Representativeness and certainty of sea surface temperature from MODIS in semi-enclosed bays

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ABSTRACT

The sea surface temperature estimated by satellites (SST$_{skin}$) may facilitate the understanding of processes that affect water quality in semi-enclosed bays. However, the representativeness and certainty of SST$_{skin}$ in semi-enclosed bays have not been fully investigated. We investigated the SST$_{skin}$ from MODIS in Tokyo Bay and Ise Bay to test the hypothesis that water-mass structure and proximity to land would affect SST$_{skin}$. Results showed that the SST$_{skin}$ from MODIS in two semi-enclosed bays can be as representative and certain as the data from previous studies in the open ocean. We found that horizontal gradients of water temperature had little effect on the certainty of SST$_{skin}$. However, we found that both the representativeness and certainty of satellite-based estimates of SST$_{skin}$ in semi-enclosed bays were reduced by seasonal and location characteristics. The representativeness and certainty of SST$_{skin}$ near the mouth of Ise Bay were compromised by the complex vertical structure of water temperature in summer. Because SST$_{skin}$ may greatly enhance understanding of the processes that affect water quality in semi-enclosed bays, our results indicate that prior validation of SST$_{skin}$ by comparison with in-situ sea surface temperature (SST$_{dep}$) is important.

1. Introduction

Measurements of sea surface temperature (SST) have been made for meteorology and oceanography since the 1800s (Shukla 1998; Kennedy 2014; Minnett et al. 2019). SSTs estimated by satellites are widely used for global climate change research because they provide estimates over a much wider area than measurements made with sensors such as moored buoys (Reynolds et al. 2002; Rayner et al. 2003).

Semi-enclosed bays are particularly vulnerable to water pollution and hypoxia, and there is a need to understand the processes that affect water quality in these areas (Kasai 2014; Nakayama et al. 2014). Semi-enclosed bays are generally formed in places where riverine freshwater discharge mixes with seawater (e.g. Fujiwara 2003; Alizadeh et al. 2018). The water mass structure in semi-enclosed bays changes with the intrusion depth of ocean water because of the density difference between the bay water and ocean water (e.g. Kasai et al. 2004; Yanagi and Hinata 2004). Water temperature is used as a basic metric of water quality in semi-enclosed bays with complex water-mass structures. SSTs in semi-enclosed bays are also used to study the effects on the temperature of urban areas through heat exchange with the atmosphere (Oda and Kanda 2009). SST data are useful for understanding the processes associated with changes in water quality in semi-enclosed bays because they cover a wide range of spatial scales and can be used to study the spatial extent of phenomena that affect water quality.

SST generally refers to the temperature of the ocean from the sea surface to a depth of about 10 m and has been categorized in different ways (Donlon et al. 2002, 2007; Kawai and Wada 2007; Minnett et al. 2019). SST estimates obtained from satellite measurements are termed SST$_{skin}$; this type of estimate only reflects the temperature at the sea surface. SSTs measured by in-situ sensors such as moored buoys are termed SST$_{dep}$; this type of measurement reflects the temperature at a depth of several meters. The SST$_{skin}$ estimated by a satellite is calculated via an algorithm, and its accuracy can be assessed by comparing it with in-situ measurements made, for example, with buoys (Walton et al. 1998; Kilpatrick et al. 2015). On a calm day, the sea surface is warmed by solar radiation, and a warm layer is formed at the surface (Fairall et al. 1996; Donlon et al. 2002; Kawai and Wada 2007). This causes diurnal variability of SST and can result in a large vertical gradient of water temperature during the day (Fairall et al. 1996; Donlon et al. 2002; Kawai, Otsuka, and Kawamura 2006; Kawai and Wada 2007). In contrast, during periods with strong winds or at night, a cool skin is formed near the sea surface because of heat exchange with the atmosphere (Fairall et al. 1996; Kawai and Wada 2007).
Minett et al. 2019). In the cool layer, SST\textsubscript{skin} decreases to about 0.2 K below the SST\textsubscript{dep} (Kawai and Wada 2007; Kilpatrick et al. 2015; Minnett et al. 2019). Because the degree of the decrease is known to be stable, nighttime data are used in the validation of SST\textsubscript{skin} data (Kilpatrick et al. 2015). Sea surface temperature in semi-enclosed bays may be affected by several other factors in addition to heat exchange with the atmospheric and solar radiation. In areas close to land, microwave satellite observations cannot be used to estimate SST\textsubscript{skin} because land contamination from the antenna sidelobes restricts data acquisition (Chelton and Wentz 2005; Reynolds and Chelton 2010). In thermal infrared satellite observations, SST\textsubscript{skin} in coastal areas differs from SST\textsubscript{dep} in the same areas as well as from SST\textsubscript{skin} in the open ocean (Smit et al. 2013; Brewin et al. 2017). Also, the differences between SST\textsubscript{skin} and SST\textsubscript{dep} can result from errors in geolocation or thermal adjacency effects (Brewin et al. 2018). In addition, because complex, three-dimensional water mass structures are formed in the semi-enclosed bays (Fujivara 2003; Kasai et al. 2004; Yanagi and Hinata 2004; Alizadeh et al. 2018), the complex structure is predicted to affect the differences between SST\textsubscript{skin} and SST\textsubscript{dep}. However, comparisons of SST\textsubscript{skin} with SST\textsubscript{dep} at a scale of several kilometers, such as in semi-enclosed bays, have been limited by a lack of field observations.

