete nutrients in the upper ocean layer, while a short melt duration in the peak of $PAR(0^+)$ can result in massive under-ice bloom and consequently an oligotrophic set-up in the pelagic system after the sea-ice retreat. To extrapolate the satellite-derived production model to under ice, we proposed to improve the sea-ice transmission models using sea-ice thermodynamic stages (i.e., melt, pond and drainage onsets, and ice-free season) (Horvat et al., 2017) detected by active microwave scatterometers, similar to (Howell et al., 2006) in the Arctic Canadian Archipelago. As an example to encourage this approach, Figure 52, presented in the Arctic Change meeting 2017, shows an evaluation of the QuikSCAT-derived sea-ice thermodynamic stages using high resolution (30 meters) multispectral imagery of Landsat.

4.2 Algae, ocean and cryosphere feed-backs: the bio-optical heating

In Arctic and Canadian sub-Polar systems, climatic changes ongoing leads to an enhancement of upper-ocean bio-optical complexity. Because open-water season lengthening leads to the arise of annual phytoplankton production (Ardyna and Arrigo, 2020), and continental drainage has driven an increase in colored dissolved organic matter (CDOM), and upper layer freshening (Morison et al., 2012; Matsuoka et al., 2016). The marine bio-optical state plays a role in ocean heating (Ohlmann and Siegel, 2000; Morel and Antoine, 1994) and atmospheric radioactive balance (Siegel et al., 1999; Bartlett et al., 1998). Bio-optical heating, in turn, influences ocean dynamics (i.e. $\nabla \vec{u}$), sea surface temperature (SST), thermal stratification (i.e. $\partial T/\partial z$) (Gera et al., 2020; Mallick et al., 2019; Zhai et al., 2011; Wu et al., 2007). For example, Zhai et al. (2011), based on an optically-coupled circulation model, reported that phytoplankton dynamics affect sea-ice thermodynamics as a consequence of its control on surface warming (> 2°C), subsurface cooling, and stabilization of water column in the Saint Lawrence Gulf, East Canada. The phytoplankton thermal energy dissipation (i.e., non-photochemical quenching) can account for 60% of the photosynthetic active quanta absorbed by phytoplankton globally (Lin et al., 2016).

The spectrum of solar incoming radiance at the sea surface is very sensitive to atmospheric conditions, bio-optical properties, and cloud structure (Siegel et al., 1999; Bartlett et al., 1998). However, the model generally negligence atmospheric influence on spectral radiance. For example, Bartlett et al. (1998) reported the spectral dependence of surface incoming radiation to cloud types in the Bering



Figure 52: Sea-ice thermodynamic stages detected by QuikSCAT and Landsat ETM+7 at 91°W 58°N in 2006 offshore the Nelson River. A) QuikSCAT time-series of σ_0 (black line), co-polarization ratio HH/VV (red line) applied to detect sea-ice stages using Howell et al. [2005, 2006, 2009] method based on dynamic thresholds, and sea-ice concentration (SIC) from passive microwaves (Comiso, 2000) (blue line). (B) Landsat ETM+7 true-color composite (RGB: bands 3, 2, and 1) on Jun 23 shows ice floes' interaction with coastal dynamic in the Nelson river plume, colored dissolved organic carbon resulting in dark waters. (C) True-color (RGB: bands 3, 2, and 1) and (D) thermal (RGB: bands 6, 5, and 4) composites equalized to highlight sea-ice patterns. During the consolidated sea-ice stage, widespread leads and long fractures (Feb 15) produce corner-reflection and high variability in the QuikSCAT time series. These features were releasing latent heat stoked in the upper ocean layer to the atmosphere as highlighted by Landsat thermal band 6 (10.40-12.50 nm). An increase of sea-ice fractures or leads, and a decrease in ice floe size, on April 4, marked the transition to the melt and pond onset. The melting process is intensified by ice floes dispersion. Around April 20, QuikSCAT detected the pond onset, while Landsat shows significant changes in the sea-ice floe size ranging from 1 to 5 km. Finally, even after QuikSCAT detection of open water onset (June 20) sea-ice floes remain as seen by Landsat corresponding to SIC of 50% (blue line, right axis). Source: Barbedo and Bélanger (2017) in Arctic change meeting, Québec City, QC (poster version: https://arcticnetmeetings.ca/pages/asm/2017/natural_sciences_marine)

