



# **A New Operational Mediterranean Diurnal Optimally Interpolated**

## 2 SST Product within the Copernicus Marine Environment

**3 Monitoring Service** 

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10 Abstract. Within the Copernicus Marine Environment Monitoring Service (CMEMS), a new operational MEDiterranean 11 Diurnal Optimally Interpolated SST (MED DOISST) product has been developed. This product provides hourly mean maps 12 (Level-4) of sub-skin SST at 1/16° horizontal resolution over the Mediterranean Sea from January 2019 to present. The product 13 is built by combining hourly SST data from the Spinning Enhanced Visible and InfraRed Imager (SEVIRI) on board Meteosat 14 Second Generation and model analyses through optimal interpolation. SEVIRI and model data are respectively used as the 15 observation source and first-guess. The differences between satellite and model SST are free, or nearly free, of any diurnal 16 cycle, thus allowing them to be interpolated in space and time using satellite data acquired at different times of the day. The accuracy of the MED DOISST product is assessed here by comparison against surface drifting buoy measurements, covering 17 18 the years 2019 and 2020. The diurnal cycle reconstructed from DOISST is in good agreement with the one observed by 19 independent drifter data, with a mean bias of  $0.041 \pm 0.001$  K and root-mean-square difference (RMSD) of  $0.412 \pm 0.001$  K. 20 The new SST product is more accurate than the input model during the central warming hours, when the model, on average, 21 underestimates drifter SST by one tenth of degree. The MED DOISST product is also able to reproduce accurately the extreme 22 diurnal warming events frequently observed in the Mediterranean Sea, which may reach amplitudes larger than 5 K during the 23 warm season. This product can contribute to improve the prediction capability of numerical weather forecast systems (e.g., 24 through improved forcing/assimilation), as well as the monitoring of surface heat budget estimates and temperature extremes 25 which can have significant impacts on the marine ecosystem.

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The full MED DOISST product (released on 04 May 2021) is available upon free registration at <a href="https://doi.org/10.25423/CMCC/SST\_MED\_PHY\_SUBSKIN\_L4\_NRT\_010\_036">https://doi.org/10.25423/CMCC/SST\_MED\_PHY\_SUBSKIN\_L4\_NRT\_010\_036</a> (Pisano et al., 2021). The reduced subset used here for validation and review purposes is openly available at <a href="https://doi.org/10.5281/zenodo.5807729">https://doi.org/10.25423/CMCC/SST\_MED\_PHY\_SUBSKIN\_L4\_NRT\_010\_036</a> (Pisano et al., 2021). The reduced subset used here for validation and review purposes is openly available at <a href="https://doi.org/10.5281/zenodo.5807729">https://doi.org/10.5281/zenodo.5807729</a> (Pisano, 2021).





30

#### 31 1 Introduction

32 In the last decades, the development of accurate satellite-based Sea Surface Temperature (SST) products required an increasing 33 effort to meet an ever-growing request from scientific, operational and emerging policy needs. Indeed, infrared and/or 34 microwave satellite radiometers allow a systematic and synoptic mapping of the ocean surface temperature (under clear-sky 35 conditions for the infrared and in the absence of rain for the microwave bands) with spatial resolutions from one to few 36 kilometers and temporal sampling from hourly to daily (Minnett et al., 2019). This almost continuous coverage represents a 37 unique characteristic of satellite thermal data, which is clearly not achievable with the use of in situ measurements alone. 38 Indeed, though in situ sensors reach significantly higher accuracy than satellite sensors, with uncertainties that can reach  $O(10^{-1})$ 39 <sup>2</sup> °C), they provide pointwise seawater temperature measurements, generally characterized by a poor and non-uniform sampling 40 of the ocean surface.

41 There is a huge variety of satellite-based SST datasets, characterized by different nominal resolutions as well as temporal and 42 spatial (global or regional) coverage, and based on different processing algorithms and satellite sensors, but designed to provide 43 highly accurate SST estimates (Yang et al., 2021). Operational datasets are typically distributed in near real time (NRT), 44 delayed-mode or as reprocessed datasets, and may include different processing levels, from single satellite passes processed 45 to provide valid SST values in the original observation geometry, the so-called Level-2 (L2), to images remapped onto a regular grid, also known as Level-3 (L3), up to the spatially complete Level-4 (L4), interpolated over fixed regular grids. These latter 46 47 are required by several applications since the lower levels are typically affected by several data voids (due to clouds, rain, land, 48 sea-ice, or other environmental factors depending on the type of sensors). The timely availability of SST data, ranging from a 49 few hours to a few days before real time, allows their use as boundary condition and/or assimilation in meteorological and 50 ocean forecasting systems (Waters et al., 2015), to improve the retrieval of ocean surface currents (Bowen et al., 2002; Rio 51 and Santoleri 2018), and monitor some weather extreme events, such as marine heatwaves (Oliver et al., 2021). The 52 reprocessing of long-term SST data records, typically covering the satellite era (1981-present), aims to provide more stable 53 and consistent datasets, complementing the NRT production, to be used to investigate climate variability and monitor changes 54 from interannual to multi-decadal timescales (Deser et al., 2010), including e.g. SST trends' estimates (Good et al., 2007; Pisano et al., 2020). The Copernicus Marine Environment Monitoring Service (CMEMS) is one of the main examples of how 55 56 satellite observations, including not only SST but a wide range of surface variables (e.g., sea surface salinity, sea surface 57 height, ocean color, winds and waves), are exploited to derive and disseminate high-level products (Le Traon et al., 2019), 58 namely L4 data in order to be directly usable for downstream applications.

59 The majority of the existing L4 SST datasets are provided as daily, weekly or monthly averaged fields (see e.g. Fiedler et al., 60 2019; Yang et al., 2021). Examples of well-known state-of-the-art SST daily datasets include the Global Ocean Sea Surface





61 Temperature and Sea Ice (OSTIA) dataset (Good et al., 2020), the European Space Agency (ESA) Climate Change Initiative 62 (CCI), the Copernicus Climate Change Service (C3S) Reprocessed Sea Surface Temperature Analyses (Merchant et al., 2019), 63 and the NOAA Daily Optimally Interpolated SST (OISST) v2.1 dataset, previously known/referred to as Reynolds SST 64 analysis (Huang et al., 2021). Though a daily resolution is generally sufficient to meet the requirements of many of the 65 oceanographic applications, it does not resolve the SST diurnal cycle, the typical day-night SST oscillation mainly driven by 66 solar heating. Within the oceanic thermal skin layer (few µm to 1 mm), SST is typically subject to a large potential diurnal cycle (especially under low wind speed and strong solar heating conditions) reaching amplitudes up to 3 K in the world oceans 67 68 (Gentemann et al., 2008; Gentemann and Minnett, 2008).

