

1 **Towards a Multi-Product Methodology for Calculating the Ocean**

2 **Monitoring Indicator of SST Extremes in the IBI Region**

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8 **Abstract.** The ongoing evaluation and refinement of the Copernicus Ocean Monitoring Indicators (OMIs) is essential to ensure
9 their scientific robustness and operational relevance. This process takes place within a context of continuous advances in
10 upstream products and the need to adapt methodologies to evolving scientific priorities and decision-making requirements. In
11 this framework, the release of new Copernicus products and the growing demand for quantifying uncertainty in indicator
12 results are particularly relevant.

13 Among the operational OMIs produced by the Iberia–Biscay–Ireland (IBI) Monitoring and Forecasting Center is the Sea
14 Surface Temperature (SST) extremes indicator, which assesses the intensity of extreme thermal events in the region. This study
15 proposes two methodological improvements to it: first, replacing the near real-time data product currently used to compute the
16 indicator with the recently developed Interim extension of its multi-year counterpart; and second, exploring the use of a multi-
17 product ensemble approach that integrates regional and global model outputs with satellite-based observations to provide an
18 initial estimate of uncertainty.

19 The methodology focuses on comparing the 2024 SST extremes OMI, computed using the existing approach, with outputs
20 generated by the revised methodologies. The evaluation uses the observationally based SST extremes OMI as a reference
21 (currently available in the Copernicus Marine catalog), and the analysis examines spatial patterns and local behaviors,
22 highlighting consistencies and discrepancies across products.

23 The results show that both the Interim dataset and the multi-product approach improve the robustness and consistency of the
24 SST extremes indicator. While the Interim dataset enhances internal coherence by reducing heterogeneity in data sources, the
25 ensemble method provides a more reliable assessment by incorporating uncertainty information. Together, these advances
26 strengthen the scientific maturity and operational value of SST extremes monitoring in the IBI region.

27 **1 Introduction**

28 Ocean indicators can be defined as measures based on scientifically validated data and methodologies that enable the
29 assessment of the state of ocean phenomena across various temporal and spatial scales, in a manner that is accessible and
30 meaningful to end users. These indicators are derived from environmental variables (e.g., temperature, salinity, sea level),
31 processes (such as primary productivity), or events (such as algal blooms or marine heatwaves) (von Schuckmann et al., 2026).
32 Given that operational Ocean Monitoring Indicators (OMIs) are developed within a dynamic and evolving framework of
33 oceanographic data production, their underlying methodologies must be periodically reviewed and updated. These continuous
34 methodological refinements are essential to ensure that OMIs remain aligned with the current state of scientific knowledge,
35 incorporate the best available upstream data, and maximize their accuracy, reliability, and operational relevance.

36 Among the operational OMIs maintained by the Iberia–Biscay–Ireland Monitoring and Forecasting Centre (IBI-MFC) is the
37 Sea Surface Temperature (SST) extremes indicator (listed as OMI-NRT in Table 1, product ref. no. 1). This OMI provides an
38 assessment of extreme SST events in the IBI region by quantifying the annual anomaly of the 99th percentile of SST. The
39 indicator is derived by calculating the difference between the 99th percentile value for a given year and the climatological
40 mean of the 99th percentile, obtained from a multi-decadal model reanalysis time series over its full temporal coverage. To
41 minimize the latency of the operational product, the indicator is computed by combining outputs from both reanalysis and near
42 real-time (NRT) Copernicus Marine products (referenced in Table 1 as IBI-REA and IBI-NRT, product refs. no. 2 and 3,
43 respectively). While the IBI-REA is used to estimate the climatological 99th percentile mean, the IBI-NRT dataset provides
44 the corresponding value for the target year. This methodological combination ensures that the indicator remains both
45 scientifically robust and operationally relevant. Its consistency is evaluated through comparisons with in situ observations, as
46 documented in Álvarez Fanjul et al. (2019).

47 The OMI-NRT indicator demonstrates both scientific maturity and operational readiness in alignment with the GOOS¹
48 framework (von Schuckmann et al., 2026). Scientifically, the indicator is verified through a robust methodology based on peer-
49 reviewed percentile analysis of SST extremes (Pérez Gómez et al., 2018), using the 99th percentile to capture high-impact
50 thermal events. It provides significant and policy-relevant information on marine heat extremes, which are known to be
51 associated with a wide range of ecological and socioeconomic impacts (Olivier, 2021, Smith et al. 2021), grounded in a multi-
52 decadal model reanalysis and operational NRT datasets from the Copernicus Marine Service. The approach is scalable and
53 adaptable to other ocean regions, supporting consistent and reproducible implementation. From an operational standpoint, the
54 indicator is justified by its relevance to coastal and marine impact assessments and is measurable through Essential Ocean
55 Variables using standardized Copernicus data products. It is accessible via the Copernicus Marine platform, updated annually,
56 and compliant with FAIR principles. These attributes collectively position the SST extremes indicator as a mature product
57 according to GOOS quality criteria.

¹ Global Ocean Observing System: <https://goosocean.org/>

58 Nevertheless, the current indicator could benefit from two methodological improvements, which are explored in the present
59 work. First, the incorporation of the recently released Interim dataset from the Copernicus IBI Multiyear product (referenced
60 as IBI-INT in Table 1, product ref. no. 2) may enhance the consistency of the upstream data used in the calculation of the
61 indicator. This is due to the reduction of heterogeneity in the modeling systems involved and the exclusive use of outputs
62 derived from the IBI Multiyear system itself. This refinement would improve the "Verified" criterion of the GOOS framework
63 by strengthening the traceability and scientific coherence of the data sources underpinning the indicator.

64 Second, the availability of multiple SST datasets in the Copernicus Marine Data Store opens the possibility of applying a multi-
65 product ensemble methodology to calculate the same indicator across different Copernicus Marine products. This would allow
66 for the generation of an uncertainty range associated with the indicator values, offering a more robust interpretation of results.
67 Incorporating such ensemble-based estimates would directly contribute to enhancing the "Significant" and "Scalable" criteria,
68 by improving the indicator's robustness and enabling its comparison across regions and systems.

69 Therefore, the objectives of this study are two: first, to assess the potential replacement of the near real-time dataset currently
70 used in the computation of the SST extremes indicator (OMI-NRT) with the recently released Interim dataset from the
71 Copernicus IBI Multiyear system (IBI-INT); and second, to evaluate the implementation of a multi-product ensemble
72 methodology based on the computation of the same indicator using different SST datasets available in the Copernicus Marine
73 catalogue. Both approaches aim to enhance the consistency, robustness, and interpretability of the indicator within the GOOS
74 quality framework.

75 To achieve these objectives, the proposed methodological refinements will be evaluated and discussed in light of independent
76 observational evidence, using in situ datasets provided by the Copernicus observational OMI product for SST extremes
77 (referenced in Table 1 as OMI-OBS, product ref. no. 8). This validation step will allow for a critical comparison of performance
78 and consistency between the existing and alternative approaches, supporting the long-term goal of improving the scientific and
79 operational maturity of the SST extremes indicator within the IBI region and beyond.