Sea and the Atlantic North coast of Halifax, Nova Scotia. Siegel et al. (1999) pointed out that clouds attenuate long waves of solar radiation and reflect back light, predominantly in the blue–green spectrum, that has already been reflected on the sea surface or backscattered in water.

The performance of ice-ocean dynamic modeling depends on the dataset assimilation quality, which must well represent the environmental parameters and processes (Lovelock, 2003). However, bio-optical feedback has been overlooked. Advance of sea-ice and ocean modeling depends on a resolve the upper-ocean layer solar heating, which is mainly controlled by solar elevation, inherent optical properties Zhai et al. (2011); Kim et al. (2016); Mallick et al. (2019); Soppa et al. (2019); Gera et al. (2020), and cloud conditions (Okamoto et al., 2003; Stephens et al., 2008; Kato et al., 2011; Van Tricht et al., 2016; Ham et al., 2017; Papavasileiou et al., 2020).

Does the quality of ocean-state modeling in the Pan-Canadian Ocean rely on how ice-ocean dynamic models resolve feed-backs among cloud structure, bio-optical heating, optically complex water, seaice, and ocean dynamics? Do riverine input of organic matter and freshwater from continental drainage intensify bio-optical heating and sea-ice losses in the Pan-Canadian Ocean? Can phytoplankton mitigate the impact of climatic changes on the cryosphere? Satellite-derived cloud structure and ocean color data ingestion are in the state-of-art of ice-ocean dynamic modeling in Pan-Canadian Ocean (Smith et al., 2020). The Figure 53 shows a conceptualization of Cloudsat cloud profile, and light attenuation dedicated to resolving ocean heating in ice-ocean models in a Pan-Canadian perspective encompassing continental shelves and adjacent areas of the Arctic Ocean, North Atlantic, and North Pacific. This deep-level synergy can solve feedbacks between the atmosphere, continental drainage, cryosphere, ocean, and phytoplankton (Smith et al., 2020) and delivery us an essential scientific question to better understand how climate changes affect the Earth system.

4.3 A pan-Arctic perspective of climatic control on fall blooms

Understanding how the rise of air-sea momentum forced by the continued loss of sea-ice coverage affects biological production is critical for predicting the future of Arctic ecosystems (Armitage et al.,



Figure 53: Pacific, Atlantic, Arctic Canadian Systems: (A) Light attenuation coefficient at 490 ($k_d(490)$: m⁻¹) calculated using the quasi-analytical algorithm (QAA: Lee et al. 2005) in July 2019. Topography is obtained from the ETOPO1 global relief model (Amante and Eakins, 2009). CloudSat Profiler Radar (CPR) track 901 (red line) and it's respective (B) cloud optical thickness (τ_{cl}) atmospheric profile obtained from 2B-TAU product processed by the CloudSat Data Processing Center (CloudSat DPC website: http://www.cloudsat.cira.colostate.edu).

2020). As a research line for next publications about atmospheric forcing on fall bloom, this section presents a panorama of fall bloom development concerning major Pan-Arctic processes: the Beaufort Gyre, the Arctic polar vortex, and Pacific and Atlantic water exchanges. Nevertheless, we recognize that regional interplays of atmosphere, ocean structure, and phytoplankton dynamics are distinct between the Arctic bio-regions (Carmack et al., 2016).