If the effects of semi-enclosed bay decreased the representativeness and certainty of SST\textsubscript{skin} as the surface layer of water temperature significantly, SST\textsubscript{skin} is not useful in the analysis of water quality in the semi-enclosed bay. In this study, we hypothesized that SST\textsubscript{skin} is affected by the complex, three-dimensional water mass structure of semi-enclosed inner bays. This hypothesis predicts that the representativeness and certainty of SST\textsubscript{skin} decrease in semi-enclosed bay, and that these decreases may occur at places near land and when the spatial gradient in water temperature is steep. To test this hypothesis, the SST\textsubscript{skin} that has been provided by the moderate resolution imaging spectroradiometer (MODIS) was used. Although the advantage of MODIS has been diminishing because of recent new satellites operated, the advantage of SST\textsubscript{skin} from MODIS remains because of its large amount of accumulated data and the high frequency of the observations. The SST\textsubscript{skin} from MODIS was compared with SST\textsubscript{dep}, which is an SST used for the analysis of water quality at present. Our goal was to assess the representativeness and certainty of the SST\textsubscript{skin} from MODIS in semi-enclosed bays and their seasonal and spatial characteristics.

2. Materials and methods

2.1. SST from MODIS

MODIS is an optical sensor on the Terra satellite (launched in 1999) and Aqua satellite (launched in 2002) measures the reflected or emitted radiance from Earth in two orbits per day. The sensor observes 36 bands in the wavelength range of 0.4–14 μm. Based on the signals observed in two bands in the thermal infrared region, SST\textsubscript{skin} is estimated with a horizontal resolution of 1 km by an algorithm based on global data (Walton et al. 1998; Kilpatrick et al. 2015). The quality of the SST\textsubscript{skin} estimates fluctuates because of the effects of clouds and large satellite zenith angles (Kilpatrick, Podestá, and Evans 2001; Merchant et al. 2005; Kilpatrick et al. 2015; Minnett et al. 2019). It is known that the accuracy of the satellite-estimated SST\textsubscript{skin} is compromised when cloud effects are present, and quality tests are conducted to eliminate cloud effects (Kilpatrick, Podestá, and Evans 2001; Merchant et al. 2005). The SST\textsubscript{skin} from MODIS (https://oceancolor.gsfc.nasa.gov/) used in this study was assigned a quality index based on the results of the NASA Goddard Ocean Biology Processing Group quality test (Donlon et al. 2007; Kilpatrick et al. 2015). Users can perform their quality assessment based on quality indices, and we used the quality index flags_sst (Table S1) to categorize the data.

2.2. Study site

The study sites, Tokyo Bay and Ise Bay, are semi-enclosed inner bays in Japan that are adjacent to urban centers. Tokyo Bay is located in a densely populated urban area. About 26 million people live in its hinterland (Oda and Kanda 2009; Irie et al. 2015). The bay is about 50 km long in the north–south direction and 15 km wide in the east–west direction. Ise Bay is also located in an urban area, and about 11 million people live in its hinterland (Kasai et al. 2004; Irie et al. 2015). It is about 60 km long in the north–south direction and 30 km wide in the east–west direction. Both bays are semi-enclosed and partially surrounded by land (Figure 1). The water-mass structures within the bays are complex because of the mixing of freshwater from rivers and oceanic water from the Kuroshio Current (Fujivara 2003; Yanagi and Hinata 2004; Nakayama et al. 2014). There are observation stations (Figure 1), which measure the water temperature (SST\textsubscript{dep}) at depths of 1–5 m. The depths of observations at the stations can be divided into two types. One type is fixed relative to a landmark, and the depth fluctuates with the level of the tide. These stations include Chiba No. 1, Nakano, Nakayama, and Mouth of Ise Bay. In the second type, the depth below the surface is constant and controlled by buoys or automatic elevators. Attention must be paid to the effect of variations of water depth on the results if the depths of the observations fluctuate with the tide level. There is another observation point at the Chiba landmark in Tokyo Bay, but it was not included in this study because of its proximity to Kemigawa.
2.3. SST data used

SST\textsubscript{skin} values in Tokyo Bay and Ise Bay were estimated by MODIS at approximately 12-hour intervals by both the Terra and Aqua satellites: once during the day (about 10:00 am to 2:00 pm) and once at night (about 9:00 pm to 2:00 am). The two satellites together, therefore, collected about four data points per day. We used only nighttime data to avoid the effect of solar radiation during the daytime. The SST\textsubscript{skin} estimates were made at points that lay within a 1-km mesh (latitude $\pm0.0045^\circ$, longitude $\pm0.0055^\circ$) centered on the SST\textsubscript{dep} observation points.

SST\textsubscript{dep} was measured at each station in Tokyo Bay and Ise Bay (Figure 1) within one-hour intervals, and used from the nearest time compared with the SST\textsubscript{skin}. The accuracy of the thermometer measured SST\textsubscript{dep} was equal and lower than 0.1 K (Table S2). The SST\textsubscript{dep} was rejected from the analysis if the variation in the SST\textsubscript{dep} among an hour was more than 10 K, or if the SST\textsubscript{dep} was outside of the range 0–40°C. The analysis of SST\textsubscript{skin} and SST\textsubscript{dep} was carried out with data collected during 2011–2020 inclusive.

\[ \Delta SST = SST_{\text{skin}} - SST_{\text{dep}} . \quad (1) \]

Also, in the same way, the certainty of SST\textsubscript{skin} is defined as less variable in the difference between SST\textsubscript{skin} and SST\textsubscript{dep}.