69 The SST diurnal cycle has several implications on mixed layer dynamics, air-sea interaction and the modulation of the lower 70 atmosphere dynamics. The most direct consequence of the SST diurnal amplitude variability is certainly on air-sea fluxes. 71 Clayson and Bogdanoff (2013) estimated that the diurnal SST cycle contributes with slightly less than that 5 Wm<sup>-2</sup> to the global 72 ocean-atmosphere heat budget with peaks of about 10 Wm<sup>-2</sup> in the Tropics. The inclusion of a realistic diurnal SST cycle in 73 atmospheric numerical simulation also has a non-negligible impact on cloud dynamics. Chen and Houze (1997) have shown 74 that in the Tropical Warm Pool, where extreme localized warming events occur, the diurnal warming can contribute to 75 modulate the evolution of convective clouds and, more in general, can impact the ocean-atmosphere coupling in numerical 76 models, producing a more realistic spatial pattern of warming and precipitation (Bernie et al., 2008). Overall, the diurnal cycle 77 of SST is generally underestimated in current ocean models and the assimilation of SST at high temporal frequency has the 78 potential to improve sea surface variability and mixed layer accuracy (Storto and Oddo, 2019).

79 In principle, the best opportunity to measure the diurnal cycle comes from infrared radiometers on board geostationary 80 satellites. Their observations are sufficiently accurate and frequent to resolve the diurnal signal variability whenever cloud cover is not too persistent. An example is provided by the Spinning Enhanced Visible Infra-Red Imager (SEVIRI) onboard the 81 82 Meteosat Second Generation (MSG) geostationary satellite covers. The operational retrieval of SST from MSG/SEVIRI 83 (managed by the European Organization for the Exploitation of Meteorological Satellites, EUMETSAT, Ocean and Sea-Ice 84 Facility, OSI-SAF) produces L3C hourly sub-skin SST products by aggregating 15 minutes (MSG/SEVIRI) observations 85 within 1 hour. The sub-skin SST is the temperature at the base of the conductive laminar sub-layer of the ocean surface, as defined by the Group of High Resolution SST (GHRSST, see e.g. Minnett et al., 2019). In practice, this is the temperature at 86 87 ~1 mm depth, and thus particularly sensitive to diurnal warming.

For the global ocean, the Operational Sea surface Temperature and sea Ice Analysis (OSTIA) diurnal product (While et al., 2017) provides daily gap-free maps of hourly mean skin SST at 0.25° x 0.25° horizontal nominal resolution, using in situ and satellite data from infrared radiometers. The skin SST is the temperature within the conductive diffusion-dominated sub-layer

91 at a depth of ~10-20 μm (as defined by GHRSST, Minnett et al., 2019). This system produces a skin SST by combining the





92 OSTIA foundation SST analysis (Good et al., 2020) with a diurnal warm-layer temperature difference and a cool skin 93 temperature difference derived from numerical models.

94 At regional scale, a method to reconstruct the hourly SST field over the Mediterranean Sea from SEVIRI data has been 95 proposed by Marullo et al. (2014, 2016). The reconstruction is based on a blending of satellite observations and numerical 96 model analyses (used as first-guess) using optimal interpolation. Though model analyses by definition also assimilate 97 observations, which could thus in principle include hourly SEVIRI data, in the present configuration they are not able to deal 98 with such frequent updates (see section 2.2), and the approach presented here represents an effective way to improve the 99 reconstruction of SST daily cycle from high-repetition satellite measurements. Previous works demonstrated the capability of 100 SEVIRI to resolve the SST diurnal variability and to reconstruct accurate L4 SST hourly fields over the Mediterranean Sea, a 101 basin that exhibits large diurnal SST variations (Buongiorno Nardelli et al., 2005; Minnett et al., 2019) that can easily exceed 102 extreme values (~5 K) as observed in the Tropical Pacific (Chen and Houze 1997), in the Atlantic Ocean and other marginal 103 seas (Gentemann et al., 2008; Merchant et al., 2008). The aim of this paper is to describe the operational implementation of a 104 diurnal optimally interpolated SST (DOISST) product for the Mediterranean Sea (MED) at 1/16° horizontal resolution, 105 building on the algorithm by Marullo et al. (2014, 2016). The assessment of the MED DOISST product covers two complete 106 years (2019-2020), thus extending previous similar validations (Marullo et al., 2016).

107

#### 108 2 The data

#### 109 2.1 Satellite data

110 Input satellite SST is derived from the SEVIRI sensor onboard the Meteosat Second Generation (Meteosat-11) satellite. 111 SEVIRI has a repeat cycle of 15 minutes over the 60S-60N and 60W-60E domain: Atlantic Ocean, European Seas and western 112 Indian Ocean. The retrieval of SST from Meteosat-11/SEVIRI is managed by EUMETSAT OSI-SAF, which provides subskin SST data as aggregated (L3C) hourly products remapped onto a 0.05° regular grid. Hourly products result from 113 114 compositing the best SST measurements available in one hour and are made available in near real time with a timeliness of 3 115 hours (see the OSI-SAF product user manual, https://osi-saf.eumetsat.int/products/osi-206). File format follows the Data 116 Specification (GDS) version 2 from the Group for High Resolution Sea Surface Temperatures (GHRSST, https://podaac-117 tools.jpl.nasa.gov/drive/files/OceanTemperature/ghrsst/docs/GDS20r5.pdf). The computation of SST in day and night 118 conditions is based on a nonlinear split window algorithm whose coefficients are determined from brightness temperature 119 simulations on a radiosonde profile database, with an offset coefficient corrected relative to buoy measurements. A correction 120 term derived from simulated brightness temperatures with an atmospheric radiative transfer model is then applied to the 121 multispectral derived SST (OSI-SAF PUM, https://osi-saf.eumetsat.int/lml/doc/osisaf cdop3 ss1 pum geo sst.pdf). L3C