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Product ref. no.	Product ID Acronym Type	Data access	Documentation:
1	IBI_OMI_TEMP_SAL_extreme_var_ temp_mean_and_anomaly (OMI-NRT) Numerical models	EU Copernicus Marine Service Product (2021)	Quality Information Document (QUID): de Pascual Collar <i>et al.</i> (2021a) Product User Manual (PUM): de Pascual Collar <i>et al.</i> (2021b)

2	IBI_MULTIYEAR_PHY_005_002 (IBI-REA for Reanalysis dataset, IBI-INT for Interim dataset) Numerical models	EU Copernicus Marine Service Product (2024a)	QUID: Levier <i>et al.</i> (2024a) PUM: Castrillo-Acuña <i>et al.</i> (2024a)
3	IBI_ANALYSISFORECAST_PHY_005_001 (IBI-NRT) Numerical models	EU Copernicus Marine Service Product (2024b)	QUID: Levier <i>et al.</i> (2024b) PUM: Castrillo-Acuña <i>et al.</i> (2024b)
4	GLOBAL_MULTIYEAR_PHY_001_030 (GLO-REA) Numerical models	EU Copernicus Marine Service Product (2023)	QUID: Drévillon <i>et al.</i> (2023) PUM: Drévillon <i>et al.</i> (2024)
5	GLOBAL_ANALYSISFORECAST_PHY_001_024 (GLO-NRT) Numerical models	EU Copernicus Marine Service Product (2024c)	QUID: Lellouche <i>et al.</i> (2024) PUM: Le Galloudec <i>et al.</i> (2024)
6	SST_ATL_SST_L4_REP_OBSERVATIONS_010_026 (SAT-REP) Satellite observations	EU Copernicus Marine Service Product (2024d)	QUID: Autret <i>et al.</i> (2024) PUM: Autret <i>et al.</i> (2023)
7	SST_ATL_SST_L4_NRT_OBSERVATIONS_010_025 (SAT-NRT) Satellite observations	EU Copernicus Marine Service Product (2022a)	QUID: Piollé <i>et al.</i> (2022a) PUM: Piollé <i>et al.</i> (2022b)
8	OMI_EXTREME_SST_IBI_sst_mean_and_anomaly_obs (OMI-OBS) In-situ observations	EU Copernicus Marine Service Product (2022b)	QUID: de Alfonso <i>et al.</i> (2022a) PUM: de Alfonso <i>et al.</i> (2022b)

81 **Table 1: List of datasets used in this work referencing the source and documentation.**

82 2 Data and methods

83 The present study aims to assess two potential modifications to the operational procedures for computing the SST extremes
 84 indicator in the IBI region. The baseline indicator taken as the starting point is that listed in Table 1 as OMI-NRT, whose
 85 methodology is described in detail below.

86 The OMI-NRT indicator evaluates SST extremes for a given target year by quantifying the anomaly of the 99th percentile of
 87 SST, computed as the difference between the 99th percentile of SST for the target year and the climatological mean of the 99th
 88 percentile derived from a multi-decadal reanalysis. The climatological baseline is obtained from the Copernicus IBI reanalysis
 89 product (referenced in Table 1 as IBI-REA), computed over the full extent of the multi-year product period (in this study,
 90 1993–2023) in order to provide the most robust climatological reference possible at each indicator update, while the SST
 91 values for the target year (in this study, 2024) are drawn from the IBI near-real-time product (referenced in Table 1 as IBI-
 92 NRT).

93 The methodology proceeds in two main steps. In the first step, the annual 99th percentile of SST is computed for each individual
 94 year of the multi-year product (IBI-REA):

$$95 \quad P_{99}^{MYP}(x, y) = \text{perc}_{99}(\{T^{MYP}(x, t) \mid t \in y\}) [1]$$

96 where $T^{MYP}(x, t)$ is the SST field from the multi-year product at spatial location x and time t , and perc_{99} denotes the 99th
 97 percentile computed over all temporal instances within year y . These annual 99th percentiles are subsequently averaged over
 98 the full reference period to obtain the climatological mean of the 99th percentile, which serves as the reference climatology:

$$99 \quad \bar{P}_{99}^{MYP}(x) = \frac{1}{N} \sum_{y=y_1}^{y_N} P_{99}^{MYP}(x, y) [2]$$

100

101 In the second step, the 99th percentile for the target year y^* is computed using the near-real-time product (IBI-NRT):

$$102 \quad P_{99}^{NRT}(x, y^*) = \text{perc}_{99}(\{T^{NRT}(x, t) \mid t \in y^*\}) [3]$$

103 where $T^{NRT}(x, t)$ is the SST field from the near-real-time product at spatial location x and time t , including all available time
 104 steps within the target year y^* .

105 Finally, the annual anomaly map of the 99th percentile for the target year is obtained by subtracting the climatological mean of
 106 the 99th percentile from the near-real-time-derived 99th percentile:

$$107 \quad A_{99}(x, y^{Yr}) = P_{99}^{NRT}(x, y^{Yr}) - \bar{P}_{99}^{MYP}(x) [4]$$

108 Positive values of A_{99} indicate that the 99th percentile of SST for the target year exceeds the climatological reference, reflecting
 109 anomalously high extreme SST conditions, whereas negative values indicate that the 99th percentile falls below the
 110 climatological reference, suggesting a relative attenuation of SST extremes during that year.

111 The first methodological modification evaluated in this study involves the replacement of the datasets currently used in the
 112 computation of the OMI-NRT indicator. This reassessment is motivated by the recent inclusion in the Copernicus Marine
 113 catalogue of a new interim dataset, part of the IBI multiyear product (referenced in Table 1 as IBI-INT). This new dataset is

suitable for the calculation of the SST extremes indicator for two main reasons. First, it is generated using the same ocean model configuration as the IBI reanalysis (IBI-REA), which ensures greater homogeneity between the computational systems involved and reduces potential biases in the indicator's estimation. Second, the IBI-INT dataset is updated on a monthly basis with a latency of 4 months relative to real time, offering a compromise between timeliness and data consistency. Based on this, the present work defines OMI-INT as an SST extremes indicator analogous to OMI-NRT, but with the IBI-NRT dataset replaced by IBI-INT. This alternative formulation seeks to balance the trade-off between the update frequency of the indicator and the homogeneity of the upstream data used in its computation.

The second methodological modification addressed in this study involves the implementation of a multi-product approach for calculating the SST extremes indicator in the IBI region. To this end, a systematic review of the Copernicus Marine catalogue was conducted to identify products suitable for applying the same percentile-based methodology used in the operational OMI-NRT indicator. For each selected product, an independent estimation of the SST extremes indicator was computed, which is subsequently treated as a member of an ensemble. Several inclusion criteria were defined to ensure methodological consistency and scientific robustness across the ensemble members: (i) products must provide gridded SST data covering the IBI region; (ii) daily temporal resolution is required to compute annual 99th percentile anomalies; (iii) the time series must be long enough to support the construction of a robust climatology of the 99th percentile; and (iv) the product must be updated with a latency that ensures sufficient proximity to real time.