To analyze the spatial structure of $\Delta$SST, we defined the origin of horizontal coordination as the horizontal location of SST\textsubscript{dep}. Then, the difference between the SST\textsubscript{dep} and the SST\textsubscript{skin} at the origin of horizontal coordination ($SST_{\text{skin}, \text{o}}$) is defined as $\Delta$SST\textsubscript{z} as follows:

\[ \Delta SST_{z} = SST_{\text{skin}, \text{o}} - SST_{\text{dep}} . \quad (2) \]

Here, if the horizontal location of estimated SST\textsubscript{skin} has an error, the difference between SST\textsubscript{skin} and SST\textsubscript{skin}, 0 is defined as $\Delta$SST\textsubscript{X}, as follows:

\[ \Delta SST_{X} = SST_{\text{skin}} - SST_{\text{skin}, \text{o}} . \quad (3) \]

From these three equations, $\Delta$SST is denoted as follows:

\[ \Delta SST = \Delta SST_{z} + \Delta SST_{X} . \quad (4) \]

In the open ocean, only the first term on the right-hand side of equation (4) has been considered in evaluations of $\Delta$SST. This equation shows that the error by the horizontal geolocation affects $\Delta$SST.

Because $\Delta$SST is an estimate for a specific time and place in the past, $\Delta$SST may not be relevant to the determination of processes that affect water quality. However, the expected $\Delta$SST gives us the relevant prediction for the process of water quality. If the expected $\Delta$SST is closer to zero, SST\textsubscript{skin} corresponds to less bias from SST\textsubscript{dep}, and it has representativeness of SST\textsubscript{dep}. Also, if the $\Delta$SST is less variable with less bias, the representativeness of SST\textsubscript{skin} is uncertain.

2.4. Data analysis

2.4.1. Representativeness and certainty of estimated SST\textsubscript{skin}

The representativeness of SST\textsubscript{skin}, defined in this study is whether SST\textsubscript{skin} is useful as the surface layer of water temperature to analyze water quality in semi-enclosed bay. That is, if the SST\textsubscript{dep} is a representative value used now, the difference between SST\textsubscript{skin} and SST\textsubscript{dep} ($\Delta$SST), expressed as the following, must be close to zero:

Figure 1. Map of Ise Bay (left) and Tokyo Bay (right). The black dot and the length of the line between the dot and land indicate the observation point and the distance measured from land, respectively.
Here, by assuming that the two terms on the right-hand side of equation (4) are independent of one another, the expectation of ΔSST is expressed as the following:

\[ E(\Delta SST) = E(\Delta SST_x) + E(\Delta SST_T) \]  

(5)

Also, the variance of ΔSST over time, \( V(\Delta SST) \), will equal the right-hand side of equation (6):

\[ V(\Delta SST) = V(\Delta SST_x) + V(\Delta SST_T) \]  

(6)

The mean and variance of ΔSST in the open ocean are −0.2 K and 0.26 K² (MODIS, Terra), respectively (Kilpatrick et al. 2015). These values provide one guide for assessing the representativeness and certainty of SSTskin values in semi-enclosed bays.

### 2.4.2. SSTskin Categorization and the land effect on their acquisitions

Because the accuracy of the SSTskin estimates is variable, we categorized SSTskin estimates using flags_sst. The SSTskin that satisfied all quality tests (flags_sst = 0) was defined as UNIF data. The UNIF data is interpreted as reliable and horizontally uniform (Table S1). Conversely, the SSTskin flagged by the uniformity test (flags_sst = 256 or 768) was defined as NO-UNIF data, which had a great spatial gradient in SSTskin (Table S1).

The acquisition rate of SSTskin was calculated as the ratio of the number of data points to the total number of data points in a month. The acquisition rate was calculated for UNIF and NO-UNIF data at the station. A generalized linear model was used to assess the effect of the land on data acquisition of SSTskin. A generalized linear model was performed with a logit function and binomial error and with an explanatory variable of a distance from land.

### 2.4.3. The mean and variance of ΔSST

The mean and variance of ΔSST were assessed as the monthly mean to take into consideration the influence of seasonal bias on the number of data points. The mean of the monthly means and the mean of the monthly variances were calculated for UNIF and NO-UNIF data at each station. The mean of the monthly means was defined as the monthly mean ΔSST. The mean of the monthly variances was defined as the monthly variance ΔSST. The differences between the UNIF and NO-UNIF data were tested by Welch’s two-sample t-test. In addition, the seasonality of ΔSST was tested by one-way analysis of variance (ANOVA) with a group of the month.

### 2.4.4. The effects of the horizontal gradient in SSTskin on ΔSST estimation

The geolocation of MODIS is adjusted by the attitude control of the satellite, but the standard deviation of its error is about 50 m (Wolfe et al. 2002). It is difficult to verify how much of the effect of this geolocation error is included in the ΔSST measured by the MODIS with a horizontal resolution of 1 km. Here, we assessed the horizontal gradients in SSTskin and the potential effect of the geolocation error on the ΔSST by using the Second-generation Global Imager (SGLI) with a horizontal resolution of 250 m, which is loaded on the G-COMC satellite (https://www.eorc.jaxa.jp/JASMES/SGLI_NRT/).

To assess the horizontal gradients in SSTskin at the STD, observation point, the SSTskin of the SGLI was arrayed at the mesh the closest to the coordinates of the STD observation point. The horizontal gradient in SSTskin was defined as the maximum difference in the SSTskin of SGLI within the eight pixels in the vicinity by assuming that the direction of the geolocation error was random. Next, the variance potential of the horizontal gradient was calculated before verifying the potential effect of the geolocation error on the ΔSST. The variance potential of the horizontal gradient was calculated as follows:

\[ \text{variancepotential} = \frac{V(\text{Maximum horizontal difference in SSTskin by SGLI})}{V(SST)} \]  

(7)

where \( V(\Delta SST) \) is the variance of ΔSST by MODIS. This ratio is calculated as the second term on the right-hand side of equation (6) divided by \( V(\Delta SST) \) by assuming that the horizontal difference in SSTskin by SGLI is intrinsic in the difference by MODIS. Because the horizontal resolution of SGLI is 250 m, the ratio is overestimated than the geolocation error in MODIS.