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- data are provided with additional information, including quality level and cloud flags. Such quality flags are provided at pixel
  level, ranging over a scale of five levels with increasing reliability: 1 (="cloudy"), 2 (="bad"), 3 (="acceptable"), 4 (="good")
  to 5 (="acceptable")
- 124 to 5 (="excellent").
- The accuracy of Meteosat-11 SST data has been assessed through comparison with co-located drifting buoys, for day and night data separately covering the period from February to June 2018 (see the OSI-SAF scientific validation report, <u>https://osi-</u> saf.eumetsat.int/lml/doc/osisaf cdop2 ss1 geo sst val rep.pdf). The mean bias and standard deviation (derived from the differences between SEVIRI SSTs and drifter measurements over a matchup database) during nighttime have been quantified in -0.1 K and 0.53 K, respectively. During daytime, the bias remains practically unchanged (-0.09 K) and the standard deviation
- 130 slightly higher (0.56 K). These statistics were derived by selecting SEVIRI SST with quality flags  $\ge$  3, and it is shown that
- 131 the quality of SST improves when choosing higher quality levels.
- For our purposes, we selected L3C SST data with quality flag  $\geq$  3, as also indicated/suggested in the OSI-SAF scientific validation report.
- 134 2.2 Model data
- 135 The model output fields of surface temperature are derived from the CMEMS Mediterranean Sea Physical Analysis and
- 136Forecastingproduct,andidentifiedasMEDSEA\_ANALYSIS\_FORECAST\_PHY\_006\_013137(https://resources.marine.copernicus.eu/product-
- 138 detail/MEDSEA ANALYSISFORECAST PHY 006 013/INFORMATION;
- 139 https://doi.org/10.25423/CMCC/MEDSEA ANALYSISFORECAST PHY 006 013 EAS6; last access: 03 November 2021; 140 Clementi et al., 2021), and routinely produced by the CMEMS Mediterranean Monitoring and Forecasting Center (Med-MFC). 141 The modelling system is based on the Mediterranean Forecasting System, MFS (Pinardi et al., 2003), a coupled hydrodynamic-142 wave model implemented over the Mediterranean basin, extended into the Atlantic Sea in order to better resolve the exchanges 143 with the Atlantic Ocean at the Strait of Gibraltar, with a horizontal grid resolution of 1/24° (~4 km) and 141 unevenly spaced 144 vertical levels (Clementi et al., 2017). The Ocean General Circulation Model is based on the Nucleus for European Modelling 145 of the Ocean (NEMO v3.6) (Oddo et al., 2014, 2009), while the wave component is provided by Wave Watch-III. The model 146 solutions are corrected by a variational data assimilation scheme (3DVAR) of temperature and salinity vertical profiles and 147 along track satellite sea level anomaly observations (Dobricic and Pinardi 2008). The CMEMS Mediterranean SST L4 product 148 (CMEMS product reference: SST\_MED\_SST\_L4\_NRT\_OBSERVATIONS\_010\_004, 149 https://resources.marine.copernicus.eu/product-
- $\frac{\text{detail/SST MED SST L4 NRT OBSERVATIONS 010 004/INFORMATION}{\text{Isst access: 03 November 2021}} \text{ is used for}$   $\frac{\text{the correction of surface heat fluxes with the relaxation constant of 110 Wm^{-2}K^{-1}}{\text{centered at midnight since the product}}$
- 152 provides foundation SST (~SST at midnight).





The Med-MFC product is produced with two different cycles: a daily cycle for the production of forecasts (i.e., ten-days forecast on a daily basis), and a weekly cycle for the production of analyses. For our purposes, only hourly mean fields of sea surface temperature, which correspond to the first vertical level of the model centered at  $\sim 1$  m from the surface, are selected.

#### 156 2.3 In situ data

In situ data have been used for validation purposes (Section 4). Specifically, only surface drifting buoys have been used due to both their closeness to the sea surface (typically ~20 cm from the surface; Reverdin et al., 2010) and to their much larger number compared to other in situ instruments, which allows a more consistent and homogeneous temporal and spatial coverage.

160 Drifter data have been obtained from the CMEMS IN SITU (INS) TAC (identified as 161 INSITU MED NRT OBSERVATIONS 013 035, https://resources.marine.copernicus.eu/product-162 detail/INSITU MED NRT OBSERVATIONS 013 035/INFORMATION; and 163 INSITU IBI NRT OBSERVATIONS 013 033, https://resources.marine.copernicus.eu/product-164 detail/INSITU IBI NRT OBSERVATIONS 013 033/INFORMATION; last access: 03 November 2021), which collects 165 and distributes a variety of physical and biogeochemical seawater measurements, provided with the same homogeneous file 166 format. Each in situ measurement, including drifters, undergoes automated quality controls before its distribution. The quality 167 of the data is expressed by control flags indexed from 0 to 9, with the value of 1 indicating best quality. Drifter data have been 168 used to compile an hourly matchup database of co-located (in space and time) diurnal optimally interpolated SST (DOISST) 169 values and model outputs (Section 4.1), and validation statistics are based on the comparison between DOISST, model SST 170 and drifting buoy measurements over the matchup database (Section 4.2).

#### 171 3 The Mediterranean diurnal optimally interpolated SST product

#### 172 **3.1 Product overview**

173 The Mediterranean diurnal optimally interpolated SST (hereafter referred to as MED DOISST) operational product consists 174 of hourly mean gap-free (L4) satellite-based estimates of the sub-skin SST over the Mediterranean Sea (plus the adjacent 175 Eastern Atlantic box, see Section 2.2) at 0.0625° x 0.0625° grid resolution, from 1st January 2019 to near real time. 176 Specifically, the product is updated daily and provides 24 hourly mean data of the previous day, centered at 00:00, 01:00, 177 02:00,..., 23:00 UTC. The MED DOISST product is published on the CMEMS on line catalogue and identified as 178 SST MED PHY SUBSKIN L4 NRT 010 036 (CMEMS product reference) and cmems obs-sst med phy-179 sst nrt diurnal-oi-0.0625deg PT1H-m (CMEMS dataset reference). A synthesis of the product characteristics is shown Table 180 1.

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#### CMEMS Product ID: SST\_MED\_PHY\_SUBSKIN\_L4\_NRT\_010\_036





	set ID: cmems_obs-sst_med_phy-sst_nrt_diurnal-oi-0.0625deg_PT1H-m		
General description	The CMEMS Mediterranean diurnal product provides near-real-time, hourly mear gap-free (L4) sub-skin SST fields over the Mediterranean Sea and the adjacer Atlantic box over a $0.0625^{\circ}x0.0625^{\circ}$ regular grid, covering the period from 2019 to present (one day before real time). This product is built from optimal interpolating the Level-3C (merged single-sensor, L3C) SEVIRI data as observations and the CMEMS Mediterranean model analyses as first-guess.		
	33°N 30°N 10°W 0° 10°E 20°E 30°E		
Horizontal resolution	0.0625° x 0.0625° (1/16°) degrees [871x253]		
Temporal resolution	Hourly		
Spatial coverage	Mediterranean Sea + adjacent North Atlantic box (W=-18.1250, E=36.2500, S=30.2500, N=46.0000)		
Temporal coverage	2019/01/01 – near real time (-14H)		
Variables	Sub-skin SST (K) Analysis Error (%)		
Format	NetCDF – CF-1.4 convention compliant		
DOI	https://doi.org/10.25423/CMCC/SST MED PHY SUBSKIN L4 NRT 010 036		
Comments	Eventual updates of this product will be described in the corresponding Product User Manual (PUM) and Quality Information Document (QUID) available on t CMEMS on line catalogue.		

182

183 **Table 1.** The CMEMS MED DOISST product description synthesis.