Based on these criteria, two additional product pairs from the Copernicus catalogue were identified as suitable for ensemble integration. First, the Global Ocean Physics modelling system provides both a reanalysis product (referenced in Table 1 as GLO-REA, product ref. no. 4) and a near real-time forecast product (referenced as GLO-NRT in Table 1, product ref. no. 5) that meet all necessary conditions. Second, satellite-derived SST observations from the European North West Shelf / Iberia-Biscay-Irish Seas High-Resolution L4 SST dataset are available in both a reprocessed delayed mode (referenced in Table 1 as SAT-REP, product ref. no. 6) and a near real-time version (referenced as SAT-NRT in Table 1, product ref. no. 7), both of which satisfy the requirements for computing the indicator.

In both cases, as with the previously defined OMI-NRT and OMI-INT indicators, the methodology involves calculating the 99th percentile anomaly of SST for the target year using near real-time products (GLO-NRT and SAT-NRT), referenced to the corresponding climatological 99th percentile derived from the respective multiyear products (GLO-REA and SAT-REP). Accordingly, this study defines the MULTI-OMI as the ensemble SST extremes indicator, computed using the same methodology as OMI-NRT but incorporating multiple Copernicus products. The ensemble comprises three members derived from: (i) IBI regional modelling data (IBI-REA and IBI-INT), (ii) global ocean modelling data (GLO-REA and GLO-NRT), and (iii) satellite-derived SST observations (SAT-REP and SAT-NRT). Each member anomaly is initially computed at the native spatial resolution of its corresponding NRT product. Prior to the ensemble aggregation, all individual anomaly fields are remapped to the IBI-NRT grid using a conservative interpolation method, ensuring a consistent spatial framework for the intercomparison of OMI-NRT, OMI-INT, and MULTI-OMI. The ensemble mean is then obtained as the simple arithmetic

mean of the three regrided member anomalies, while the associated uncertainty is estimated from the standard deviation computed across the three ensemble members. This ensemble-based approach enables a probabilistic interpretation of the results rather than a purely deterministic one. Following the methodology of the baseline indicator (OMI-NRT), the climatological 99th percentiles are computed over the longest period commonly available across all multi-year and reprocessed datasets. Since the different products considered present slight differences in their temporal coverage, a common reference period of 1993–2023 is adopted for all ensemble members, as this interval is fully covered by all multi-year and reprocessed products (IBI-REA, GLO-REA, and SAT-REP), ensuring methodological consistency and comparability across ensemble members and the operational baseline indicator (OMI-NRT).

Since this study aims to assess the sensitivity of the SST extremes indicator to the methodological modifications proposed above, it is necessary to establish a common reference dataset against which the results of each variant can be evaluated. For this purpose, the Copernicus Marine SST extremes indicator derived from observational data (referenced in Table 1 as OMI-OBS, product ref. no. 8) is used as the benchmark. This indicator follows the same percentile-based methodology as OMI-NRT, with the key difference that it is computed using non-gridded in situ data provided by the Copernicus Marine In Situ Thematic Assembly Centre. These observational datasets are derived from quality-controlled measurements collected by fixed stations and provide an independent and realistic representation of SST conditions in the IBI region. However, the reference period of OMI-OBS is subject to additional constraints imposed by the nature of the in situ data. Since observational records from fixed stations may contain temporal gaps, only stations with a minimum of 10 years of data and a minimum annual data coverage of 70% are retained for the computation of the climatological 99th percentile. These quality thresholds follow the criteria established in the original OMI-OBS methodology and are necessary to ensure the statistical robustness of the climatology derived from non-gridded in situ observations.

3 Results of indicator using interim and near real-time products

The first objective of this study is to assess how the substitution of near real-time SST data with the recently released Interim dataset from Copernicus affects the estimation of the SST extremes indicator in the IBI region. As described in Section 2 (Data and Methods), this analysis is conducted by comparing two configurations: the current operational setup (OMI-NRT), which uses near real-time data (IBI-NRT) for the target year, and an alternative formulation (OMI-INT), which replaces it with the Interim dataset (IBI-INT). Both configurations apply the same methodological framework, differing only in the input dataset used for 2024. This comparison allows us to evaluate the sensitivity of the indicator to upstream data choices and to explore whether the use of a more homogeneous modeling framework improves internal consistency and overall robustness.

Figure 1 presents the results of the SST extremes indicator for the year 2024, computed using the OMI-NRT and OMI-INT configurations. The anomaly maps displayed include shaded regions that indicate areas where the absolute value of the 2024 anomaly exceeds one or two standard deviations of the interannual distribution of the 99th percentile, as derived from the IBI-

REA climatological reference (1993–2023). This visualization allows for the identification of regions where the anomalies are unusually high relative to the historical variability of SST extremes.

The anomaly fields from both OMI configurations consistently reveal that 2024 was characterized by predominantly positive SST anomalies across the IBI region, with broad agreement between products in highlighting widespread warm signals. Both configurations identify a continuous tongue of positive anomalies extending from approximately 36°N to 48°N, strongly impacting the Cantabrian coast and large portions of the French Atlantic coastline, where anomalies frequently exceed one standard deviation and locally surpass the two-standard-deviation threshold, pointing to exceptionally intense events. A similar coherent pattern is observed in the Mediterranean, where both products display dominant positive anomalies, most pronounced in the Alboran Sea. However, notable differences emerge in regions of high natural variability and in the spatial extent and intensity of anomalies. Along the Portuguese coast and Gulf of Cádiz, OMI-NRT tends to produce broader and more intense negative anomalies compared to OMI-INT, while in the northeastern Atlantic near 54°N, negative anomalies exceeding one standard deviation in the OMI-NRT configuration represent the most pronounced discrepancies. Conversely, positive anomaly regions exhibit opposite behavior, with both the Atlantic anomaly tongue extending toward the Bay of Biscay and Mediterranean warm anomalies appearing more extensive and generally stronger in the OMI-INT configuration. These systematic differences suggest the presence of biases between the IBI-NRT and IBI-INT datasets relative to the climatological reference provided by IBI-REA, which will be examined in detail in Section 5 (Assessment of SST indicator configurations using in situ observations).