Because the G-COMC satellite was launched in 2017, the variance potential was calculated during the period 2018 to 2020 for UNIF and NO-UNIF data. A quality index was assigned to the SSTskin of the SGLI, and the most accurate datum was extracted (Kurilhara 2020). However, the data of Urayasu could not be extracted based on the quality index; those data were flagged because of their proximity to land.

### 3. Results

#### 3.1. The acquisition rate of UNIF and NO-UNIF data

The acquisition rate of UNIF data was distributed spatially and seasonally in Tokyo Bay (Figure 2a) and Ise Bay (Figure 2b). The spatial acquisition rate was relatively lower along the coastal line than that in the center of bays. The rate ranged from 0% to 40% at the observation points with spatial contrast in winter, and from 11% to 28% in summer at the observation points. A generalized linear model showed that the acquisition rate was positively correlated with distance from land for months except for July–September in Ise Bay, and for months except for July in Tokyo Bay (Figure 3). The slope of the positive relationship was steeper in the winter months in both bays.
Figure 2. Spatial distribution of the acquisition rate in the \( \text{SST}_{\text{skin}} \) of UNIF data in (a) Tokyo Bay and (b) Ise Bay.

Figure 3. Relationship between the acquisition rate in UNIF data and the distance from land. Dots show the data points, and lines show significant regression lines estimated by a generalized linear model with the logit function. Blue and red indicate Tokyo Bay and Ise Bay, respectively.
The acquisition rate of NO-UNIF data was also distributed spatially and seasonally in Tokyo Bay (Figure 4a) and Ise Bay (Figure 4b). However, the spatial distribution was opposite to the acquisition rate of UNIF data. The acquisition rate of NO-UNIF data was negatively correlated with the distance from land, except in July, August, and December in Tokyo Bay (Figure 5). The rate of NO-UNIF data was negatively correlated with distance from land during March, April, May, September, and October in Ise Bay (Figure 5) and was positively correlated between December and February.

3.2. Mean and variance of ΔSST

The monthly mean ΔSST in UNIF data varied from −0.4 K (Kemigawa) to −0.1 K (Nakanose) in Tokyo Bay (Figure 6a) and from −0.2 K (Back of Ise Bay) to 0.0 K (Mouth of Ise Bay) in Ise Bay (Figure 6b). These results were comparable to the mean of the Terra satellite in the open ocean (Kilpatrick et al. 2015). The monthly mean ΔSST was significantly lower in NO-UNIF data than that in the UNIF data in Tokyo Bay except at Nakanose (Welch’s two-sample t-test: \( t = 2.103, P = 5.346 \times 10^{-2} \) (Figure 6a). The monthly mean ΔSST in NO-UNIF data was significantly lower than that in UNIF data at No. 1 buoy, Back of Ise Bay, and Center of Ise Bay (Figure 6b).

The maximum monthly variance ΔSST was 0.20 K² at Nakanose, Tokyo Bay, in UNIF data (Figure 7a), which was slightly lower than the Terra variance of 0.26 K² for the open ocean (Kilpatrick et al. 2015). However, the monthly variance ΔSST was higher at Nakayama, Mouth of Ise Bay, and No. 1 buoy in Ise Bay than the Terra variance (Figure 7b). Also, the distribution of the monthly variance ΔSST was wider in these three locations. The monthly variance ΔSST was significantly larger in NO-UNIF data than that in UNIF data at all locations in Tokyo Bay (Figure 7a) and at locations except at No. 1 buoy (Wilcoxon signed-rank test: \( V = 12, P = 0.131 \) in Ise Bay (Figure 7b). These results indicate that the NO-UNIF data was more uncertain than the UNIF data.

3.3. Spatiotemporal characteristics of mean and variance of ΔSST

The one-way ANOVA showed significant differences among months in the ΔSST in UNIF data at locations except at Urayasu, No. 1 buoy, and No. 3 buoy (Figure 8).

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**Figure 4.** Spatial distribution of the acquisition rate in the SSTskin of NO-UNIF data in (a) Tokyo Bay and (b) Ise Bay.
and see Table S3 for their statistics). The difference among months was also significant in NO-UNIF data at Urayasu and No. 3 buoy, where are the closest locations from land at each bay. These results indicate that the representativeness and certainty of the SST\textsubscript{skin} varied spatiotemporally.

The ΔSST in UNIF data was positively biased in the summer months at Mouth of Ise Bay and Nakayama (Figure 8), with a significant difference among months. These locations have a complex structure of water mass in this season. In an example month, July 2016, water temperatures from in-situ measurements at Back of Ise Bay, Center of Ise Bay, Mouth of Ise Bay, and Nakayama formed thermal stratification (Figure 9a). However, the SST\textsubscript{dep} at Nakayama and Mouth of Ise Bay fluctuated briefly because of tidal effects and then approached the water temperature at depths of 10 and 20 m. The SST\textsubscript{skin} at that time was lower in a localized region near the mouth of the bay (Figure 9b). In other words, these results indicate that the water mass in the lower layer, which was initially cooler than in the upper layer because of thermal stratification, reached the upper layer through the mixing of water masses, and the SST\textsubscript{dep} decreased. However, the SST\textsubscript{skin} did not
decrease as much as the SST_{dep} (Figure 9a). This phenomenon was frequently observed during high tide at Mouth of Ise Bay and Nakayama (Figure 9a and Figure S1), and it is an explanation that ΔSST was biased positively in the summer months. The variance potential was close to zero at these locations (Table 1). In
addition, although the observation depth of SST_{dep} at Nakayama and Mouth of Ise Bay changes with the tides, the correlation between tide level and ΔSST was not significant (correlation coefficient: r = −0.219, at Nakayama). That is, the positive bias of ΔSST is suggested to occur strongly by the vertical structure of water temperature.