In the Beaufort Sea, a high-pressure system typically gives rise to anticyclonic wind-driven surface stress generating the Beaufort Gyre (Morison et al., 2021; Armitage et al., 2020). Ekman-transport convergence elevates the sea surface height and deepens the halocline at the center of the Beaufort Gyre while storing the melt-freshwater inside the Beaufort Gyre and increasing the total freshwater content of the Arctic Ocean. Increased stratification because of freshening limits the transport of nutrients from deep layers and adjacent shelves, and constraints algae production (Morison et al., 2021; Armitage et al., 2020; Carmack et al., 2016). Conversely, the strengthening of the Arctic polar vortex, which is observed in positive phases of the Arctic Oscillation (Wang, 2021; Cornish et al., 2020; Armitage et al., 2018; Stroeve et al., 2011), can reverse the Beaufort Gyre in a cyclonic cell. Consequently, Beaufort Gyre releases freshwater into sub-arctic seas, relieves the Arctic upper-layer stratification (Morison et al., 2021; Solomon et al., 2020). As discussed by Hill et al. (2018), the weakening of stratification and shallowing of the Atlantic water mass can facilitate the impact of atmospheric forcings on the vertical transport of nutrients and favors the occurrence of fall blooms in the north Canadian basin.

Pacific and Atlantic water inflows have increased in the last decades in response to climatic changes, in a process referred to as Arctic Borealization (Polyakov et al., 2020). In the Atlantic-Arctic sector, the subsurface intrusions of Atlantic Water throughout the Fram Strait and the Barents Sea, and riverine inflow from the wide Siberian watershed intensify the upper layer stratification (Polyakov et al., 2020; Carmack et al., 2006). Storms and seasonal atmospheric cooling ocean can promote vertical transport of nutrients into the euphotic zones increasing fall production in nutrient-limited phytoplankton communities over the eastern Arctic shelves (Crawford et al., 2020; Ardyna and Arrigo, 2020; Ardyna et al., 2014). On the other hand, the intrusion of nutrient-rich Pacific Water throughout
the Bering Strait sustains high phytoplankton production in the western Arctic Ocean. Consequently, wind-driven and convective turbulence can collapse an ideal water column structure for light-limited phytoplankton communities resulting in a negative impact on phytoplankton production on western Arctic shelves (Ji et al., 2019; Coupel et al., 2015).

global conclusion

5.1 Synopsis

To investigate the environmental control of algae dynamics in the eastern Canadian Arctic, we focus on the Hudson Bay System. This thesis is the first to address phytoplankton dynamics in the Hudson Bay from remote sensing ever published. Satellite observations of ice-edge blooms and sea-ice retreat enlightened how climatic-changes impact the balance between under-ice and pelagic production throughout marginal ice edge zones. We applied wide synergy embracing ocean color satellites, seaice remote sensing, climatic reanalysis, dynamic modeling, and in situ marine bio-optics to expose the mechanism to trigger, maintain, photo-acclimation, and the potential productivity of phytoplankton fall blooms. After enlightened the phytoplankton dynamics in the Hudson Bay, in the optic of remote sensing, we analyzed the phytoplankton production assessment to unveil the sensitivity of satellitederived production to environmental forcings and parametrizations.

5.2 Major contributions on this thesis

5.2.1 Marginal ice blooms

In the first chapter, we quantified the impact of the timing of sea-ice retreat on ice-edge bloom magnitude using two decades of ocean color remote sensing. Although sea ice masks under-ice blooms, satellite observations of chlorophyll-*a* concentration in ice-edge zones allowed us to estimate phytoplankton phenology throughout marginal ice zones. Sympagic communities and under-ice-blooms have less time to consume nutrients in marginal ice zones when sea-ice retreats early, therefore, allowing massive ice-edge blooms. Oppositely, snow-ice melting, ponds, and delays on sea-ice retreat permit long-exposure of light beneath ice-pack leading to depletion of upper layer nutrients stocks before ice-edge bloom development. This process drives an oligotrophic upper layer set-up and the development of sub-surface chlorophyll-*a* maximum.