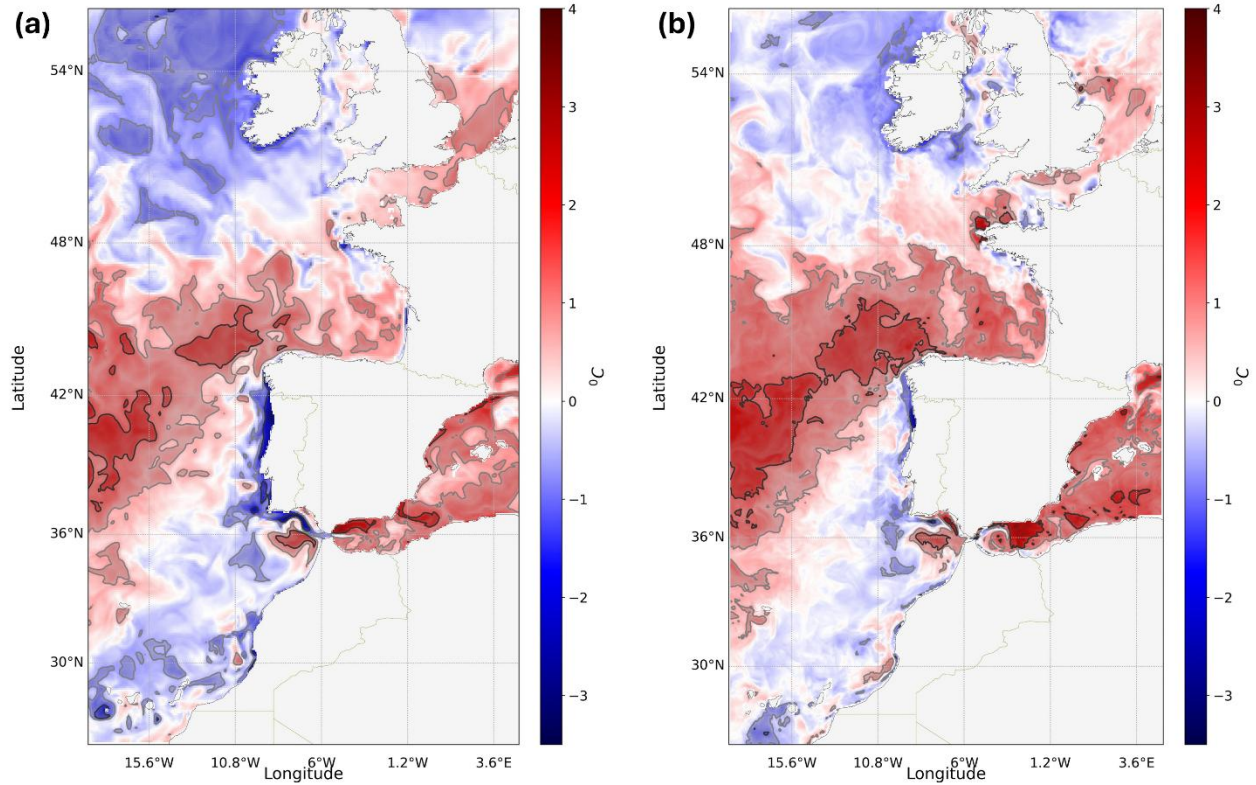
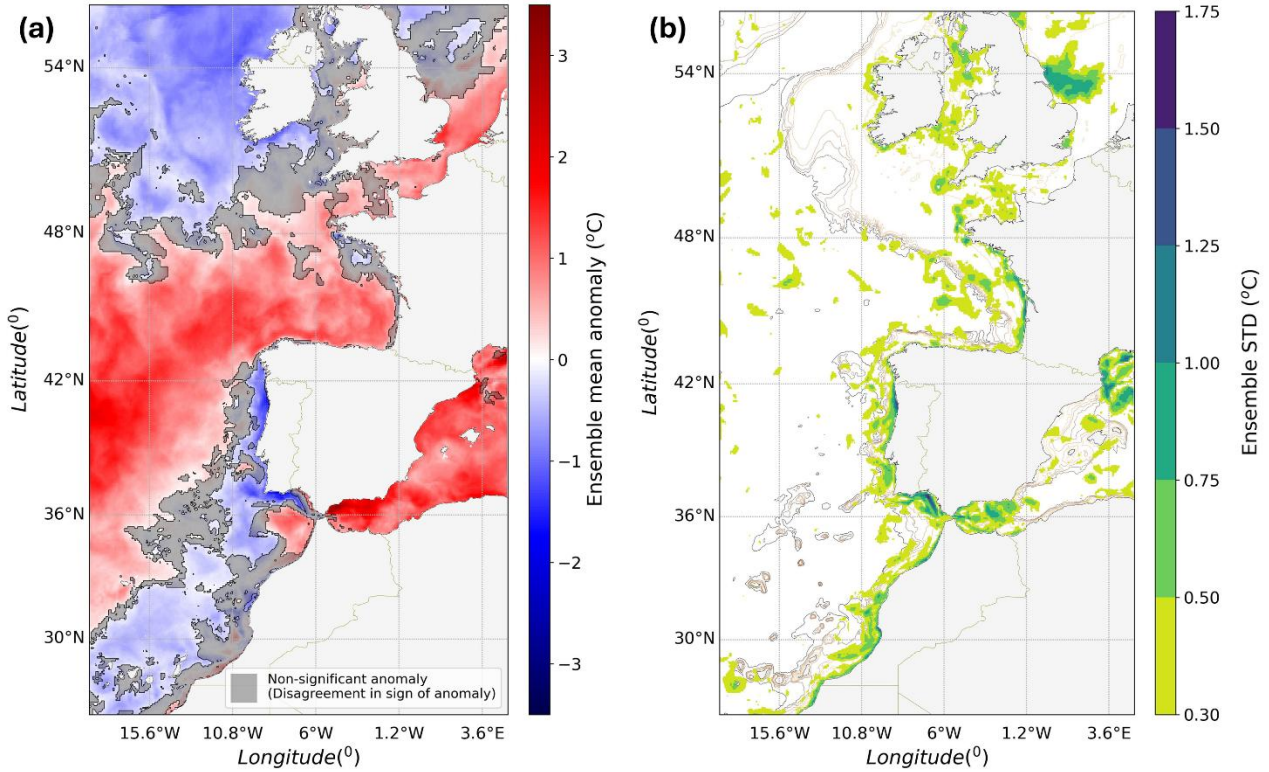


Figure 1: Anomaly in 2024 of the 99th percentile of the annual SST distribution (blue/red shading), referenced to the climatological mean for the period 1993–2023 derived from the IBI reanalysis product (IBI-REA). Panel (a) shows results obtained using the OMI-NRT configuration, which combines IBI-REA and the near real-time product IBI-NRT, while panel (b) displays results using the OMI-INT configuration, which replaces IBI-NRT with the Interim dataset IBI-INT. Grey and black contour lines, along with partial grey shading, indicate regions where the absolute anomaly exceeds one and two standard deviations, respectively, of the interannual distribution of the 99th percentile during the reference period.

4 Analysis of multi-product indicator results

The second improvement explored in this work is the adoption of a multi-product ensemble approach, referred to as MULTI-OMI. As described in the Data and Methods section, this configuration combines three independent estimates of the 2024 SST extremes indicator derived from distinct Copernicus datasets: regional model outputs, global model outputs, and satellite-based SST observations. The ensemble mean provides a consolidated estimate of SST anomalies, while the ensemble spread serves as an indicator of the robustness of the results across the different upstream data sources. Figure 2 shows both the ensemble mean of the anomaly in the 99th percentile of SST for 2024 and the corresponding ensemble standard deviation, allowing for the identification of regions with high inter-product agreement, as well as those with greater sensitivity to the choice of data product. Areas with elevated standard deviation values indicate reduced inter-product consistency and therefore require more

215 cautious interpretation. The ensemble spread thus provides a practical measure of the indicator's robustness, helping to identify
 216 regions where the signal is most reliable and where it should be interpreted with greater care.
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 221 **Figure 2: Results of the multi-product SST extremes indicator computed using the MULTI-OMI configuration. (a) Ensemble mean**
 222 **of the 2024 anomaly of the 99th percentile of annual SST (blue/red shading) computed with respect to the reference period 1993-**
 223 **2023. Grey shading indicates regions where at least one ensemble member shows an opposite sign of the SST anomaly, in which case**
 224 **the anomaly sign is considered non-significant. (b) Standard deviation (STD) of the ensemble. Only STD values above 0.3 °C are**
 225 **shown (contour shading), along with bathymetric contour lines at 50, 100, 500, 1000, 1500, 2000, and 3000 m depth (contour lines**
 226 **over ocean areas).**