184

#### 185 **3.2 Processing chain**

186 The system implements the DOISST scheme developed by Marullo et al. (2014). The system ingests merged single-sensor

187 (L3C) SEVIRI data as the observation source, and the CMEMS Mediterranean Sea model outputs as first-guess. It has been

188 shown that the diurnal signal in the hourly anomaly SST field (satellite-model) is reduced by about one order of magnitude

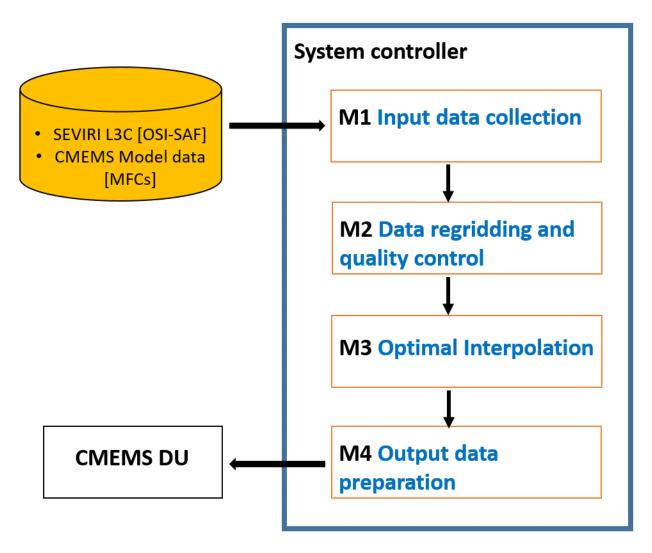
189 with respect to the full signal, thus allowing to interpolate SST anomalies using satellite data acquired at different times of the





https://resources.marine.copernicus.eu/product-

- day (Marullo et al., 2014). Several trials over a large variety of environmental conditions have shown that the temporal window to be used for the selection of input observations is  $\pm 24$  hours.
- 192 The data sub-sampling strategy, inversion technique and numerical implementation of the optimal interpolation
- scheme are based on the CMEMS NRT MED SST processing chain (Buongiorno Nardelli et al., 2013), which provides daily
- 194 mean fields of foundation SST over the Mediterranean Sea (CMEMS product reference:
- 195 SST\_MED\_SST\_L4\_NRT\_OBSERVATIONS\_010\_004,
- 196 <u>detail/SST\_MED\_SST\_L4\_NRT\_OBSERVATIONS\_010\_004/INFORMATION;</u> last access: 03 November 2021). Here, the
- 197 diurnal SST chain is organized in three main modules (Fig. 1).



198

199 **Figure 1.** Schematic diagram of the processing chain used for the MED DOISST SST product.





200

Module M1 manages the external interfaces to get both upstream L3C SST and model data: hourly mean L3C sub-skin SST data at 0.05° grid resolution are downloaded from OSI-SAF; hourly seawater potential temperatures at 1.0182 meter are obtained from the CMEMS Mediterranean Sea model outputs.

Module M2 extracts and regrids (through bilinear interpolation) L3C data and model outputs over the CMEMS Mediterranean
 Sea geographical area. A selection over SEVIRI is performed by flagging the pixels with quality flag < 3.</li>

Module M3 performs a space-time optimal interpolation (OI) algorithm. L4 data are obtained as a linear combination of the SST anomalies, weighted directly with their correlation to the interpolation point and inversely with their cross-correlation and error. Correlations are typically expressed through analytical functions with predefined spatial and temporal de-correlation lengths. Here, the covariance function  $f(r, \Delta t)$  is the one defined in Marullo et al. (2014), and given as the product of a spatial and temporal component:

211

 $f(r, \Delta t) = f(r) * f(\Delta t) = [a*exp(-r/R) + (1.-a)/(1.+r)c] * exp(-(\Delta t/T)d)$ 

213

where r is the distance (in km) between the observation and the interpolation point;  $\Delta t$  is the temporal difference (in hours) between the observation and the interpolation point; R = 200 km is the decorrelation spatial length; T = 36 h is the decorrelation time length; the other parameters are set as follows: a = 0.70, c = 0.26, d = 0.4. All these parameters have been deduced from a statistical analysis of the satellite SST data.

The input data are selected only within a limited sub-domain (within a given space-time interval), with a temporal window of  $\pm 24$  h (Marullo et al., 2014) and a spatial search radius of about 700 km (Buongiorno Nardelli et al., 2013). A check to avoid data propagation across land is performed between each pixel within the sub-domain and the given interpolation point (eventually discarded if there are land pixels between the straight line connecting the two points).

The interpolation error (analysis\_error field in the L4 file, Table 1) is obtained from the formal definition of the error variance derived from optimal interpolation theory (e.g., Bretherton et al., 1976). This error ranges between [0,100%], meaning that all observations are used (no first-guess data are used) when the error is zero, while only first-guess data are used (i.e no observations available) when the error is 100%.

- 226 The optimal interpolation algorithm is synthetized as follows:
- Hourly SEVIRI and model SSTs in a space/time window of 700 km/ ±24 h around the interpolation position/time are
   ingested;
- SEVIRI data with quality flag  $\geq$  3 are retained;





- Regridding over the Mediterranean Sea;
  Hourly model SSTs are subtracted from valid SSTs producing SST anomalies;
  SST anomalies are used as data input for the optimal interpolation analysis;
  Optimal interpolation is run using the covariance function defined above;
- The model SST is added to the optimally interpolated output again.

#### 235

The only difference with the original method is that all the input observations are interpolated, while in Marullo et al. (2014)
valid SST observations are left unchanged (not interpolated).

#### 238 **4 Validation of diurnal product**

#### 239 4.1 Validation framework

The accuracy of the MED DOISST product has been assessed through comparison with independent co-located (in space and time) surface drifting buoy data (matchups). The validation framework is based on the compilation of a matchup database between DOISST and drifters measurements covering the full years 2019 and 2020. The large number of drifters provides a rather homogeneous and continuous spatial and temporal coverage over the whole period (Fig. 2) allowing a robust statistical approach.

245 Firstly, a pre-selection of high-quality drifter data is performed, retaining only temperatures with quality flag equal to 1 (good) 246 or 2 (probably good) (see section 2.3). Then, the validation is carried out on hourly basis, building a matchup database by 247 collecting the closest (in space) SST grid point to the in situ measurement within a symmetric temporal window of 30 minutes 248 with respect to the beginning of each hour. A final quality control iteratively identifies drifter temperatures for which the 249 module of the difference between satellite and drifter temperature exceeds n-times the standard deviation  $\sigma$  of the distribution 250 of all these differences ( $\delta$ ). At each step of decreasing n, data that falls out of the interval  $I = [mean(\delta) - n \cdot \sigma, mean(\delta) + \sigma,$ 251  $n \cdot \sigma$  are flagged as outliers and then not included in the next step. The process starts for n=10 and stops at n=3. This last quality control removes ~1% of the total original sampling (as expected from a gaussian distribution) of drifter data that clearly 252 253 revealed anomalous temperature values.

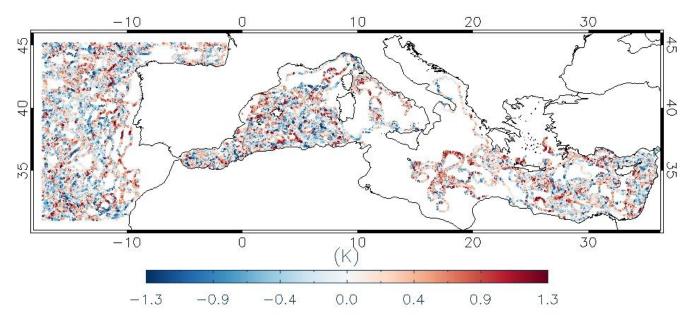
- Validation statistics are quantified in terms of mean bias and Root-Mean-Square Difference (RMSD) from matchup temperature differences (namely, SST minus drifter). Each statistical parameter is associated with a 95% confidence interval computed through a bootstrap procedure (Efron 1994).
- In order to evaluate the DOISST performance with respect to the model, the same validation procedure has been applied to themodeled SST.
- 259



#### 260 **4.2 Comparison with drifters**

#### 261 **4.2.1 The mean diurnal cycle**

The spatial distribution of DOISST and drifter matchups over the 2019-2020 period, along with their pointwise bias (i.e., DOISST minus drifter measurement) shows a rather homogeneous coverage over the most of the CMEMS MED domain (Fig. 2), although some areas are characterized by quite low coverage, such as the North Adriatic Sea or North Aegean Sea. The spatial distribution also evidences a positive tendency of the bias indicating that, on average, DOISSTs are warmer than drifters' temperatures.



