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Comparison of Remotely-Sensed Sea Surface Temperature and Salinity Products With *in Situ* Measurements From British Columbia, Canada

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Sea surface temperature (SST) and salinity (SSS) are essential variables at the ocean and atmosphere interface when considering risk factors for disease in farmed and wild fish stocks. Ecological research has witnessed a recent trend in use of digital and satellite technologies, including remote-sensing tools. We explored spatial coverage of remotely-sensed SST and SSS data and compared them with *in situ* measurements of water temperatures and salinity, which led to suggested adjustments to the remotely-sensed data for its use in aquaculture research. The *in situ* data were from farms and wild surveillance sites in coastal British Columbia, Canada, from 2003 to 2016. Concurrent SST and SSS values were extracted from remotely-sensed products and compared with 20,513 and 20,038 *in situ* records for water temperature and salinity, respectively, from 232 different sites. Among nine SST products evaluated, the UKMO OSTIA SST (UK Meteorological Office) had the highest retrieval, and highest concordance correlation coefficient (0.86), highest index of agreement (0.93), fewest missing values, and smallest mean and SD values for bias, when compared to *in situ* measurements. A mixed linear regression model with UKMO OSTIA SST as the predictor for *in situ* measurements estimated an adjustment coefficient of 0.89°C for UKMO OSTIA SST. None of the three SSS products evaluated provided appropriate corresponding values for *in situ* sites, suggesting that spatial coverage for the study area is currently lacking. This study demonstrates that, among SST products, UKMO OSTIA SST is currently best suited for aquaculture studies in coastal BC. The near real-time availability of these data with the estimated adjustment would allow their use in forecast models, surveillance of pathogens, and the creation of risk maps.

Keywords: sea surface temperature, sea surface salinity, *in situ*, satellite remote sensing, MODIS, aquaculture

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INTRODUCTION

Maritime aquaculture activities are affected by oceanographic properties that regulate physical and biogeochemical processes throughout the ecosystem. Critical environmental variables such as water temperature, salinity, and oxygen influence fish bioenergetics, health, and reproduction, and can affect interactions between farmed and wild fish, as well as other ecosystem functions

(Bowden, 2008; Maynard et al., 2016). There is a need for broad-scale oceanographic data to support assessment and management of stocking density, farm-fallow cycles, and fish health. These data are also critical for establishing the initial and boundary conditions of ecosystem models used for ecosystem-based management, allowing assessment of ecological carrying capacity and environmental effects (Filgueira et al., 2013). Environmental data (e.g., water temperature and salinity) are often recorded at farm sites, but often *in situ* data have missing values, while corresponding *in situ* data for wild salmon habitat rarely exist. Remotely-sensed (RS) data, captured via satellites, may be used as a substitute to fill data gaps at lower costs than *in situ* or ship-based sampling. In addition, RS tools may contribute to sustainable blue growth in the aquaculture sector by providing observation-based evidence in support of decisions for monitoring and mitigating diseases, and in adapting to changes associated with warming oceans (Santos, 2000; Zagaglia et al., 2004; Williams et al., 2010; Bojinski et al., 2014).

Ecological, oceanographic, and biogeographical research have seen increased use of digital and satellite technologies (Ferreira et al., 2012), which can provide synoptic data at high spatial and temporal resolutions for studying the Earth's surface, atmosphere, and oceans (Horning et al., 2010). Satellite sensors provide data for oceanographic and climate models that promote forecasting and prediction for fisheries and aquaculture management.

Active and passive satellite RS can be used to measure variables at the ocean surface, including surface roughness, wave height, suspended particulate matter, sea surface temperature (SST), sea surface salinity (SSS), and ocean color (Le Traon et al., 2015). The World Meteorological Organization has designated SST and SSS as essential climate variables at the interface of the ocean and atmosphere (Ishii et al., 2005; Hollmann et al., 2013; GCOS, 2015). While RS measurement of SST is well-established (Casey et al., 2010), salinity has not yet achieved comparable spatial resolution (Lagerloef et al., 1995, 2008). These data are available for several combinations of spatial and temporal resolutions (Savtchenko et al., 2004), and at multiple processing levels, ranging from uncalibrated raw data to fully integrated modeled products. However, attempts to incorporate this wealth of data into practical research in areas such as aquaculture are often hindered by a lack of understanding of the products' uncertainties, spatial and temporal heterogeneity in oceanographic properties (particularly in coastal areas where aquaculture occurs), and the lack of consistency and continuity among the satellite-derived products (Hollmann et al., 2013).

Sea surface temperature and salinity are important variables, from the perspective of disease and the productivity of farmed and wild fish stocks (Mueter et al., 2002; Malick and Cox, 2016; Maynard et al., 2016). Temperature regulates metabolic processes in finfish, including respiration, growth and feed conversion ratios (Handeland et al., 2008), and has an impact on the immune system (Bowden, 2008). Temperature also affects the ability of the surrounding ecosystem to metabolize waste products and uneaten feed, influencing oxygenation, and creating an important link between fish and ecosystem health (Findlay and Watling, 1997). Connectivity within and among wild and farmed fish populations is dependent upon abiotic factors such as temperature, salinity, and ocean circulation, which affect survival and dispersion of parasites and pathogens (Stien et al., 2005; Stucchi et al., 2011; Rogers et al., 2013; Rees et al., 2015). The spatial dynamics of parasites and pathogens of fish are likely to be affected by weather events, seasonality, and climate change, which may influence dispersal and population structures with implications for fish health (Harvell et al., 1999; Marcogliese, 2001; Altizer et al., 2006). As such, accurate measurements of temperature and salinity are prerequisites for the creation of oceanographic circulation models used in various aspects of aquaculture planning and regulation (Brewer-Dalton et al., 2015; Foreman et al., 2015).