The change in the observation depth of SST_{dep} with the tides also occurred at Nakanose and Chiba No. 1 in Tokyo Bay, and the correlation was not significant (correlation coefficient: r = −0.039, at Chiba No. 1). Although the ΔSST was not biased in the summer months at Chiba No. 1, which is not located at the bay mouth, the ΔSST was positively biased in the summer months at Nakanose, which is located at the bay mouth (Figure 8). The short-term variations in SST_{dep} due to tidal effects were also observed at Nakanose (Figure 5), as the variations in SST_{dep} in the mouth of Ise Bay.

The mouth of bays were locations where the spatial gradients in SST_{skin} tended to step in winter (Figure 10 and Figure 11). As a result, the acquisition rate was low in UNIF data (Figure 2) and high in NO-UNIF data (Figure 4) in the months.
two-sample t-test showed that the ΔSST in NO-UNIF data in winter did not differ significantly from the UNIF data at Tomiura ($t = 0.923$, $P = 0.372$, in February), Mouth of Ise Bay ($t = 1.599$, $P = 0.117$, in February), and Nakayama ($t = 1.050$, $P = 0.298$, in January) (Figure 8). The variance potential was close to zero at these locations (Table 1). In other words, the real spatial distribution of SST was determined to cause the data to be NO-UNIF.

The large negative bias in monthly mean ΔSST occurred in NO-UNIF data than that in UNIF data at Urayasu, Tokyo Bay (Figure 6a) and Back and Center of Ise Bay (Figure 6b). Because the acquisition rate is biased spatially along the coastal lines in both bays and around these locations (Figure 2 and Figure 4), the negative bias in ΔSST is judged to arise from different data populations.

The maximum variance potential was 0.07 in the UNIF data at Kawasaki (Table 1). The variance potential in NO-UNIF data at Back of Ise Bay was 0.24 ($n = 6$). However, the variance potential was also close to zero in the NO-UNIF data except at Back of Ise Bay. The potential effect of geolocation error in MODIS is still uncertain but is likely low. Because the variance potential is overestimated than the geolocation error in MODIS, these results indicate that the geolocation error in MODIS caused little uncertainty in estimates of SST$_{\text{skin}}$ compared to the effect of vertical gradients on differences in water depth between SST$_{\text{skin}}$ and SST$_{\text{dep}}$.

4. Discussion

4.1. Summary of representativeness and certainty of SST$_{\text{skin}}$ in semi-enclosed bays

The SST$_{\text{skin}}$ from MODIS in the two semi-enclosed bays was as representative and certain as those in the open ocean when the data from the bays were uniform (UNIF data). However, the geographical characteristics of semi-enclosed bay affected the representative and certain of the SST$_{\text{skin}}$: 1) the deviation from SST$_{\text{dep}}$ (ΔSST) was biased toward the negative side, resulting in the loss of representativeness, at places near land by the loss of the horizontal uniformity of the SST$_{\text{skin}}$, 2) the complex structure of water mass induced by the hydrodynamics in semi-enclosed bay decreased the representative of the SST$_{\text{skin}}$, and 3) encountering between waters from inner bay and ocean at the bay mouth decreased the horizontal uniformity SST$_{\text{skin}}$ and caused to judge being unreliable data; however, the representativeness SST$_{\text{skin}}$ was not affected. The variance potential of geolocation error was slight at most locations.

Figure 10. Spatial distribution of monthly mean SST$_{\text{skin}}$ in Tokyo Bay (a) UNIF and (b) NO-UNIF data. The unit of the color bar is the degree of Celsius.
4.2. Influence of thermal effects from land

The acquisition rate in UNIF data was positively correlated to distance from land in both bays. In Tokyo Bay, the acquisition rate in UNIF data decreased proportionally to distance from land in months except in July, August, and December (Figure 3), whereas the acquisition rate in NO-UNIF data increased proportionally to distance from land (Figure 5). This relationship showed that the proximity to the land affected the decrease in horizontal uniformity of SSTskin. One of the reasons for this relationship may be the increase in the horizontal gradient of SSTskin because of the decrease in SSTskin near land by nighttime cooling over land (Brewin et al. 2018). In fact, at Tomiura in Tokyo Bay, the acquisition rate in UNIF data was lower in the winter than in other seasons, whereas the acquisition rate in NO-UNIF data was higher, indicating the influence of the increased horizontal gradient of SSTskin (Figure 2a, Figure 4a, and Figure S3).

However, as an exception, at Urayasu in Tokyo Bay, which is located adjacent to land, the acquisition rate in UNIF data was zero in winter, and the acquisition rate in both NO-UNIF and UNIF data was poorer than at the other points. The data not judged as NO-UNIF or UNIF data were mainly judged as land, cloud, or unreliable data compared to the reference data (Table S1). The data was mainly judged as land or unreliable data compared to the reference data because the influence of clouds could occur equally at all locations, as noted below. The monthly mean ΔSST in NO-UNIF data at Urayasu was −1.1 K and lower than at the others (Figure 6a). This result indicated that the quality test did not work successfully at Urayasu.