267

Figure 2. Spatial distribution of the matchup points along with their punctual bias (i.e., SST minus drifter data, K) over the
 CMEMS Mediterranean domain from 2019/01/01 to 2020/12/31.

270 271

272 The DOISST product shows effectively an overall small positive mean bias of  $0.041 \pm 0.001$  K and a RMSD of  $0.412 \pm 0.001$ 

273 K (Table 2). A negative bias of  $-0.100 \pm 0.001$  K and slightly larger RMSD of  $0.467 \pm 0.001$  K characterize model SSTs.

274

	Period	Mean bias (K)	RMSD (K)	Matchups
DOISST	2019-01-01 to	$0.041 \pm 0.001$	$0.412\pm0.001$	548959
	2020-12-31			
Model	2019-01-01 to	$-0.100 \pm 0.001$	$0.467\pm0.001$	548959
	2020-12-31			



Table 2. Summary statistics of DOISST and model outputs. Mean bias (K) and RMSD (K) are derived from temperature
 differences against drifters' data over the period 2019-2020.

#### 277

- The hourly mean bias of DOISST and model shows similar but opposite behaviour (Fig. 3, and Table 3). In both cases, the bias clearly exhibits a diurnal oscillation during the 24 hours but, while the bias of DOISST increases positively during the central diurnal warming hours, the one of the model increases negatively. The DOISST mean bias is practically null between 17:00 to 06:00 local time, ranging between -0.001 and 0.03 K, and highest (~0.1 K) between 10:00 and 13:00 local time. The bias of the model oscillates around ~-0.07 K between 23:00 and 07:00 local time. Then, it increases (in absolute value) reaching the peak of ~-0.16 K between 11:00 and 14:00 and decreases successively. Similar results are obtained for the RMSD, which increases with diurnal warming (Fig. 3, Table 3). However, the RMSD of DOISST is less impacted by diurnal variations,
- characterized by an amplitude of ~0.04 K against ~0.14 K of the model.

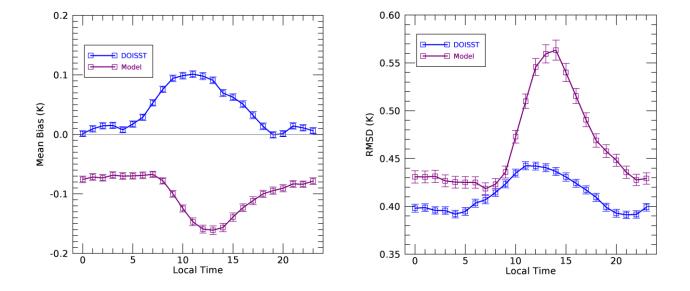


Figure 3. Mean bias (K) and RMSD (K) relative to MED DOISST (blue line) and model (purple line) based on the differences against drifters' data. Mean bias and RMSD are given as hourly mean over the period 2019-2020.





Hour	Mean BIAS	RMSD (K)	BUOY-AVAIL	Mean BIAS (K)	RMSD (K)
(local	(K)	(DOISST)		(Model)	(Model)
time)	(DOISST)				
HH: 00	$0.001\pm0.005$	$0.398 \pm 0.004$	22807	$-0.076 \pm 0.006$	$0.431\pm0.006$
HH: 01	$0.009\pm0.005$	$0.399 \pm 0.004$	23004	$-0.072 \pm 0.006$	$0.431\pm0.006$
HH: 02	$0.014\pm0.005$	$0.396\pm0.004$	22798	$-0.073 \pm 0.005$	$0.431\pm0.006$
HH: 03	$0.015\pm0.005$	$0.396 \pm 0.004$	23078	$-0.068 \pm 0.006$	$0.427\pm0.006$
HH: 04	$0.008\pm0.005$	$0.392\pm0.004$	22857	$-0.070 \pm 0.005$	$0.425\pm0.006$
HH: 05	$0.017\pm0.005$	$0.395\pm0.004$	22806	$-0.070 \pm 0.005$	$0.425\pm0.006$
HH: 06	$0.029 \pm 0.005$	$0.403\pm0.004$	22819	$-0.069 \pm 0.006$	$0.425\pm0.006$
HH: 07	$0.053\pm0.005$	$0.407\pm0.004$	23379	$-0.067 \pm 0.005$	$0.419\pm0.006$
HH: 08	$0.076\pm0.005$	$0.415\pm0.004$	23501	$-0.078 \pm 0.006$	$0.423 \pm 0.006$
HH: 09	$0.094\pm0.005$	$0.423 \pm 0.004$	23481	$-0.100 \pm 0.006$	$0.436\pm0.006$
HH: 10	$0.099\pm0.006$	$0.435\pm0.004$	23270	$-0.125 \pm 0.006$	$0.473\pm0.007$
HH: 11	$0.101\pm0.006$	$0.442\pm0.004$	23311	$-0.147 \pm 0.006$	$0.510\pm0.007$
HH: 12	$0.098 \pm 0.006$	$0.442\pm0.004$	23129	$-0.159 \pm 0.007$	$0.546\pm0.009$
HH: 13	$0.091\pm0.006$	$0.440\pm0.005$	22836	$-0.161 \pm 0.007$	$0.560\pm0.009$
HH: 14	$0.070\pm0.006$	$0.436\pm0.004$	22673	$-0.157 \pm 0.007$	$0.563\pm0.011$
HH: 15	$0.062\pm0.006$	$0.431\pm0.004$	22418	$-0.139 \pm 0.007$	$0.540\pm0.009$
HH: 16	$0.051\pm0.006$	$0.424\pm0.004$	22368	$-0.123 \pm 0.007$	$0.515\pm0.008$
HH: 17	$0.032\pm0.006$	$0.417 \pm 0.004$	22019	$-0.111 \pm 0.006$	$0.491\pm0.007$
HH: 18	$0.014\pm0.006$	$0.410\pm0.004$	21916	$-0.100 \pm 0.006$	$0.469\pm0.007$
HH: 19	$-0.001 \pm 0.005$	$0.399 \pm 0.004$	22117	$-0.095 \pm 0.006$	$0.458\pm0.007$
HH: 20	$0.001 \pm 0.005$	$0.393 \pm 0.004$	22458	$-0.090 \pm 0.006$	$0.448 \pm 0.006$
HH: 21	$0.014\pm0.005$	$0.391 \pm 0.004$	23229	$-0.083 \pm 0.005$	$0.436 \pm 0.006$
HH: 22	$0.011 \pm 0.005$	$0.392\pm0.004$	23272	$-0.084 \pm 0.006$	$0.428 \pm 0.006$
HH: 23	$0.006 \pm 0.005$	$0.399 \pm 0.004$	23413	$-0.078 \pm 0.006$	$0.429 \pm 0.006$

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Table 3. Summary statistics of MED DOISST and model products based on the differences against drifters' data over the
 matchup points. Mean bias (K), RMSD (K) and number of matchups are given as hourly mean over the period 2019-2020.