Since most marine finfish aquaculture occurs within the coastal zone, salinity and temperature regimens can be dynamic (Groner et al., 2016). Salinity near salmon farms is influenced by fresh water inflow from rivers and precipitation, coastal and oceanic water exchange, mixing of the water column (due to wind and tides), estuarine circulation, and inlet bathymetry. Water temperature is influenced by many of these same factors, as well as by atmospheric and oceanic heat exchange (Jones and Beamish, 2011; Jones and Johnson, 2015).

Gridded oceanic RS data are usually satisfactory for offshore areas and larger spatial or temporal scales, such as regional phenomena or weekly/ monthly aggregates (Castillo and Lima, 2010; Smit et al., 2013). However, the same data may not be equally suitable in coastal waters, where the spatial resolution of SST and SSS satellite products, with pixel edge lengths of 1 km or larger, are generally too coarse to adequately capture coastline features (Urquhart et al., 2012). Satellite remote sensing in coastal zones can be complicated by weather patterns and dissolved organic compounds of terrestrial origin, such as tannins, that may attenuate signals and yield unreliable results. As a result, many processed RS products apply a land mask that excludes mixed pixels in nearshore areas and use temporal averaging to account for missing observations. Previously published studies comparing *in situ* water temperature measurement in coastal waters suggest significant differences in agreement among RS SST products across geographical regions (Castillo and Lima, 2010; Smit et al., 2013; Williams et al., 2013; Stobart et al., 2015; Wu et al., 2016).

Given the large spatial extent of aquaculture in British Columbia (BC) and the spatio-temporal variability of influential factors on environmental determinants, investigation of corresponding RS-data for use in aquaculture research in BC is prudent to assess their reliability as surrogates for *in situ* measurements. The objectives of this study were to explore the spatial coverage of remotely-sensed SST and SSS data for coastal areas of BC, to compare RS data with *in situ* measurements of water temperatures and salinity, and to suggest adjustments for the use of such data in aquaculture research.

MATERIALS AND METHODS

Sources of Data

In Situ Data

In situ water temperature and salinity data were collected by salmon farm operators and the Broughton Archipelago

Management Plan research project (BAMP, 2010) during wild fish surveillance for sea lice. Most farms ($n = 19$) and wild fish surveillance sites ($n = 192$) were in the Broughton Archipelago, while a smaller number of sites (5 farm and 16 wild sites) were located in Muchalat Inlet on the west coast of Vancouver Island, British Columbia (**Figure 1**). Salinity and temperature measurements were taken at wild sites using either YSI® 85 or YSI® 6-series multi-parametric sondes (YSI Incorporated, www.ysi.com). At farm sites, these were measured using an RHS-10ATC refractometer (Huake Instrument Co, Guangdong, China), and an OxyGuard Handy Polaris portable meter (Arriagada et al., 2016). Farm measurements were taken at the surface (<20 cm) and at depths of 1, 5, 10, and 15 m, while wild site measurements were taken at the surface (<20 cm) and at depths of 1 and 5 m. Water temperature and salinity were recorded up to two decimal points in degrees Celsius and parts per thousand (ppt) respectively, daily, for the whole year, for each salmon farm site (when sites were active), at the same location and at approximately the same time each morning. Wild fish surveillance measurements were collected weekly between March and July of each year at different times during the day. We had access to *in situ* data from 2003 to 2016. *In situ* data were checked for consistency, and likely data entry errors were replaced with missing values.

Remote Sensing Data

We used level 3 and 4 gridded RS data products in this study. The level 3 "composite" products provide data for variables mapped on uniform space-time grids, usually with some averaging, but do not perform any gap-filling or interpolation. The level 4 "analysis" products are generated by combining several sources of SST data (e.g., satellites, moorings, and ship-based observations) through statistical interpolation and temporal averaging (Martin et al., 2012). These products provide gap-free gridded outputs (Parkinson et al., 2006), and are thought to provide the best available estimates of SST/SSS through data assimilation of available datasets. They provide global coverage and foundational estimates free of diurnal variation (Piolle et al., 2010; Donlon et al., 2012), which are representative of bulk ocean properties; in contrast to the skin or sub-skin estimates provided by the infrared (IR) or microwave satellite sensors (Beggs, 2010; Donlon et al., 2012). Hereafter, the terms "level 3 composite products" and "level 4 analysis products" refer to direct satellite-derived level 3 data, or estimates based on analysis and interpolation of SST/SSS products, respectively. We assessed products that were freely available, widely used, active at the time of study, and effective for coastal data retrieval (Yuan, 2009).