In Ise Bay, during March–May and October, the acquisition rate in UNIF data decreased proportionally to distance from land (Figure 3), whereas the acquisition rate in NO-UNIF data increased proportionally to distance from land (Figure 5). However, during December–February, the acquisition rate in UNIF data and NO-UNIF data at No. 1 buoy, No. 2 buoy, and No. 3 buoy in the east area of Ise Bay were lower than 10% (Figure 2b and Figure 4b). This SSTskin was mainly judged as land or unreliable data compared to the reference data (Table S1) because the influence of clouds could occur equally at all locations, as noted below. In Ise Bay, the relationship between the acquisition of SSTskin and the proximity to the land was not simply because the shape of the bay is more complex than that of Tokyo Bay (Figure 2 and Figure 4). In other words, the interaction with the shape of the bay is a factor that reduces the representativeness of SSTskin in semi-enclosed bays.
4.3. Influence of water-mass structures peculiar to semi-enclosed bays

The variance potential of the SST_{skin} of SGLI with a horizontal resolution of 250 m compared to the ΔSST by MODIS was 0.07 at maximum, except at Back of Ise Bay. Considering that the standard deviation of the geolocation error of MODIS is about 50 m (Wolfe et al. 2002), the ratio caused by this geolocation error to the uncertainty of MODIS ΔSST was lower than the variance potential. The certainty of ΔSST was dominated by the vertical gradient, with little effect from the horizontal gradient. However, the variance of ΔSST by MODIS at Back of Ise Bay was lower than at the other points, given the small number of NO-UNIF data, and this may be attributable to a lack of power. This is an issue to be addressed in the future.

Two specific patterns of water-mass structure affected the mean and standard deviation of ΔSST in Ise Bay. The first pattern involved deviation of SST_{skin} from SST_{ref} in Mouth of Ise Bay and Nakayama. The reason is that thermal stratification in summer fluctuates greatly because of vertical mixing below the surface during high tide. Kasai et al. (2004) described that vertical mixing at the mouth of Ise Bay occurred by the intrusion of oceanic water, and the water below the pycnocline was well mixed during spring tide in summer. However, the SST_{skin} above the pycnocline had no relationship with the vertical mixing. The representativeness and certainty of ΔSST were reduced by the vertical gradient, even in the UNIF data.

The second pattern was observed at Mouth of Ise Bay and Nakayama in winter when the temperature in the coastal water is lower than the temperature in the open ocean. The feature of this pattern was that the ΔSST in NO-UNIF data did not differ from the ΔSST in UNIF data, although the horizontal gradient increased because of the encounter of the water masses. In other words, this pattern indicates that NO-UNIF data cannot in general be rejected. Intrusions of oceanic water are among the processes that change water quality in semi-enclosed bays, and these NO-UNIF data may play an important role in understanding such processes.

4.4. Influence of clouds

The NO-UNIF data included cases where the effect of clouds could not be excluded (Figure S4). However, because the cloud distribution was not affected by the shapes of Tokyo Bay and Ise Bay, this cloud effect could occur equally at all locations. The difference between the monthly mean ΔSST in NO-UNIF data and the monthly mean ΔSST in UNIF data was lower at Mouth of Ise Bay and Nakayama (Figure 6a and Figure 6b), which are far from land, than at Urayasu, which is adjacent to land. The implication in Tokyo Bay and Ise Bay is that even if cloud effects are determined to be NO-UNIF, they have little influence on the representativeness of SST_{skin}. However, this result is not universal because the effect of clouds depends on the frequency of cloud formation.

4.5. Deployment to data use

The MODIS quality index can be used to determine the horizontal uniformity of SST_{skin} and as a guide to evaluating the representativeness and certainty of SST_{skin} even in semi-closed inner bays. However, in semi-enclosed bays, there are variations in the representativeness and certainty of SST_{skin} that depend on the location and season because of the unique structures of the associated water masses. At Nakayama, the UNIF monthly standard deviation for July was 1.4, seven times larger than for February (0.2) (Figure 8). In addition, at Mouth of Ise Bay and Nakayama, which are the encounter of the open ocean, the NO-UNIF data in winter were found to be representative and certain. The NO-UNIF data also included data affected by clouds, which tend to lower SST_{skin} but clouds may have had little effect on the representativeness of points far from land. To understand changes in water quality, it is important to carefully organize the types of data, their usability, and limitations (Table 2) and increase the volume of usable data as much as possible.

Even when the horizontal gradients of SST_{skin} are small, the SST_{skin} is flagged as flags_sst = 32 when the difference between the SST_{skin} and the reference data of MODIS SST_{skin} (OISST data; Table S1) occurred, and the flagging SST_{skin} was defined as SSTREFDIFF data.

| Data type | Availability and limitations | Response |
|-----------|-----------------------------|----------|
| UNIF data (Data that has passed all quality tests) | The data are comparable to the results in the open ocean (Kilpatrick et al. 2015) and are representative and certain. | The locations and seasons where vertical mixing is likely to occur should be identified in advance and data from those locations and seasons should be avoided. |
| NO-UNIF data (Data that has failed the uniformity test) | These data for stations close to land are not representative. By contrast, the data for water masses far from land is representative and certain and can be used to make corrections. | Encounters between different water masses are important in elucidating the mechanisms of environmental change, and it is desirable to devise ways to use them. |
| SSTREFDIFF data (Data that has failed the reference test) | Although not fully investigated in this study, in the winter season when most of these data were found, they were as representative and certain as the UNIF data. | This phenomenon is observed mainly in specific places during the winter when there is a difference in water temperature between the bay and the open sea, and it is desirable to devise ways to use them. |
The flagging of such data is caused by the coarse resolution (0.25°) of the reference data relative to the topography (Reynolds et al. 2007; Dufois et al. 2012; Kilpatrick et al. 2015). This problem is particularly common in winter when the temperature in the coastal water is lower than the temperature in the open ocean (Kilpatrick, Podestà, and Evans 2001; Dufois et al. 2012). In our study area, SSTREFDIFF data were observed mainly in winter at Nakanose, No. 1 Buoy, and No. 3 Buoy (Figure S3). The mean and variance in SSTREFDIFF data at Nakanose in Tokyo Bay were almost the same as those in UNIF data (Figure S5), and SSTREFDIFF data could also be used.