227 The spatial distribution of SST anomalies in the ensemble mean (Figure 2a) reproduces the main patterns identified in the
 228 OMI-NRT and OMI-INT configurations, particularly in regions where the anomaly signal clearly exceeds climatological
 229 variability (exceedance of the one- and two-standard-deviation thresholds). In particular, a tongue of positive anomalies
 230 extends across the open Atlantic and reaches into the Gulf of Biscay, affecting the Cantabrian coast of the Iberian Peninsula.
 231 Similarly, widespread positive anomalies dominate the Mediterranean basin, especially in the Alboran Sea. Negative anomalies
 232 along the Portuguese coast and the Gulf of Cádiz also closely match those obtained from the OMI-NRT configuration,
 233 confirming the dominance of this cold signal across different datasets.

234 It is worth noting that the adoption of the MULTI-OMI configuration represents a fundamental shift in the nature of the
235 indicator, moving from a deterministic to a probabilistic framework. While OMI-NRT and OMI-INT each produce a single,
236 deterministic estimate of the SST extremes indicator, MULTI-OMI provides a distribution of plausible outcomes derived from
237 independent data sources. In this context, the ensemble mean should not be interpreted merely as a more accurate single
238 estimate, but rather as the central tendency of a range of plausible outcomes, each reflecting the SST extreme conditions as
239 captured by a different observational or modelling system. The ensemble spread, quantified here through the standard deviation
240 across members, thus serves as a natural proxy of the uncertainty associated with the indicator, providing users with actionable
241 information on the confidence of the results. In this regard, Figure 2a also includes a significance criterion based on the sign
242 agreement across ensemble members, which allows for the identification of regions where the indicator should be interpreted
243 with particular caution. Regions where the anomaly signal is not considered significant—shaded in grey—are those where at
244 least one ensemble member shows an opposite sign of the SST anomaly, indicating a lack of agreement among members on
245 the direction of the anomaly. These regions are generally confined to areas with low anomaly magnitudes, where, according
246 to the applied criteria, even small discrepancies among members can result in a non-significant outcome. Additionally, three
247 notable coastal areas of non-significant anomalies are observed, where the weak anomaly signal coincides with greater
248 discrepancies among ensemble members. The first region is located along the northwestern African coast, in the vicinity of
249 the Saharan upwelling system, an area known to be characterized by high high-frequency variability due to the interaction
250 between coastal upwelling dynamics and mesoscale processes (Desbiolles et al., 2014; Barton et al., 2004). Here, the strong
251 short-term variability characteristic of coastal upwelling likely contributes to the divergence in ensemble estimates. The second
252 area extends along the French Atlantic coast, from the Spanish border to the Brittany Peninsula, where model disagreement
253 may stem from complex coastal dynamics, the influence of shallow nearshore waters, and variable spatial resolution among
254 products. The entire Irish Sea appears as a region of non-significant anomalies, likely reflecting the heightened uncertainty in
255 resolving fine-scale variability within shallow, semi-enclosed waters, which in turn amplifies discrepancies across ensemble
256 members.

257 Figure 2b shows the standard deviation of the ensemble, which highlights areas where discrepancies between ensemble
258 members are largest, indicating a potential decrease in the reliability of the indicator estimates. The highest values are
259 predominantly concentrated along coastal areas and the continental slope. The most pronounced maxima appear in regions
260 where strong coastal dynamics and sharp bathymetric gradients coincide, such as the Gulf of Cádiz and the upwelling zones
261 off both the Iberian Peninsula and the northwestern African coast. A well-defined band of increased discrepancy is also evident
262 along the Armorican Slope in the Bay of Biscay, as well as in the coastal margins of the French Atlantic façade. In these areas,
263 the magnitude of inter-member differences is such that it can render the anomaly sign non-significant near the coast. In the
264 Mediterranean, particularly in the Alboran Sea, elevated discrepancies are observed in association with mesoscale structures
265 and gyres generated by the inflow of Atlantic water through the Strait of Gibraltar (Macias et al., 2016).

5 Assessment of SST indicator configurations using in situ observations

The results of the three SST extremes indicator configurations (OMI-NRT, OMI-INT, and MULTI-OMI) are now compared with in situ observational data from the Copernicus product OMI-OBS for 2024. The objective is to evaluate the degree of agreement between the gridded indicator estimates and observed SST extremes, and to understand how methodological choices influence the consistency and reliability of the results (see Figure 3).

Figure 3a displays the spatial distribution of the 2024 SST anomaly in the 99th percentile, as estimated by the MULTI-OMI ensemble mean, overlaid with anomaly values derived from in situ observations (OMI-OBS). Observational points are categorized according to whether they fall within or outside the uncertainty range defined by the ensemble mean $\pm$ standard deviation. The results reveal a widespread agreement in the sign of the anomalies between MULTI-OMI and OMI-OBS, indicating consistency in the detection of warm and cold events. However, the inclusion of observed values within the ensemble uncertainty range reveals instances in which they fall outside the bounds defined by the ensemble standard deviation, even when the sign of the anomaly matches. This behavior does not display a clear spatial distribution and is more clearly illustrated (and commented) in Figure 3b.

Figure 3b presents a Taylor diagram (Taylor, 2001) comparing the performance of the three indicator configurations, using OMI-OBS as the reference. The results for OMI-INT show that replacing near real-time data with the Interim dataset yields a modest improvement in overall performance. This improvement is particularly evident in the spatial standard deviation ratio, which in OMI-INT lies closer to unity than in OMI-NRT, indicating that the former provides a more accurate estimation of the spatial variability of the 99th percentile anomaly, along with a slight enhancement in spatial correlation. The superior performance of OMI-INT over OMI-NRT supports the inclusion of the former as the IBI regional modelling member of the MULTI-OMI ensemble, while OMI-NRT is consequently discarded as an ensemble member. In light of this, the remainder of the analysis focuses on the MULTI-OMI configuration, which incorporates OMI-INT as its regional modelling component. Regarding the MULTI-OMI configuration, it is important to interpret the results within the context of applying deterministic metrics to a probabilistic product. In this case, the Taylor diagram was computed using the ensemble mean as a deterministic representation of the indicator. From this perspective, the MULTI-OMI configuration behaves as expected for ensemble-based methodologies. On the one hand, the ensemble mean yields a higher correlation with observations, likely due to a more accurate representation of average anomaly values across the region. On the other hand, this increase in correlation comes at the expense of a reduced ability to capture variability. Since the ensemble mean averages out the anomaly fields of its members, the spatial variability of the resulting field is inherently reduced compared to that of any individual member. This smoothing effect leads to a spatial standard deviation of the ensemble mean that is lower than that of the observations, which is reflected in the Taylor diagram as a displacement of the MULTI-OMI point away from the reference standard deviation line. Nevertheless, despite this limitation, the ensemble mean of the MULTI-OMI configuration achieves a noticeable reduction in the centered root-mean-squared error (RMSE), as shown in the Taylor diagram, which is consistent with a reduction in the RMSE computed directly from the data, decreasing from 0.76 °C for OMI-NRT to 0.65 °C for MULTI-OMI. This highlights that, even when

299 using only the ensemble mean as a deterministic estimate, the multi-product approach yields a net improvement in
300 performance, demonstrating its potential to enhance the accuracy of SST extremes indicators.