The daily SST level 3 composite product, with 4.6 and 9 km spatial resolution captured via the MODIS (Moderate Resolution Imaging Spectroradiometer)[1] sensor on board the Aqua and Terra satellites, and the daily SSS level 3 composite product with 1 degree spatial resolution, captured via SSS sensors on board the Aquarius satellite, were obtained from the Ocean Color website (https://oceancolor.gsfc.nasa.gov/). These daily SST and SSS level 3 composite products are processed and maintained by the NASA Ocean Biology Processing Group. A second daily SSS level 3 composite product from the Soil Moisture and Ocean Salinity (SMOS) satellite of the European Space Agency was acquired, along with daily SST and SSS level 4 analysis products from the Copernicus Marine Environment Monitoring Service of the European Union (CMEMS)[2]. **Table 1** presents the details on the SST and SSS products evaluated, indicating source availability and spatial-temporal resolution.

Remotely-sensed data for the corresponding *in situ* sites (wild and farm) were retrieved from each of the selected SST and SSS products for the study duration (2003–2016), using the *raster* (Hijmans and van Etten, 2014) and *ncdf4* (Pierce, 2012) packages for the R software environment (R Core Team, 2015).

Statistical Comparison

The statistical analyses were performed using Stata (Release 14.1; StataCorp, College Station, TX, USA, 2015) and R version 3.4.1 (R Core Team, 2015) using packages hydroGOF (Zambrano-Bigiarini, 2011) and nlme (Pinheiro et al., 2017). The *in situ* measurements at 1 m depth were deemed to be the best/most reasonable depth to compare with RS measurements. A number of metrics were used to assess the relationship between products and *in situ* measurements. First, the difference between the two measurements (value from the overlapping pixel of the RS product minus the *in situ* measurement, referred to as "bias") was computed. The mean, standard deviation (SD), and root mean square error (RMSE) of these biases were estimated. Pearson correlation coefficients and concordance correlation coefficients (CCC) between pairs of measurements were also computed. The CCC (Lin, 1989) provides an indication of agreement between two measurements (see Appendix for formula), with values close to 1 indicating very good agreement and values approaching zero reflecting very poor agreement. As in the case of Pearson's correlation, this coefficient is dimensionless; however, CCCs are penalized (adjusted downward) to account for both location- and scale-shifts between measurements, as opposed to simply describing their linear dependence (Pearson correlation).

The spatial footprint of the *in situ* measurements was point-based, while that of the composite and analysis products was a 2-dimensional pixel that occasionally encompassed multiple *in situ* points. To evaluate the impact multiple sites within a pixel could have on our metrics we averaged all *in situ* measurements for a given day, within a pixel, and compared this value to the measurements from the RS products.

We also compared larger temporal windows (weekly and monthly averages), as these better reflect the temporal scales likely to be encountered in aquaculture research. We used index of agreement (d-index) to compare *in situ* measurements with RS products; this approach has been widely used to assess the performance of hydrologic models (Zambrano-Bigiarini, 2011). The d-index (see Appendix for formula) represents the

[1]NASA. *Goddard Space Flight Center, Ocean Ecology Laboratory, Ocean Biology Processing Group. Moderate-resolution Imaging Spectroradiometer (MODIS) Aqua Sea Surface Temperature Data; 2014 Reprocessing*. Greenbelt, MD: NASA OB.DAAC. (Accessed July 3, 2016).

[2]CMEMS. *Copernicus Marine Environment Monitoring Service (European Union)*. Available online at: http://marine.copernicus.eu