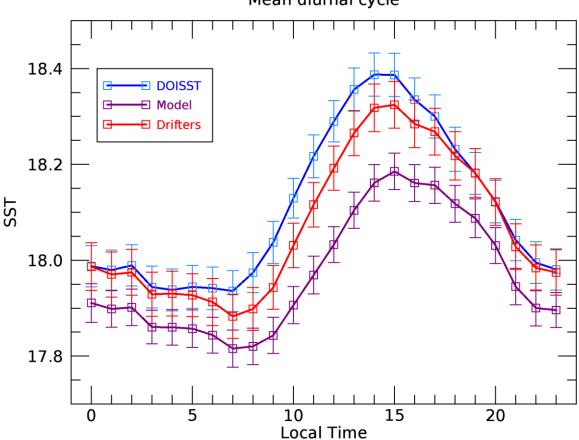
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The mean diurnal cycle of DOISST (namely, the 24-hour mean SSTs estimated over the matchup dataset) is in very good agreement, within the error confidence interval, with the SST cycle reconstructed from drifters (Fig. 4). The two diurnal cycles are practically coincident between 17:00 and 06:00, while they are biased by ~0.1 K between sunrise and 16:00, coherently with the DOISST bias oscillation (Fig. 3). This bias could be related to skin SST getting warmer faster than 20 cm temperature. The diurnal cycle of model SST maintains always below that of in situ temperatures, evidencing larger differences during the central diurnal warming hours (Fig. 4). However, apart from the biases likely induced by the different depths, the SST





amplitude as estimated from the DOISST and the model is ~2.3% larger and ~16% smaller than that of drifters, respectively,
suggesting that the model tends to underestimate diurnal variations.



Mean diurnal cycle

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Figure 4. Mean diurnal cycle for MED DOISST (blue line), model (purple line) and drifters (red line) computed over the matchups from 2019 to 2020.

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A delay of ~1 hour of the model with respect to DOISST and in situ on the onset of diurnal warming and in reaching the maximum is also evident. This delay could be explained as the physical result of delayed solar heating of the skin layer sensed by the satellite and of the first model layer. This may also be a consequence of the different packaging of the SEVIRI and model SST data into the hourly files: model hourly SST fields are centered at half of every hour (e.g., 12:30), while SEVIRI L3C at the beginning of each hour (e.g., 12:00) and obtained from collating data within one hour (from 11.30 to 12:29).





309 The capability of DOISST to capture and realistically reproduce diurnal variability is further investigated by analysing the 310 seasonally averaged SST diurnal cycle (Fig. 5), computed as for the mean diurnal cycle (by using the matchup dataset) but 311 over seasons: winter (December to February, D-J-F), spring (March to May, M-A-M), summer (June to August, J-J-A) and 312 autumn (September to November, S-O-N). The effect of warming in the diurnal SST excursion is clearly more pronounced 313 during spring and summer than winter and autumn, and reconstructed well in DOISST. During the warmer seasons, the 314 DOISST shows the lower biases (Table 4), estimated in  $0.036 \pm 0.001$  K (spring) and  $0.012 \pm 0.003$  (summer). Conversely, 315 the model reaches its higher biases, namely  $-0.101 \pm 0.001$  K (spring) and  $-0.117 \pm 0.003$  K (summer). The good agreement 316 between DOISST and drifters during winter and autumn (Table 4) reveals that the hourly DOISST fields are reconstructed 317 accurately also under cloudy conditions, which are more frequent during these seasons (Kotsias and Lolis, 2018).

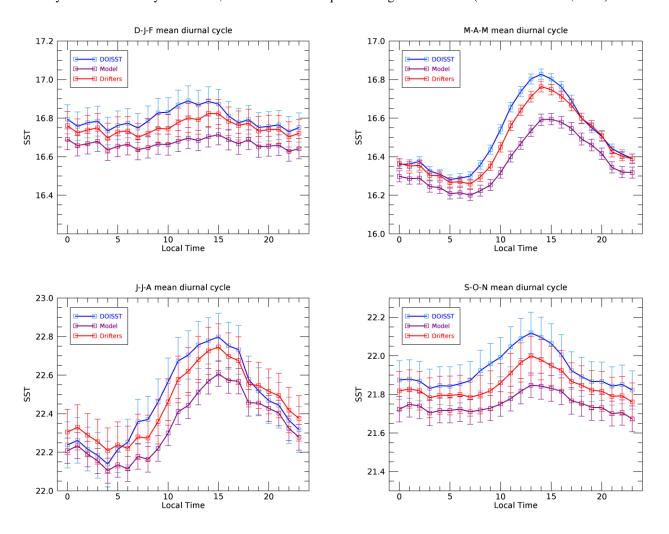




Figure 5. Seasonal mean diurnal cycle over the period 2019-2020 for MED DOISST (blue line), model (purple line) in situ (red line).



321

	Period	Mean bias (K)	RMSD (K)	Matchups
D-J-F	DOISST	$0.045\pm0.003$	$0.428 \pm 0.002$	
	Model	$-0.084 \pm 0.004$	$0.563 \pm 0.003$	90247
M-A-M	DOISST	$0.036 \pm 0.001$	0.383 ± 0.001	308448
	Model	$-0.101 \pm 0.001$	$0.389\pm0.002$	506446
J-J-A _	DOISST	$0.012 \pm 0.003$	$0.483\pm0.002$	74107
	Model	$-0.117 \pm 0.003$	$0.486\pm0.004$	
S-O-N _	DOISST	$0.079\pm0.003$	$0.429\pm0.002$	76157
	Model	$-0.098 \pm 0.004$	$0.590\pm0.004$	/015/

Table 4. Summary statistics of DOISST and model outputs. Mean bias (K) and RMSD (K) are derived from temperature differences against drifters' data during winter (D-J-F), spring (M-A-M), summer (J-J-A) and autumn (S-O-N) over the period 2019-2020.

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327 The capability of DOISST to reproduce diurnal warming events is analysed in the following section.

### 329 4.2.2 Diurnal warming events

Diurnal warming (DW) can be defined as the (positive) difference between the SST at a given time of the day and the foundation SST (see e.g. Minnett et al., 2019), i.e. the water temperature at a depth such that the daily variability induced by the solar irradiance is negligible. In many cases, the foundation SST coincides with the night minimum SST, namely the temperature that is recorded just before sunrise.

The capability of DOISST to describe diurnal warming events is analysed here in comparison with SEVIRI L3C, model and drifter data. The evaluation is carried out by computing daily DWAs from drifters and building a matchup dataset of DWAs as estimated from DOISST, SEVIRI L3C and model data. The inclusion of SEVIRI data is aimed at evaluating the impact of optimal interpolation on the input SEVIRI SSTs. The diurnal warming amplitude (DWA) is estimated here as a difference between the maximum occurred during daytime (10:00-18:00 local time) and the minimum during nighttime (00:00-06:00 local time) (see also Takaya et al., 2010; While et al., 2017).