301 Figure 3c presents the same comparison as in panel (a), using a representation that facilitates the identification of discrepancies
302 in the magnitude of the estimated anomalies. Several mismatches can be observed, which may be partly attributed to the use
303 of the ensemble spread as a proxy for uncertainty. While the computation of formally robust confidence intervals would require
304 the generation of long-term simulations for the interim and reprocessed systems, which currently fall outside the scope of this
305 contribution, the ensemble standard deviation provides a practical first-order estimate that is sufficient to identify regions of
306 reduced inter-product agreement and to motivate further in-depth analysis. Additionally, many observational platforms are
307 located near the coast, where gridded products (regardless of whether they originate from models or satellite observations)
308 often exhibit higher uncertainty due to complex dynamics and limited spatial resolution. This is also evident in the absence of
309 OMI-NRT values at some coastal stations, a limitation caused by land-sea masking and insufficient data coverage close to the
310 shoreline. Likewise, the absence of uncertainty bars for MULTI-OMI at certain locations indicates that only one ensemble
311 member contributed data at those stations, preventing the estimation of an uncertainty range.

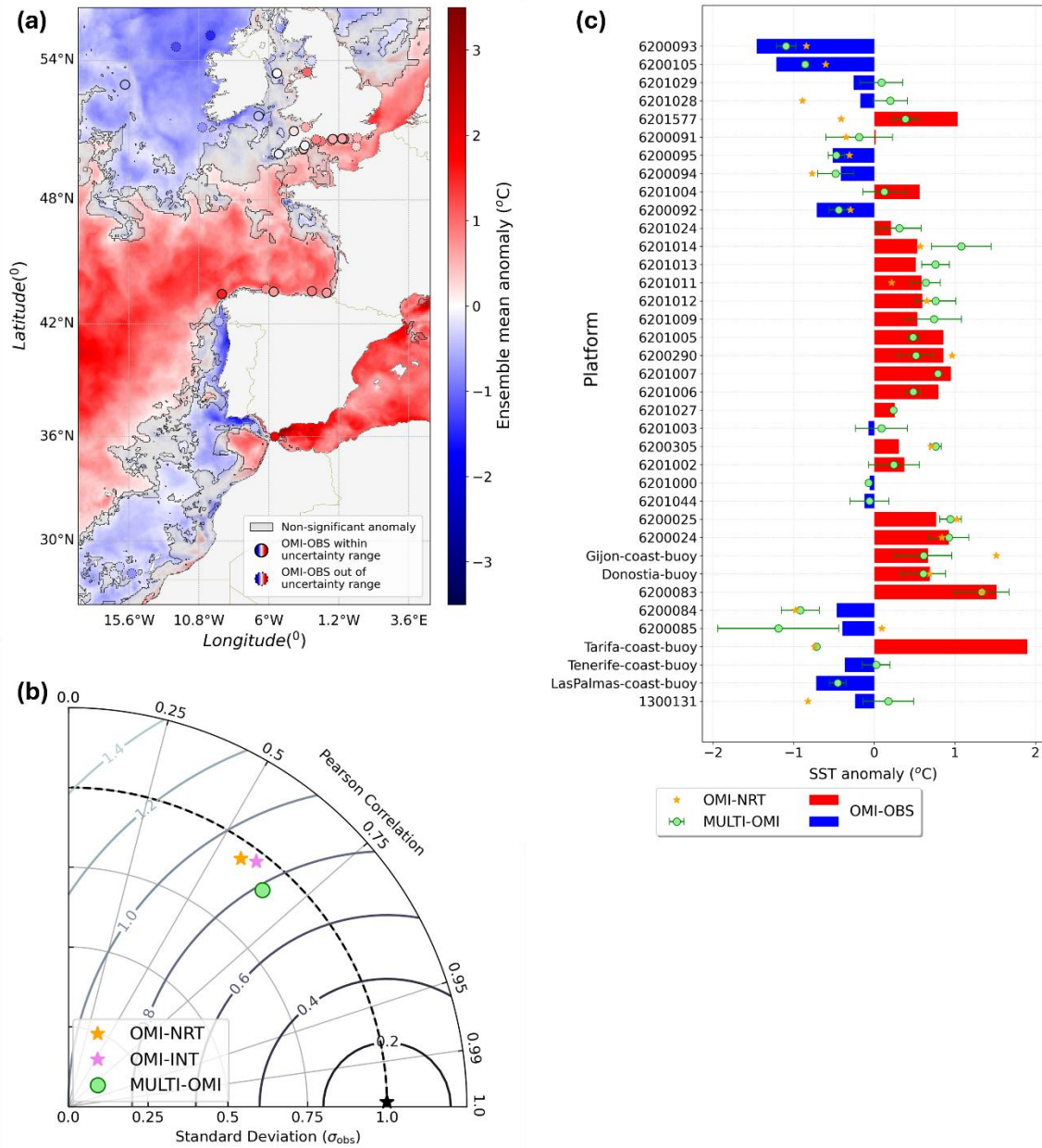


Figure 3: (a) Anomaly in 2024 of the 99th percentile of the annual SST distribution from the MULTI-OMI configuration (shading, same as in Figure 2a), shown alongside corresponding anomalies computed from in situ observations provided by the OMI-OBS product (colored circles). Circles with solid black outlines indicate locations where the observed anomaly lies within the uncertainty range defined by the MULTI-OMI ensemble mean $\pm$ standard deviation. Circles with dashed outlines represent locations where the observed anomaly falls outside this range. (b) Taylor diagram showing the performance of the three configurations (OMI-NRT, OMI-INT, and MULTI-OMI) relative to in situ observations (OMI-OBS). (c) Anomaly values for the 99th percentile of the annual SST distribution in 2024 computed from OMI-OBS (blue and red horizontal bars, indicating negative and positive anomalies, respectively), compared with estimates from MULTI-OMI (green circles with uncertainty bars) and OMI-NRT (orange stars). The OMI-OBS values are displayed using bars just to facilitate the visualization and identification of the reference data. Platforms are ordered by decreasing latitude along the vertical axis.