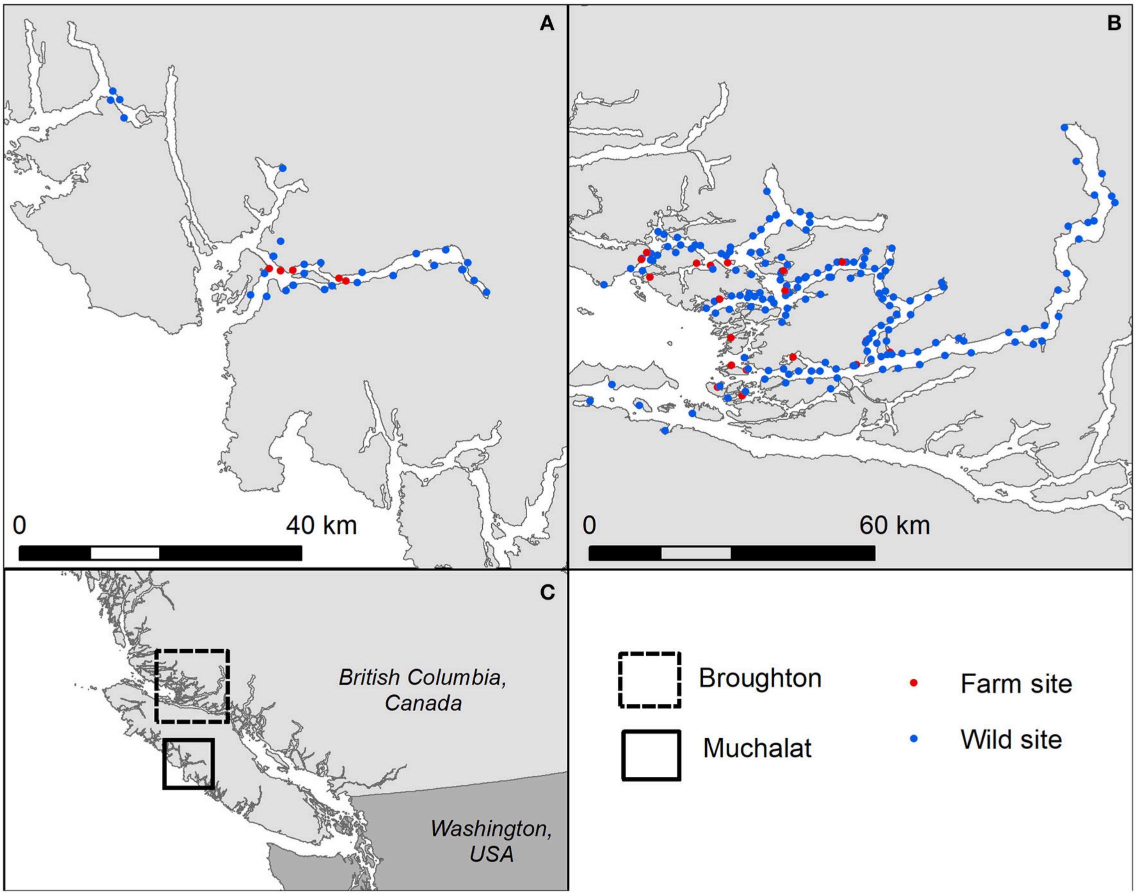

FIGURE 1 | Locations where *in situ* water temperature measurements and corresponding satellite-derived SST values were obtained for each of the study regions **(A)** Muchalat Inlet and **(B)** Broughton Archipelago, with **(C)** inset map showing administrative boundaries of British Columbia.

ratio between RMSE and the potential error between the two measurements (Willmott, 1984; Swierczynska et al., 2016). It is also dimensionless, with a value that ranges from 0 (no agreement at all) to 1 (perfect agreement), and is sensitive to differences between two measurements.

Finally, in order to adjust for differences, a mixed linear regression model was fitted to predict the *in situ* measurement, using the best performing RS product as the predictor, with sampling site as a random effect (allowing capture of the variability in both the intercept and the coefficient of the predictor), and accounting for autocorrelation between residuals of daily measurements within each site with a first-order autoregressive (AR1) or exponential autocorrelation structure. In order to meet the assumption of linearity, the fitted model also tested functional forms of the predictor using quadratic terms (both as fixed and random effects) and evaluated the fit of the model using both the significance of the additional terms and likelihood ratio test for the nested models. For this analysis, pixels were not included as a random effect due to limited replication at that level.

RESULTS

The total numbers of available daily *in situ* measurements, from the years 2003–2016, for water temperature and salinity at 1 m depth, were 20,513 (18,093 from farm sites) and 20,038 (18,563 from farm sites), respectively. The mean *in situ* water temperature and salinity was 10.07°C (range 2.60–21.80) and 23.44 ppt (range 0–33), and varied between the two study areas. The seasonal means for water temperature and salinity were 7.27, 10.44, 13.16, and 8.87°C, and 24.94, 22.43, 22.88, and 23.70 ppt, respectively. Due to many days of cloud cover and the fact that some sites (32, mostly wild surveillance sites) were beyond the satellite coverage area (see **Figure 2**), a smaller number of matched observations was available for comparison for the SST products. The groups of spatio-temporally (by site and date) matched *in situ* and SST measurements varied for each of the products (see **Table 2**).

The mean bias (°C), its SD, and the RMSE for each RS SST product, along with the corresponding Pearson correlation coefficient, CCC, index of agreement (d-index), and proportions of missing data are summarized in **Table 2**. Of the SST products

TABLE 1 | Summary of the level 3 composite and level 4 analysis and modeled SST/SSS products evaluated in the present study.

Name of products	Source	Type	Resolution		Comments	Availability[g]
			Spatial	Temporal		
A. SST PRODUCTS						
Aqua SST 11 μ	MODIS[a]/NASA[b]	Level 3 composite	∼4 km	Daily	Day	July 2002-present
Aqua NSST 11 μ					Night	
Aqua SST4 4 μ					Night	
Aqua SST9 4 μ			∼9 km		Night	
Terra SST 11 μ			∼4 km		Day	February 2000-present
Terra NSST 11 μ					Night	
UKMO OSTIA SST*	UKMO[c]	Level 4 analysis	1/20 degree (∼6 km)		Day+Night	April 2006-present
ODYSSEA SST*	CERSAT[d]		0.1 degree (∼11 km)		Night	August 2007-present
G1SST (Global 1 km SST)*	JPL[e]		1 km		Day+Night	August 2010-present
B. SSS PRODUCTS						
Aquarius SSS	NASA[b]	Level 3 Composite	1 degree (∼110 km)	Daily	–	August 2011-present
SMOS SSS*	European Space Agency		1 degree (∼110 km)		–	January 2010-present
Global Ocean Physics SSS*	Mercator Ocean[f]	Modeled[h]	1/12 degree		–	December 2006-present