5. Conclusions
This study showed that the SST\textsubscript{skin} from MODIS in two semi-enclosed bays can be as representative and certain as the data from previous studies in the open ocean (Kilpatrick et al. 2015). This study showed a new finding that horizontal gradients of water temperature had little effect on the certainty of SST\textsubscript{skin}. However, we also found a significant effect of land on the acquisition of good data and the compromised representativeness and certainty of the SST\textsubscript{skin} by the complex vertical structure of water temperature, which may be formed in summer at the mouth of the bay.

Recent studies have described coastal satellite SST variations in terms of spatiotemporal effects (Smit et al. 2013; Brewin et al. 2018). This study differed from those previous studies in that it examined the factors that contribute to these variations. The results suggest that SSTs estimated by satellites are an effective tool for understanding the processes that change water quality in semi-enclosed bays. However, seasons and locations unique to semi-enclosed bays were found to affect the representativeness and certainty of SST\textsubscript{skin}. The results underscore the importance of prior validation of SST\textsubscript{skin} data in semi-enclosed bays by comparison with in-situ measurements of SST\textsubscript{dep}.

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Disclosure statement
No potential conflict of interest was reported by the author(s).

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References
Alizadeh, M.J., M.R. Kavianpour, M. Danesh, J. Adolf, S. Shamsibehd, and K.-W. Chau. 2018. “Effect of River Flow on the Quality of Estuarine and Coastal Waters Using Machine Learning Models.” Engineering Applications of Computational Fluid Mechanics 12 (1): 810–823. doi:10.1080/19942060.2018.1528480.
Brewin, R.J.W., L. de Mora, O. Billson, T. Jackson, P. Russell, T. G. Brewin, J.D. Shutler, et al. 2017. “Evaluating Operational AVHRR Sea Surface Temperature Data at the Coastline Using Surfers.” Estuarine, Coastal and Shelf Science 196:276–289. doi:10.1016/j.ecss.2017.07.011.
Brewin, R.J.W., D.A. Smale, P.J. Moore, G. Dall’Olmo, P.J. Miller, B.H. Taylor, T.J. Smyth, J.R. Fishwick, and M. Yang. 2018. “Evaluating Operational AVHRR Sea Surface Temperature Data at the Coastline Using Benthic Temperature Loggers.” Remote Sensing 10: 6. doi:10.3390/rs10060925.
Chelton, D.B., and F.J. Wentz. 2005. “Global Microwave Satellite Observations of Sea Surface Temperature for Numerical Weather Prediction and Climate Research.” Journal of the American Meteorological Society 86 (8): 1097–1115. doi:10.1175/BAMS-86-8-1097.
Donlon, C.J., P.J. Minnett, C. Gentemany, T.J. Nightingale, I. J. Barton, B. Ward, and M.J. Murray. 2002. “Toward Improved Validation of Satellite Sea Surface Skin Temperature Measurements for Climate Research.” Journal of Climate 15 (4): 353–369. doi:10.1175/1520-0442 (2002)015<0353:TIVOS>2.0.CO;2.
Donlon, C., I. Robinson, K.S. Casey, J. Vazquez-Cuervo, E. Armstrong, O. Arino, C. Gentemany, et al. 2007. “The Global Ocean Data Assimilation Experiment High-Resolution Sea Surface Temperature Pilot Project.” Bulletin of the American Meteorological Society 88 (6): 1197–1213. doi:10.1175/BAMS-88-8-1197.
Dufois, F., P. Penven, C. Peter Whittle, and J. Veitch. 2012. “On the Warm Nearshore Bias in Pathfinder Monthly SST Products over Eastern Boundary Upwelling Systems.” Ocean Modelling 47: 113–118. doi:10.1016/j.ocemod.2012.01.007.
Fairall, C.W., E.F. Bradley, J.S. Godfrey, G.A. Wick, J.B. Edson, and G.S. Young. 1996. “Cool-Skin and Warm-Layer Effects on Sea Surface Temperature.” Journal of Geophysical Research C: Oceans 101 (C1): 1295–1308. doi:10.1029/95JC03190.
Fujiiwara, T. 2003. “Buoyancy-Driven Current during Cooling Periods in Ise Bay, Japan.” Journal of Geophysical Research: Oceans 108: 8. doi:10.1029/2002jc001521.
Irie, M., A. Yamanaka, T. Tabuchi, and S. Tabela. 2015. “Quantification of Human Activities and Influence of Fishery on Internal Cycle System in Basins of Three Major Bays, Japan.” Journal of Japan Society of Civil Engineers, Ser. B3 (Ocean Engineering) 71 (2): 1832–1837. doi:10.2208/jseceo.71.832.
Kasai, A. 2014. “Hypoxia Controlled by Hydrodynamics.” Aqua-BioScience Monographs 7 (4): 117–145. doi:10.5047/absm.2014.00704.0117.

Kasai, A., T. Fukiwara, T. Kimura, and H. Yamada. 2004. "Fortnightly Shifts of Infrusion Depth of Oceanic Water into Ise Bay." Journal of Oceanography 60 (5): 817–824. doi:10.1007/s10872-002-05774-5.

Kawai, Y., K. Otsuka, and H. Kawamura. 2006. “Study on Diurnal Sea Surface Warming and a Local Atmospheric Circulation over Mutsu Bay.” Journal of the Meteorological Society of Japan 84 (4): 725–744. doi:10.2151/jmsj.84.725.