323 Beyond the deterministic improvement achieved through the multi-product approach (Figure 3c), it is also important to
 324 evaluate the advantages offered by adopting a probabilistic methodology. Table 2 summarizes the confusion matrices for the
 325 OMI-NRT and MULTI-OMI configurations, comparing their estimates of the sign (positive or negative) of the 99th percentile
 326 SST anomaly in 2024 against in situ observations provided by OMI-OBS. The analysis is restricted to the 22 observational
 327 stations for which valid OMI-NRT data are available. In the case of MULTI-OMI, instances classified as “non-significant”,
 328 i.e., where the ensemble members disagree on the sign of the anomaly, are reported separately and not considered either correct
 329 or incorrect estimates.
 330 Overall, the MULTI-OMI configuration demonstrates a high level of agreement with observations, correctly predicting the
 331 anomaly sign at 18 out of 22 stations (81.8%), matching the performance of OMI-NRT in terms of total correct classifications.
 332 However, the nature of the errors differs between the two configurations. MULTI-OMI does not produce any false positives
 333 and only one false negative, whereas OMI-NRT yields both false positives (1) and false negatives (3). This suggests that
 334 MULTI-OMI is more conservative in regions of uncertainty, likely due to its ensemble-based structure, which avoids assigning
 335 a sign when model agreement is insufficient. This cautious behavior is reflected in the “non-significant” category, which
 336 accounts for 3 out of 22 stations (13.6%) in the MULTI-OMI configuration.
 337 In summary, although both configurations achieve the same overall accuracy with respect to the observed anomaly signs, the
 338 MULTI-OMI configuration enables the identification of areas of high uncertainty that, through their exclusion, support the
 339 reliability of the anomalies in the rest of areas, even if these have low magnitudes. Accuracy ratio for the MULTI-OMI
 340 configuration in areas with anomalies that are considered significant is 94.7% (18 out of 19), which is higher than the 81.8%
 341 reached in the OMI-NRT configuration (18 out of 22).

Sign of the estimated/observed anomaly		OMI-OBS	
		+	-
OMI-NRT	+	10 (45.4%)	1 (4.6%)
	-	3 (13.6%)	8 (36.4%)
MULTI-OMI	+	11 (50.0%)	0 (0.0%)
	-	1 (4.6%)	7 (31.8%)
	Non-significant	1 (4.6%)	2 (9.1%)

342 **Table 2: Confusion matrix comparing the performance of the MULTI-OMI and OMI-NRT configurations against in situ**
 343 **observations (OMI-OBS) for the estimation of the sign (positive or negative) of the 99th percentile SST anomaly in 2024. Each cell**
 344 **shows the number of stations and the corresponding percentage (relative to the total of 22 stations with valid OMI-NRT data) for**
 345 **which the estimated anomaly sign matches or deviates from the observed sign. In the MULTI-OMI results, the “non-significant”**
 346 **category refers to cases where the ensemble anomaly is not statistically significant, i.e., where at least one ensemble member disagrees**
 347 **on the sign of the anomaly. Cells shaded in green indicate correct classifications (true positives or true negatives), cells in red indicate**
 348 **incorrect classifications (false positives or false negatives), and white cells correspond to nonsignificant cases, which are not**
 349 **considered either correct or incorrect.**

6 Conclusions

The continuous evolution of the Copernicus Marine catalogue, with the incorporation of new and improved modelling and observational products, provides both the motivation and the opportunity for periodic methodological reassessment of existing Ocean Monitoring Indicators. In this context, the present study has evaluated two methodological alternatives to the operational OMI for SST extremes in the IBI region (OMI-NRT): (i) the replacement of the near-real-time IBI dataset with the interim version of the IBI multiyear product (OMI-INT), and (ii) the development of a multi-product ensemble approach integrating regional model, global model, and satellite-derived SST estimates (MULTI-OMI). Both modifications were designed to reduce potential biases in the original product while providing enhanced robustness and user-oriented uncertainty information.

To achieve this, three different OMI configurations were analyzed. The first, OMI-NRT, corresponds to the current operational setup, which estimates annual SST extremes by calculating the anomaly of the 99th percentile of near real-time SST values with respect to a climatology derived from a multi-decadal reanalysis. The second configuration, OMI-INT, replaces the near real-time dataset with the Interim version of the IBI multiyear product, preserving the reference climatology while improving internal coherence by relying on a more homogeneous modeling framework. The third configuration, MULTI-OMI, introduces a novel multi-product ensemble approach that combines three pairs of gridded SST datasets, including both numerical model outputs and satellite-derived observations. This configuration allows for the computation of ensemble means and associated uncertainty ranges, enabling a more comprehensive and probabilistic representation of SST extremes in the region.

The performance of these three configurations was assessed using standard statistical metrics, including mean bias and RMSE, and classification-based validation techniques. All comparisons were made with respect to the OMI-OBS product, which derives SST extremes from in situ observational data. This provided an independent and robust benchmark evaluating each configuration's ability to reproduce the magnitude and sign of 99th percentile SST anomalies for the year 2024.

The results obtained in this study lead to several relevant conclusions regarding the methodological alternatives analyzed. First, the OMI-INT configuration shows a moderate improvement over the current operational configuration (OMI-NRT). This improvement is probably associated with the greater consistency of the upstream data, since in the OMI-INT configuration both the climatological baseline and the target-year data are derived from products generated using the same ocean model configuration (IBI-REA and IBI-INT, respectively), thereby reducing potential biases introduced by the use of heterogeneous modeling configurations, i.e. the combination of data generated with IBI-REA and IBI-NRT. These results support the adoption of the IBI-INT dataset as a more consistent alternative to IBI-NRT in future operational updates of the indicator. Beyond the numerical improvements, the methodological coherence offered by using a single modeling system justifies the adoption of the Interim dataset in future operational contexts.

The MULTI-OMI configuration has also provided valuable insights through its ensemble-based probabilistic approach. The spatial distribution of SST anomalies for 2024, as estimated by MULTI-OMI, confirms the presence of strong positive anomalies in the Mediterranean and across the open Atlantic toward the Bay of Biscay. At the same time, MULTI-OMI identifies several regions—particularly along the northwestern African coast, the Atlantic coast of France, and the entire Irish

Sea—where the anomaly is classified as non-significant due to disagreement among ensemble members. These areas are associated with high dynamical variability, such as coastal upwelling systems, complex shelf dynamics, or limited model agreement in semi-enclosed basins. Moreover, the spatial distribution of ensemble spread highlights regions of elevated uncertainty, which tend to concentrate along continental slopes, coastal upwelling systems, and mesoscale gyre structures, such as those found in the Gulf of Cadiz, the Portuguese coast and the Alboran Sea.

Regarding the benefits of applying a multi-product methodology, the use of the ensemble mean in MULTI-OMI demonstrates that its advantages outweigh the minor limitations observed. While ensemble averaging tends to dampen extreme values—reducing the amplitude of high or low anomalies—it leads to a net reduction in overall error, as evidenced by the decrease in RMSE from 0.76 °C (OMI-NRT) to 0.65 °C (MULTI-OMI). This makes the MULTI-OMI configuration clearly superior in the metrics evaluated through the Taylor diagram. The improvement indicates greater accuracy in estimating anomalies near the mean. Furthermore, beyond deterministic gains, the probabilistic nature of the ensemble allows uncertainty information to be directly incorporated into the indicator. This type of information can be essential for decision-making, as it helps reduce classification errors—particularly false positives and false negatives—when determining the sign of the anomaly.