[a] *Moderate Resolution Imaging Spectroradiometer on board Aqua and Terra satellites respectively (Minnett et al., 2004).*
[b] *https://oceancolor.gsfc.nasa.gov/cgi/l3; 4 and 11 μ define short- and long-wavelength SSTs.; SST4 and SST9 designate spatial resolution of 4 and 9 km.*
[c] *Meterological Office UK; data sources include remote-sensing devices with IR and microwave sensors, and in situ data from ships, drifting, and moored buoys (Donlon et al., 2012).*
[d] *French ERS Processing and Archiving Facility (Autret and Piollé, 2007; Piolle et al., 2010).*
[e] *Jet Propulsion Laboratory; data sources include IR and microwave satellite sensors and in-situ SSTs (Chao et al., 2009).*
[f] *http://www.mercator-ocean.fr/en*
[g] *Updated near real-time.*
**Obtained via the Copernicus Marine Environment Monitoring Service of European Union (http://marine.copernicus.eu).*
[h] *The modeled product employ knowledge of ocean dynamics and assimilate other SSS products.*

evaluated, UKMO OSTIA SST (UK Meteorological Office), a level 4 analysis product, had by far the highest retrieval (fewest missing data), the largest correlation coefficient (0.88), CCC (0.86), and d-index (0.93), and the smallest mean and SD for the bias (−0.14 and 1.40, respectively). The plots of the *in situ* water temperature measurements for the SST products are presented in **Figure 3**, which indicates a noticeably strong linear relationship, with some dispersion, between *in situ* water temperature and UKMO OSTIA SST.

Of the 14,506 spatio-temporally matched *in situ* measurements with UKMO OSTIA SST, 61% were single measurements within a pixel and day, while 36% of the measurements included two sites within the same pixel and day. The maximum number of sites within a pixel and day was four. After accounting for multiple *in situ* sites within a pixel/day ($n = 11{,}595$), the mean bias and the SD of the mean bias was 0.06 and 1.4°C, respectively, while the correlation coefficient and the CCC were 0.87 and 0.85, respectively.

The correlation coefficients (0.89 and 0.90) and the CCCs (0.87 and 0.88) increased marginally when weekly and monthly averages of UKMO OSTIA SST were compared with *in situ* measurements, suggesting a marginal increase in similarity when measurements were averaged over a longer period. However, the magnitude of the bias remained unchanged (−0.14), with a slight decrease in variability (SD: 1.30 and 1.22, respectively). Similarly, the correlation coefficients were higher for the subset of the data that included only farm sites, than for those from wild surveillance sites (0.90 compared to 0.83, respectively), as was the case for the CCCs (0.88 and 0.64). This suggests higher variability in the *in situ* measurements from wild surveillance sites.

The retrieval rates of level 3 composite SST values and their respective statistical comparison with *in situ* data, using Terra and Aqua satellites with 9 km spatial resolution, were not different from SST values retrieved from Aqua satellites with 4 km spatial resolution (**Table 2**); thus, summary statistics for those SST products are not presented. Among other level 4 analysis SST products, G1SST (Global 1 km SST) had very limited coverage for our study sites, with many missing values, and the ODYSSEA SST had poor correlation (<0.30) with *in situ* measurements, so detailed statistics for these products are not presented.

Due to the higher variability of *in situ* measurements from the wild surveillance sites, the regression model included only measurements from farm sites. A mixed linear regression model with UKMO OSTIA SST as the predictor for *in situ* measurement estimated an average coefficient of 0.89°C ($p < 0.001$) for UKMO OSTIA SST across sites that varied between 0.22 and 1.56°C, 95% of the time (**Table 3**).

None of the level 3 composite SSS products (Aquarius and SMOS) evaluated provided corresponding values for *in situ* records, mostly due to their lack of spatial coverage (see **Figure 2D**) for the study area. The modeled SSS product did have partial coverage for our study area, but the retrieved values had poor correlation (<0.20) with *in situ* salinity measurements, and detailed statistics for these products are not presented.