Kawai, Y., and A. Wada. 2007. "Diurnal Sea Surface Temperature Variation and Its Impact on the Atmosphere and Ocean: A Review." Journal of Oceanography 63 (5): 721–744. doi:10.1007/s10872-007-0063-0.

Kennedy, J.J. 2014. "A Review of Uncertainty in in Situ Measurements and Data Sets of Sea Surface Temperature." Reviews of Geophysics 52 (1): 1–32. doi:10.1002/2013RG000434.

Kilpatrick, K.A., G.P. Podesta, and R. Evans. 2001. "Overview of the NOAA/NASA Advanced Very High Resolution Radiometer Pathfinder Algorithm for Sea Surface Temperature and Associated Matchup Database." Journal of Geophysical Research: Oceans 106 (C5): 9179–9197. doi:10.1029/1999jc000065.

Kilpatrick, K.A., G. Podesta, S. Walsh, E. Williams, V. Halliwell, M. Szczodrak, O.B. Brown, P.J. Minnett, and R. Evans. 2015. "A Decade of Sea Surface Temperature from MODIS." Remote Sensing of Environment 165: 27–41. doi:10.1016/j.rse.2015.04.023.

Kurihara, Y. 2020. GCOM-C/SLI Sea Surface Temperature (SST) ATBD (Version 2). https://suzaku.eorc.jaxa.jp/GCOM_C/data/ATBD/ver2/V2ATBD_01AB_SST_Kurihara_r1.pdf.

Merchant, C.J., A.R. Harris, E. Maturi, and S. MacCallum. 2005. "Probabilistic Physically Based Cloud Screening of Satellite Infrared Imagery for Operational Sea Surface Temperature Retrieval." Quarterly Journal of the Royal Meteorological Society 131 (611): 2735–2755. doi:10.1256/qj.05.15.

Minnett, P.J., A. Alvera-Azcárate, T.M. Chin, G.K. Corlett, C. L. Gentemann, I. Karagali, X. Li, et al. 2019. "Half a Century of Satellite Remote Sensing of Sea-Surface Temperature." Remote Sensing of Environment 233. doi:10.1016/j.rse.2019.111366.

Nakayama, K., T. Shintani, K. Shimizu, T. Okada, H. Hinata, and K. Komai. 2014. "Horizontal and Residual Circulations Driven by Wind Stress Curl in Tokyo Bay." Journal of Geophysical Research: Oceans 119 (3): 1977–1992. doi:10.1002/2013JC009396.

Oda, R., and M. Kanda. 2009. "Observed Sea Surface Temperature of Tokyo Bay and its Impact on Urban Air Temperature." Journal of Applied Meteorology and Climatology 48 (10): 2054–2068. doi:10.1175/2009JAMC2163.1.

Rayner, N.A., D.E. Parker, E.B. Horton, C.K. Folland, L. V. Alexander, D.P. Rowell, E.C. Kent, and A. Kaplan. 2003. "Global Analyses of Sea Surface Temperature, Sea Ice, and Night Marine Air Temperature since the Late Nineteenth Century." Journal of Geophysical Research: Atmospheres 108: 14. doi:10.1029/2002jd002670.

Reynolds, R.W., and D.B. Chelton. 2010. "Comparisons of Daily Sea Surface Temperature Analyses for 2007-08." Journal of Climate 23 (13): 3545–3562. doi:10.1175/2010JCLI3294.1.

Reynolds, R.W., N.A. Rayner, T.M. Smith, D.C. Stokes, and W. Wang. 2002. "An Improved in Situ and Satellite SST Analysis for Climate." Journal of Climate 15 (13): 1609–1625. doi:10.1175/1520-0442(2002)015<1609:rissstm>2.0.co;2.

Reynolds, R.W., T.M. Smith, C. Liu, D.B. Chelton, K.S. Casey, and M.G. Schlax. 2007. "Daily High-Resolution-Blended Analyses for Sea Surface Temperature." Journal of Climate 20 (22): 5473–5496. doi:10.1175/2007JCLI1824.1.

Shukla, J. 1998. "Predictability in the Midst of Chaos: A Scientific Basis for Climate Forecasting." Science 282 (5389): 728–731. doi:10.1126/science.282.5389.728.

Smit, A.J., M. Roberts, R.J. Anderson, F. Dufois, S.F.J. Dudley, T. G. Bornman, J. Olbers, J.J. Bolton, and I. Álvarez. 2013. "A Coastal Seawater Temperature Dataset for Biogeographical Studies: Large Biases between in Situ and Remotely-Sensed Data Sets around the Coast of South Africa." PLoS ONE 8: 12. doi:10.1371/journal.pone.0081944.

Walton, C.C., W.G. Pichel, J.F. Sapper, and D.A. May. 1998. "The Development and Operational Application of Nonlinear Algorithms for the Measurement of Sea Surface Temperatures with the NOAA Polar-Orbiting Environmental Satellites." Journal of Geophysical Research: Oceans 103 (C12): 27999–28000. doi:10.1029/98JC02370.

Wolfe, R.E., M. Nishihama, A.J. Fleig, J.A. Kuyper, D.P. Roy, J. C. Storey, and F.S. Patt. 2002. "Achieving Sub-Pixel Geolocation Accuracy in Support of MODIS Land Science." Remote Sensing of Environment 83 (1–2): 31–49. doi:10.1016/S0034-4257(02)00085-8.

Yanagi, T., and H. Hinata. 2004. "Water Exchange between Tokyo Bay and the Pacific Ocean during Winter." Ocean Dynamics 54 (3–4): 452–459. doi:10.1007/s10236-003-0055-6.