340 The scatter plots of DOISST, SEVIRI and model vs in situ-measured DWA have been computed for the years 2019-2020 (Fig.

6) and organized during spring-summer and winter-autumn seasons (Fig. 7). This choice is aimed at comparing the behaviour

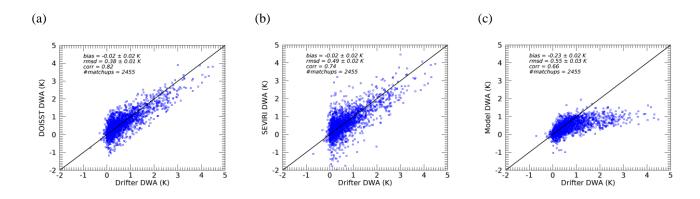
342 of the three products as a function of the seasons, since larger DWA intensities are expected in the spring-summer period.





Overall, there is a good agreement between DOISST and drifter DWAs (Fig. 6a) as confirmed by an almost null mean bias (-0.02 K), low RMSD (0.38 K) and high correlation coefficient (0.82). The largest DW amplitudes reach values as high as 4 K in both DOISST and drifter data. SEVIRI (Fig. 6b) shows the same bias (-0.02 K) of DOISST in reconstructing DWAs but higher RMSD (0.49 K) and lower correlation (0.74). It is relevant to note that the spread of SEVIRI DWAs around the line of perfect agreement is reduced in DOISST, which coherently has a lower RMSD. The model (Fig. 6c) clearly underestimates diurnal amplitudes larger than 1 K, and it is characterized by the highest mean bias (-0.23 K) and RMSD (0.66 K), and lowest correlation coefficient (0.66).

The majority of DWA events lie between 0-1 K all over the year, but higher values are effectively reached during spring and summer (Fig. 7). During these seasons, it appears more evident the capability of DOISST to better describe DWAs larger than 1 K (mean bias = -0.04 K; RMSD = 0.42 K; corr. = 0.83) compared to SEVIRI (mean bias = -0.05 K; RMSD = 0.53 K; corr. = 0.76) and especially to the model (mean bias = -0.27 K; RMSD = 0.65 K; corr. = 0.63). A similar behaviour is obtained during winter and autumn when DWA events exceeding 1 K are also observed, and such intense amplitudes are not found in the model-derived DWAs. Additionally, the good agreement between DOISST and drifters still confirms that interpolated data do not suffer from the increased cloud cover during winter and autumn periods.



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Figure 6. DWA scatter plots for (a) DOISST, (b) SEVIRI L3C and (c) model vs drifters over the period 2019-2020.





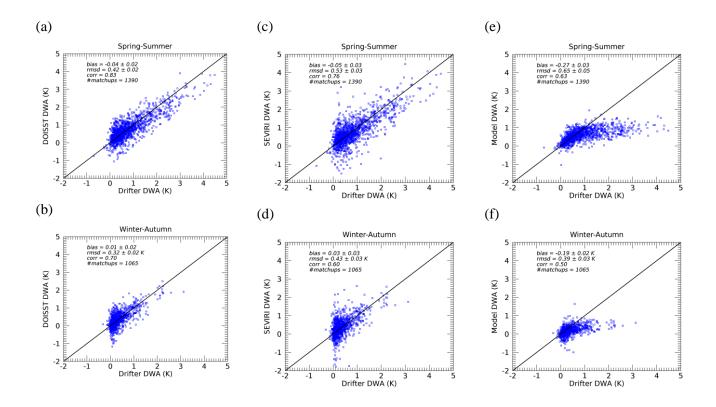


Figure 7. DWA scatter plots for DOISST (a,b), SEVIRI L3C (c,d) and model (e,f) vs drifters during Spring (M-A-M) and
 Summer (J-J-A), and Winter (D-J-F) - Autumn (S-O-N), over the period 2019-2020.

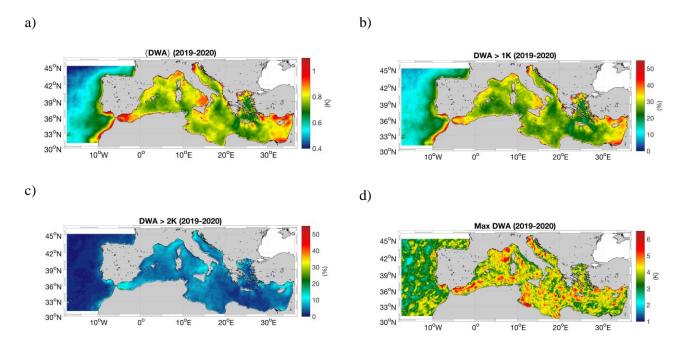
363 Having demonstrated the reliability of DOISST in the DWA estimate, we analyze its capability to reproduce the typical spatial 364 variability and intensity of DW events in the Mediterranean Sea, a basin characterized by a frequent occurrence of intense DW 365 events (Böhm et al., 1991; Buongiorno Nardelli et al., 2005; Gentemann et al., 2008; Merchant et al., 2008). In our investigation 366 area, the 2019-2020 mean DWA ranges from a minimum of 0.4 K in the Atlantic ocean box off the Strait of Gibraltar, to a 367 maximum of 1.2 K in several regions of the Mediterranean Sea (Fig. 8a) where individual diurnal warming events exceeding 368 1 or even more than 2 K are quite frequent (Minnet et al. 2019; Marullo et al. 2016; Marullo et al 2014; see in particular Fig. 369 3 in Minnet et al., 2019]. The largest DWA were observed in the Levantine Basin, in the North Adriatic Sea and in 370 correspondence with the Alboran Gyre. Less intense, though still remarkable, mean DWA patches reaching 0.9 K are found 371 around the southern tip of the Italian Peninsula as well as in the coastal Ligurian Sea. In the same areas, it is found that the 372 frequency of DW events larger than 1 K and 2 K can reach up to 55% and 10% of the analyzed time series, respectively 373 (bearing in mind that our time series is given by the total number of days in 2019 and 2020) (Fig. 8b-c).

374





The magnitude of the maximum SST diurnal oscillation is also investigated. The spatial distribution of the maximum DWA observed through 2019-2020 in the Mediterranean Sea (6°W to 36°E and 30°N to 46°N) (Fig. 8d) shows that the largest amplitudes reach and exceed 3 K in 98% of the basin and local DWA patches exceeding 6 K are also ubiquitous, confirming that the Mediterranean is one of the areas with the largest DWs of the global ocean (Minnet et al. 2019, and references therein).