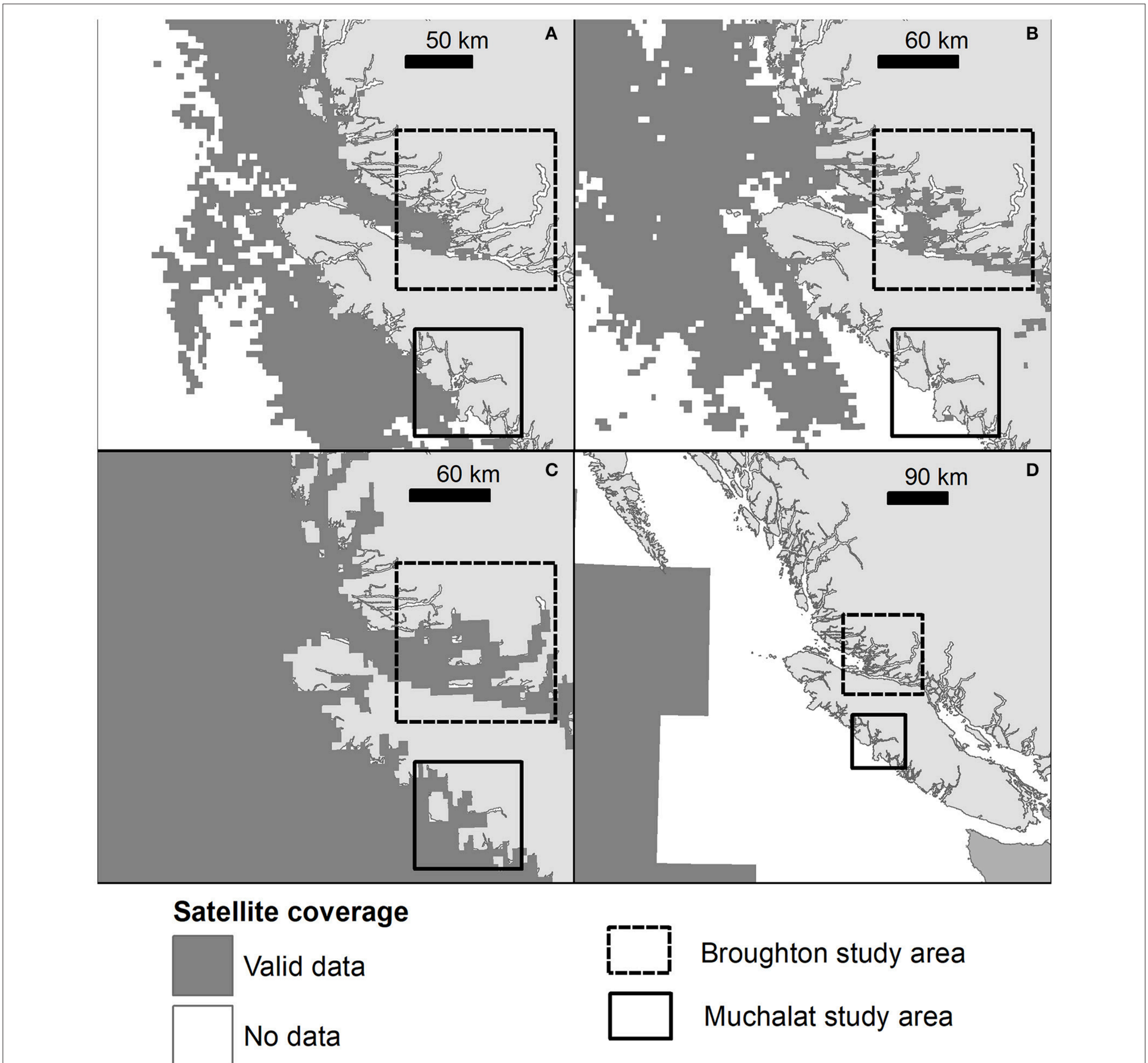

FIGURE 2 | Representation of coverage (for randomly picked dates) of some of the level 3 composite and level 4 analysis SST and SSS product/s for the study sites. **(A)** Aqua NSST 11 μ, **(B)** Aqua SST 4 μ, **(C)** UKMO OSTIA, SST, and **(D)** Aquarius SSS (right). Maps on the top panel and bottom left are on the same scale.

DISCUSSION

The main objective of this study was to evaluate whether satellite-derived SST and SSS products provide representations of temperature and salinity in marine ecosystems that would make them suitable as surrogates for environmental variables in aquaculture research. To the best of our knowledge, this is the first study to utilize existing *in situ* data from fish farms and wild surveillance programs to assess the suitability of RS SST and SSS products.

Our study demonstrated that of the SST products considered, the UKMO OSTIA SST was the most representative of the water temperature profile in coastal BC, Canada. A linear mixed model, after adjusting for autocorrelation, suggested that between-site variation was significant. The UKMO OSTIA SST (a level 4 analysis product) uses satellite SST data provided by international agencies via the Group for High Resolution SST (http://www.ghrsst.org), which include data from both microwave and IR satellite instruments, as well as *in situ* SST data (Donlon et al., 2012). The SST level 3 composite products we evaluated were

TABLE 2 | Mean bias and correlations between remotely-sensed (level 3 composite and level 4 analysis) SST products and *in situ* water temperature (at 1 m depth) from 2003 to 2013[!].

SST Products	N[a]	Missing data (%)[b]	Mean bias (°C)	SD[c] of the bias	RMSE[d]	Correlation[e]	CCC[f]	d-index[g]
Aqua SST 11 µ	747	95.4	−0.83	4.156	2.214	0.642	0.525	0.72
Aqua NSST 11 µ	737	94.6	−1.13	3.193	1.923	0.771	0.665	0.81
Aqua SST4 4 µ	3,533	82.2	−1.40	2.377	1.712	0.834	0.743	0.86
UKMO OSTIA SST	14,506	1.61	−0.14	1.40	1.384	0.880	0.860	0.93

[!] *UKMO OSTIA SST data availability started in April 2006.*
[a] *Number of spatially and temporally (by site and date) matched in situ and SST records.*
[b] *Missing values calculated after removing all the sites that were consistently beyond the coverage area for all of the above products.*
[c] *Standard deviation.*
[d] *Root mean square error.*
[e] *Pearson correlation coefficient.*
[f] *Concordance correlation coefficient.*
[g] *Index of agreement.*