Another advantage of the multi-product approach lies in its capacity to improve spatial coverage, especially in coastal zones. The use of multiple gridded data sources with differing resolutions and origins (e.g., numerical models and satellite products) increases the likelihood of capturing valid information in regions where a single product might offer limited or no coverage. The present work left open some new paths to be explored, for example it encourages the analysis of the multi-product methodology over decadal time scales. Such a study would allow for the statistical characterization of error distributions and the estimation of uncertainty intervals with controlled confidence levels. This would enable the generation of statistically consistent uncertainty ranges for the SST extremes indicator. Additionally, analyzing the temporal variability of SST maxima would provide insight into the climatic variability of extreme thermal events and support the development of trend analyses and spatial maps of SST extremes in the IBI region.

Since the goal of this study is to improve the original operational indicator for SST extremes, it is important to reflect on the operational implications of the proposed multi-product approach, as illustrated in Figure 2. This figure shows the type of outputs that can be delivered by a modified operational OMI based on ensemble methods. However, if the underlying philosophy of a multi-product methodology is to consolidate all available sources of information, then the configuration shown in Figure 2 has an important limitation: it excludes one of the key datasets available in the Copernicus Marine catalogue—namely, the in situ observational product used to compute OMI-OBS.

While the ideal solution would be to incorporate OMI-OBS directly as an additional member of the ensemble, the integration of non-gridded in situ data into a gridded multi-product framework presents significant methodological challenges. These include spatial interpolation, and ensemble consistency, all of which require careful treatment and lie beyond the scope of the present study.

As a practical compromise, a hybrid approach is proposed and illustrated in Figure 4. In this solution, the ensemble-based map from MULTI-OMI is retained as the primary product, but in regions where the anomaly is classified as non-significant, the

417 corresponding observational value from OMI-OBS is overlaid, provided such data are available. This strategy allows for the
418 integration of observational insight precisely in the areas where model-based uncertainty is highest.
419 Such an approach enables the retention of meaningful information in regions where ensemble uncertainty prevents a reliable
420 interpretation, thereby improving the utility of the indicator in operational contexts without compromising the methodological
421 integrity of the ensemble system.
422

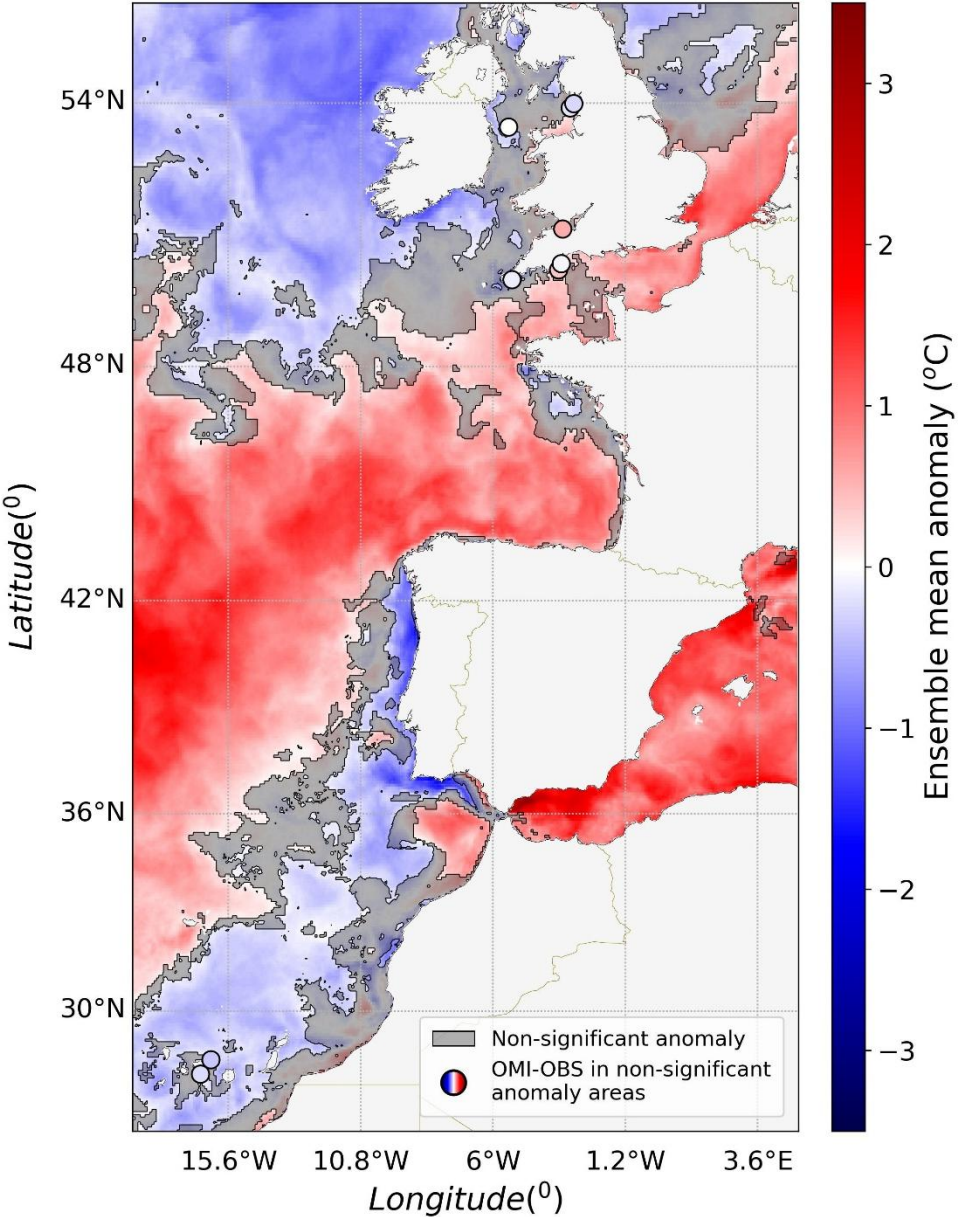


Figure 4: Map of the 2024 SST anomaly in the 99th percentile with respect to the reference period 1993-2023 as estimated by the MULTI-OMI ensemble mean (color shading), combined with in situ observational data from OMI-OBS (red and blue circles) in regions where the ensemble anomaly is classified as non-significant (grey shading) by MULTI-OMI.

The results of this study demonstrate that the MULTI-OMI configuration provides methodological and operational improvements over the current OMI-NRT framework, as evaluated through the GOOS quality criteria. By integrating multiple independent gridded datasets—including both model-based and satellite-derived sources—MULTI-OMI enhances the traceability, robustness, and coverage of the indicator. It improves the reliability of SST extreme estimates, reduces overall errors, and incorporates uncertainty in a way that directly supports informed decision-making. Additionally, its greater adaptability to coastal regions and varied spatial contexts strengthens both its scalability and accessibility. Taken together, these advancements position MULTI-OMI as a significant step forward toward a more scientifically mature and operationally relevant OMI, aligned with the evolving needs of climate monitoring and marine risk assessment.

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Author contribution

APC led the manuscript writing and revisions, and contributed to data analysis and generation of the OMI-INT and MULTI-OMI indicator configurations. AAV performed the main data analysis across all indicator configurations and contributed to manuscript writing and revisions. AG, MAAM and BPG contributed to the generation of the OMI-OBS indicator data and participated in the conceptualization of the study and manuscript revisions. SC and MGS contributed to manuscript revisions.

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