5.2.2 The northwest Hudson Bay (Kivalliq) polynya

The westerly winds and low atmospheric temperatures in the positive phase of the North Atlantic Oscillation/Arctic Oscillation (NAO/AO) activate the Kivalliq polynya (i.e., the northwest Hudson Bay polynya) in winter. Alone the NAO index can explain as much as 40% of the variance in the MIZ bloom intensity in the polynia. The activation of Kivalliq polynya intensifies sea-ice production/export, brine rejection, vertical mixture, and nutrient replenishment from the deep-nutrient pool in winter. These pre-conditions result in massive ice-edge blooms during the spring-to-summer transition. On the other hand, in a warming Arctic scenario, zonal heat-flux exchanges between the Arctic and low-latitudes result in a relaxation of the north polar vortex, waving of polar jets, and weakening of westerlies, which leads to a less dynamic Kivalliq polynya in winter, is a vibrant ecosystem for marine polar life and drives the production in Hudson Bay. These results should alert the scientific community and Canadian society about the negative impacts of Arctic warming on the ecosystem functioning of the Hudson Bay System.

5.2.3 Ocean color assessment of phytoplankton photophysiology in complex waters

Ocean color was proven efficient to phytoplankton photo physiology even in optically complex waters. Two decades of ocean color satellites revealed seasonal fluctuations of $b_{bp}(555):[chla]$, a proxy for $C_{phy}:[chla]$. The most expressive seasonal event of photoacclimation occurs in the summer. When oligotrophy and insulation (i.e., high solar elevation) facility the proliferation of small cells with low intracellular chlorophyll content, which leads to bay-wide satellite observations of a high $C_{phy}:[chla]$. We investigated ocean color satellite-derived phytoplankton photo physiology to assess fall bloom productivity. Even that, large cells with high intra-cellular high-pigment content advected from subsurface chlorophyll maximum can result in satellite-derived overestimation of production and biomass. Fall blooms had a similar signature of C_{phy} :[*chla*] observed in blooming phytoplankton in marginal ice zones in spring. In north polar seas, the fall bloom phenomenon is potentially productive and composed of an assembly of two phytoplankton communities well-acclimated to low light and turbulence, one seed from the sub-surface by mixing and the other remained in the upper layer since summer.

5.2.4 Environmental controls of algae phenology in Hudson Bay revisited

The double bloom feature, i.e., ice-edge blooms in spring and fall blooms intercalate with an oligotrophic set up in summer, became the dominant phenology in Hudson Bay as well as in Pan-Arctic. Satellite ocean color has proven effective to depict the algae processes in marginal ice zone and the seasonal variability of photophysiology. However, little is known about the environmental processes controlling the transition of oligotrophy in the summer to fall bloom phenomenon. Therefore, how do fall blooms are triggered and maintained? Here, to enlighten how the interplay of atmospheric forcing and water column structure influence phytoplankton phenology in Hudson Bay. An embracing synergy depicted the very distinct pattern of ice edge-blooms, summer oligotrophy, and fall blooms in terms of atmospheric forcing, water column structure, and stratification.

The nutrient stocks from winter pre-conditions, drainage continental, and freshwater lenses produced by ice melting are a conduit to algae production in the upper layer in marginal ice zones. The sea-ice break-up reconnects atmospheric and ocean fluxes. Then, the atmospheric heat transference to the ocean actuates expanding mixer layer depth and ventilating pycnocline. This process leads the freshwater lens dissipation until the stratification typology changes from salinity-gradient- to temperature-gradient-controlled. Consequently, satellite ocean color observed an oligotrophic setup of low phytoplankton abundance in the upper layer, concomitant to the development of sub-surface chlorophyll-*a* maximum in summer. In the fall season, the atmospheric-cooling ocean disrupts stratification and upper-layer structure. This process leads pycnocline and mixed layer to trespass the euphotic-zone

depth increasing the nutrient transport by mixture to the upper ocean layer that triggers fall blooms.

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