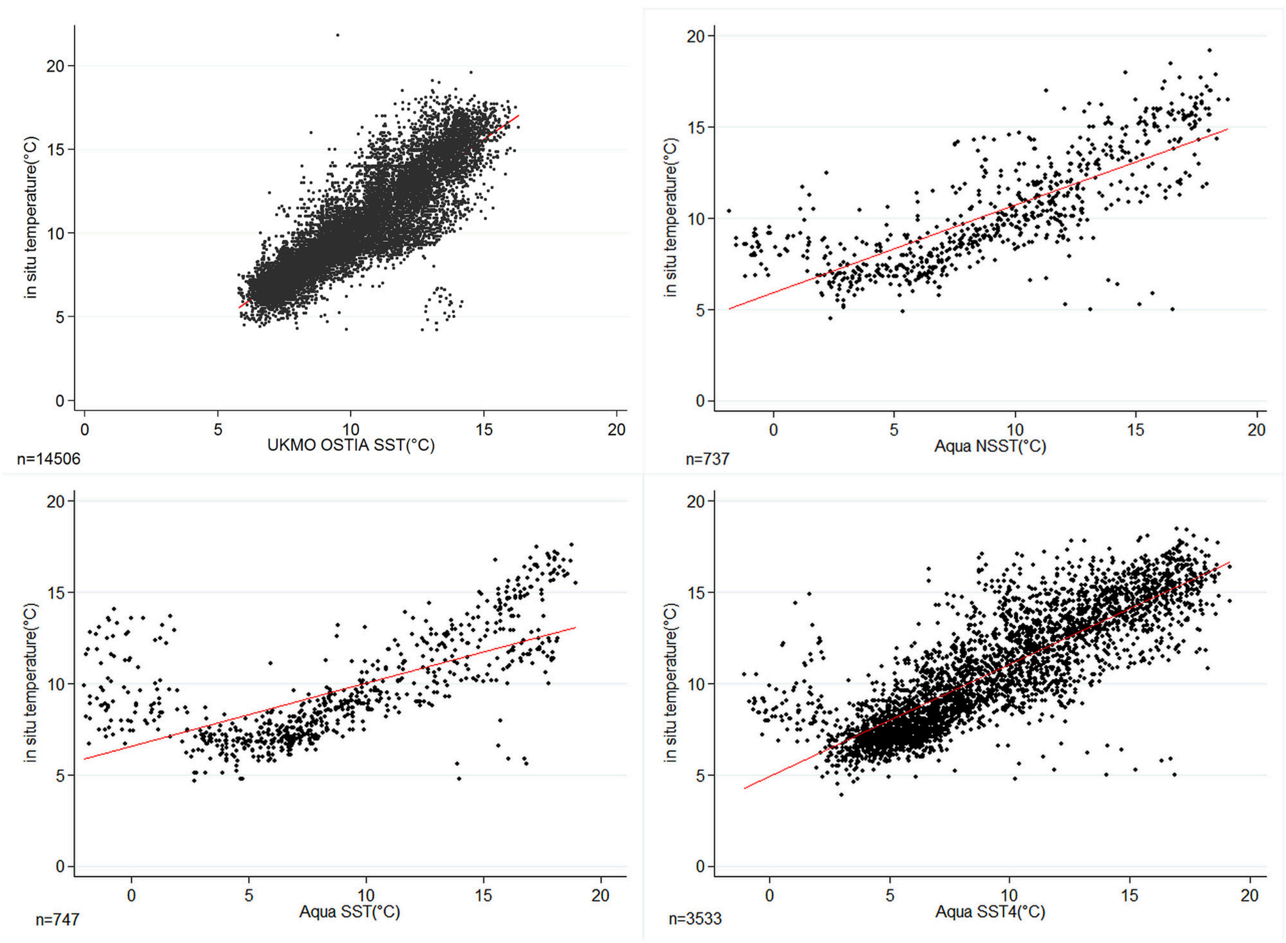

FIGURE 3 | Scatter plots of *in situ* water temperature (at 1 m depth) to that of each of the satellite-derived SST products (level 3 and level 4) for several sites in the Broughton Archipelago and Muchalet Inlet in coastal British Columbia.

often missing information for the study sites, likely due to poor satellite coverage, application of a land mask, or cloud cover (Webster et al., 1996; Guan and Kawamura, 2003). Similar observations for coastal areas have been noted by other studies (Castillo and Lima, 2010; Smit et al., 2013), but the proportion of missing values (80–90%) for some products in our study area was strikingly high, something not reported in previous studies. Nevertheless, the magnitude of bias and correlation between the

TABLE 3 | Estimates from the linear mixed model, with UKMO OSTIA SST as the predictor, to adjust for *in situ* measurements (outcome) from coastal British Columbia, with sites as the random intercept and UKMO OSTIA SST as random slope ($n = 12{,}759$).

Parameter	Coefficient	SE[a]	*p*-value	[95% Confidence interval]	
Intercept	0.931	0.634	0.142	−0.312	2.174
UKMO SST	0.890	0.081	<0.001	0.731	1.050
RANDOM-EFFECTS PARAMETERS					
SiteID: Identity					
SD[b] (Intercept)	2.665				
SD[b] (UKMO OSTIA SST)	0.344				
Correlation (Intercept, UKMO OSTIA SST)	−0.995				
Residual: AR(1)					
Rho	0.792	.	.	.	
SD[b] (Residual)	0.978				

[a]Standard Error.
[b]Standard Deviation.

in situ and RS level 3 composite SST products were comparable to those of other published studies (Castillo and Lima, 2010; Williams et al., 2013).

Our analysis also suggested that the UKMO OSTIA SST measurements were in closer agreement to *in situ* measurements from farm sites than for wild surveillance sites. The wild surveillance site measurements were captured from shallower waters close to coastlines, and this may have resulted in lower correlation coefficient and CCC values. None of the SSS products evaluated appeared promising for use in aquaculture studies, either due to lack of coverage or very poor correlation with *in situ* measurements. One of the underlying reasons for this is that, to date, all level 3 composite and modeled SSS products have focused on open ocean rather than coastal applications. The spatial resolution of data from the ESA's Soil Moisture and Ocean Salinity as well as NASA's Aquarius missions are too coarse for coastal and estuarine environments (**Figure 2D**; Urquhart et al., 2012). In time, finer resolutions, such as that offered by NASA's Soil Moisture Active Passive mission, or novel methods based on selected wavelengths of RS reflectance may provide improved estimates of SSS (Urquhart et al., 2012; Qing et al., 2013).