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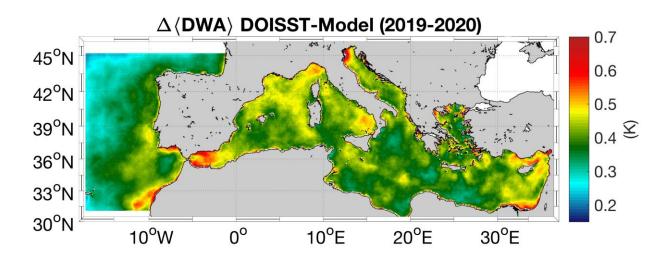
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Figure 8. a) Mean diurnal warming amplitude (DWA) derived from DOISST; b) Percentage (over the total number of days in
 the 2019-2020 period) of DOISST DWA larger than 1 K; c) Percentage of DOISST DWA larger than 2 K; d) Maximum
 observed DOISST DWA. All the maps refer to the 2019-2020 period.

When compared to the model, DOISST exhibits mean DWAs with larger intensity than model outputs in all the locations of the study area (Fig. 9). The  $\Delta$ DWA, defined as DWA<sub>DOISST</sub> minus DWA<sub>Model</sub>, is always larger than 0.2 K and locally reaches extreme values of ~1 K. The extent of the  $\Delta$ DWA generally increases in areas where the DOISST mean DWA is larger, such as in the Alboran Sea, Ligurian Sea, Levantine Basin and Southern Tyrrhenian, suggesting a tendency of the model to underestimate the largest DW events.







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Figure 9. Mean amplitude of the SST DW. Differences between the mean DWA seen by the DOISST product and themodel outputs (first layer).

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#### 393 **5 Data availability**

394 The Mediterranean diurnal optimal interpolated SST product is distributed as part of the CMEMS catalogue, and identified as 395 SST MED PHY SUBSKIN L4 NRT 010 036 (CMEMS product reference) and cmems obs-sst med phy-396 sst\_nrt\_diurnal-oi-0.0625deg\_PT1H-m (CMEMS dataset reference) (https://resources.marine.copernicus.eu/product-397 detail/SST MED PHY SUBSKIN L4 NRT 010 036/INFORMATION, last access: 03 November 2021, https://doi.org/10.25423/CMCC/SST MED PHY SUBSKIN L4 NRT 010 036; Pisano et al, 2021). Access to the product 398 399 is granted after free registration as a user of CMEMS at https://resources.marine.copernicus.eu/registration-form (last access: 400 03 November 2021). Once registered, users can download the product through a number of different tools and services, 401 including the web portal Subsetter, Direct-GetFile (DGF) and FTP. A Product User Manual (PUM) and QUality Information 402 Document (QUID) are also available as part of the CMEMS documentation (https://resources.marine.copernicus.eu/product-403 detail/SST MED PHY SUBSKIN L4 NRT 010 036/DOCU MENTATION, last access: 03 November 2021). Eventual 404 updates of the product will be reflected in these documents. The basic characteristics of the DOISST product are summarized 405 in Table 1. The reduced subset used here for validation and review purposes is openly available at 406 https://doi.org/10.5281/zenodo.5807729 (Pisano, 2021).





407

#### 408 **6 Summary and conclusions**

409 A new operational Mediterranean diurnally varying SST product has been released (May 2021) within the Copernicus Marine 410 Environment Monitoring Service (CMEMS). This dataset provides optimally interpolated (L4) hourly mean maps of sub-skin 411 SST over the Mediterranean Sea at 1/16° horizontal resolution, covering the period from 1<sup>st</sup> January 2019 to near real time (1 412 day before real time) (Pisano et al., 2021). The diurnal optimal interpolated SST (DOISST) product is obtained from a blending 413 of hourly satellite (SEVIRI) data and model outputs via optimal interpolation, where the former are used as the observation 414 source and the latter as background. This method has been firstly proposed by Marullo et al. (2014), validated over one year 415 (2013) in Marullo et al. (2016), and implemented here operationally. The validation of the operational product was also 416 extended over two years (2019-2020).

417 DOISST proved to be rather accurate when compared to drifter measurements, and correctly reproduced the diurnal variability 418 in the Mediterranean Sea. The accuracy of DOISST results in an overall, almost null, mean bias of ~0.04 K and RMSD of 419  $\sim$ 0.41 K (Table 2). This product is also more accurate than the input model, which shows a mean bias of  $\sim$ -0.1 K and RMSD 420 of ~0.47 K. A warm (positive) and cold (negative) bias characterizes the DOISST and the model, respectively, also during 421 seasons (Fig. 5). These opposite biases are likely related to the different nature of the SST provided by DOISST, model and 422 drifter data, i.e. sub-skin (upper first millimeters from the surface), averaged 1 m depth and 20 cm depth, respectively, and then consistent with the physical consequence of a reduction of the temperature with depth due to the vertical transfer heat 423 424 process. The DOISST RSMD generally keeps lower values compared to the model, ranging from a minimum of ~0.40 K (vs 425 ~0.42 K for the model) to a maximum of ~0.44 K (vs ~0.56 K for the model).

426 Compared to its native version (Marullo et al., 2016), the DOISST product maintains the same RMSD (estimated in 0.42 K) 427 but displays a lower mean bias (estimated as -0.10 K). The reduced bias could be ascribed to the fact that valid SEVIRI SST 428 values are always interpolated in DOISST, while they are left unchanged in the original method. The DOISST bias is also 429 lower than that of the OSTIA diurnal product, which produces gap-free hourly mean fields of skin SST for the global ocean, 430 and has been found to underestimate the diurnal range of skin SST by 0.1-0.3 °C (While et al., 2017).

The analysis of the SST diurnal cycle as estimated from both DOISST, model and drifter data shows that the diurnal oscillation in SST is well reconstructed by the DOISST while the model tends to underestimate this amplitude mainly during the central warming hours (Fig. 4), and during spring and summer (Fig. 5). Specifically, DOISST overestimates the mean diurnal amplitude by ~2.3% compared to that of drifters, while the model underestimates it by ~16%. This is particularly evident in the analysis of diurnal warming (DW) events, where diurnal warming amplitudes (DWAs) as estimated by DOISST, model and SEVIRI data are compared vs drifter-derived DWAs. This analysis shows that amplitudes exceeding 1 K as measured by





drifters are well reconstructed by DOISST (Fig. 6a) with a mean bias of ~-0.02 K while model SSTs show significantly lower values, with a mean bias of ~-0.23 K (Fig. 6c). The underestimation of the diurnal warming amplitude (DWA) by the model could be related to several factors, such as that the vertical resolution does not resolve the vertical temperature profile within the warm layer, the physics and atmospheric forcing implemented in the model, and/or the assimilation of the foundation SST fields used for the correction of surface heat flux.

The comparison with reconstructed SEVIRI DWAs (Fig. 6b) demonstrates that optimal interpolation does not change the SEVIRI bias, which is practically null for both SEVIRI and DOISST (~-0.02 K), while it reduces the SEVIRI RMSD, from ~0.49 K (SEVIRI) to ~0.38 K (DOISST). The seasonal analysis also reveals that DOISST is not impacted by the different environmental conditions in the Mediterranean Sea, in particular from the much frequent cloudiness during winter and autumn periods.

447 Overall, the DOISST product is able to accurately reconstruct the SST diurnal cycle, including diurnal warming events, for the
 448 Mediterranean Sea and can thus represent a valuable dataset to improve the study of those processes that require sub-daily
 449 frequency.

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- 451

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457

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