It should also be noted that certain inherent characteristics of the SST products affect both the retrieval rate and the correlation with *in situ* measurements. For example, SST products from IR sensors, such as those on MODIS, are sensitive to cloud cover (a primary cause of missing data), while those from microwave sensors are sensitive to precipitation, land contamination, and surface roughness (Donlon et al., 2012). Microwave sensors are limited to much coarser spatial resolution than products derived from IR bands. As a result, IR sensors can retrieve SSTs to within around 1 km of land (dependent on the land mask used), whereas microwave sensors cannot likely retrieve useable SST data within around 75 km of land, far from most aquaculture production areas. Further, IR light is fully attenuated within the top 1 mm of the water column while microwave penetrates only a little deeper (a few mm). In contrast the *in situ* measurements that we used were typically from a depth of 1 m, so it is possible that we were effectively comparing different segments of the water column when using the level 3 composite SST products.

Similarly, the smaller disagreement between the level 4 analysis product, UKMO OSTIA SST, and *in situ* measurements may be explained by the fact that the modeled product estimates water temperature through data assimilation from many sources over an integrated surface layer of ∼1 m, more closely matching the methods for *in situ* measurements. Another likely explanation is that *in situ* measurements at 1 m depth, despite time differences, correlated more strongly because there is less variability (due to diurnal variability, wind, weather, and currents) than at the surface (Donlon et al., 2012). The results may also have been influenced by a temporal mismatch, as instantaneous *in situ* measurements do not necessarily coincide with the RS data representing either day-time or night-time mean values, introducing a potential source of error and the possibility of aliasing. Additionally, there will inevitably be some mismatch in spatial scale, as the RS and modeled products integrate data over a larger area (1–100 km pixel size) when compared to the point-based *in situ* observations.

Lastly, in some areas within the study region there were multiple *in situ* observations recorded within single spatial extents (grid pixels) of the RS composite and analysis products. The aggregation of sites within pixels inevitably led to an overall reduction in the between-site variability and the complete removal of variability among sites within grid pixels when extracting RS data for use at individual sites. This issue may create limitations for researchers when using RS data rather than *in situ* observations. The extent of the limitation will depend on the application and objectives of the aquatic research, being most significant when capturing among-site variability is important.

The present study reinforces the findings of previous research (Castillo and Lima, 2010; Smit et al., 2013; Williams et al., 2013; Stobart et al., 2015; Wu et al., 2016). The type of SST product used (i.e., composite vs. analysis, satellite, and sensor types), the methods used for capturing *in situ* measurements, the location of the study area, and the temporal and spatial resolution used for aggregating the RS data are among the key factors associated with a true representation of water temperature profiles in the study area. The evidence suggests significant differences in agreement between satellite products across different regions (Castillo and Lima, 2010; Smit et al., 2013; Williams et al., 2013; Stobart et al., 2015; Wu et al., 2016), which highlights the need for similar studies in other aquaculture areas to assess the suitability of SST products.

Since available *in situ* water temperature data sources (in our case salmon farms and wild surveillance data) may have substantial numbers of missing values and temporal gaps, the present study provides evidence that satellite data can complement, if not be a substitute for, existing temperature data, though satellite estimates of SSS are not currently suitable for aquaculture applications. This could significantly improve monitoring capabilities relative to *in situ* observations (Urquhart et al., 2012), as *in situ* data are not always openly available and often have a lag time (depending on the field collection regimen). The near real-time and free availability of these satellite-based data make them suitable for use in forecast models, in monitoring and surveillance of pathogens, and in creating risk maps for fish health.

AUTHOR CONTRIBUTIONS

KT, RV, TP, and CR designed the study; TP and CR were instrumental in acquiring *in situ* data; KT, RV, and JB acquired and processed the remote-sensed data; KT, RV, and HS performed the analysis; KT wrote the first draft of the manuscript and everyone contributed in revising the manuscript.

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Conflict of Interest Statement: The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

APPENDIX

1. **Concordance correlation coefficient:** The concordance correlation coefficient (Lin, 1989), $\hat{\rho_c}$, between two vectors (x and y) of length N is computed as

$$\hat{\rho_c} = \frac{2s_{xy}}{s_x^2 + s_y^2 + (\bar{x} - \bar{y})^2}$$

where the means, the variances and the covariance is respectively computed as:

(a) the means

$$\bar{x} = \frac{1}{N}\sum_{n=1}^{N} x_n$$

$$\bar{y} = \frac{1}{N}\sum_{n=1}^{N} y_n$$

(b) the variances

$$s_x^2 = \frac{1}{N}\sum_{n=1}^{N} (x_n - \bar{x})^2$$

$$s_y^2 = \frac{1}{N}\sum_{n=1}^{N} (y_n - \bar{y})^2$$

(c) and the covariance

$$s_{xy} = \frac{1}{N}\sum_{n=1}^{N} (x_n - \bar{x})(y_n - \bar{y})$$

2. **Index of agreement:** The index of agreement (Willmott, 1984), *d-index*, between two vectors (x and y) of length N is computed as

$$d - index = 1 - \frac{\sum_{n=1}^{N} (x_n - y_n)^2}{\sum_{n=1}^{N} (|x_n - \bar{x}| + |y_n - \bar{x}|)^2}$$