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MODELLING THE DIURNAL VARIABILITY OF SST AND ITS VERTICAL EXTENT

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ABSTRACT

Sea Surface Temperature (SST) is a key variable in air-sea interactions, partly controlling the oceanic uptake of CO₂ and the heat exchange between the ocean and the atmosphere, amongst others. Satellite SSTs are representative of skin and sub-skin temperature, i.e. in the upper millimetres of the water column where most of the heat is absorbed and where the exchange of heat and momentum with the atmosphere occurs. During day-time and under favourable conditions of low winds and high insolation, diurnal warming of the upper layer poses challenges for validating and calibrating satellite sensors and merging SST time series. When radiometer signals, typically from satellites, are validated with in situ measurements from drifting and moored buoys a general mismatch is found, associated with the different reference depth of each type of measurement. A generally preferred approach to bridge the gap between in situ and remotely obtained measurements, is through modelling of the upper ocean temperature. Models that have been used for this purpose vary from empirical parametrisations mostly based on the wind speed and solar insolation to ocean models that solve the 1 dimensional equations for the transport of heat, momentum and salt. GOTM is a model resolving the basic hydrodynamic and thermodynamic processes related to vertical mixing in the water column, that includes most of the basic methods for calculating the turbulent fluxes. Surface heat and momentum can be either calculated or externally prescribed while the model includes a 2-band parametrisation for the penetration of light in the water column. From the analysis it has been found that the data used to initialise the model, especially the temperature profiles, along with the selected light extinction scheme hold a key role in the agreement of the modelled output with observations. To improve the surface heat budget calculation and distribution of heat in the water column, the GOTM code was modified to include an additional method for the estimation of the total outgoing long-wave

radiation and a 9-band parametrisation for the light extinction, correspondingly. New parametrisations for the stability functions, i.e. the quantities in the turbulent diffusivity expressions associated with vertical mixing, have been included. Preliminary results demonstrate the successful implementation of the new parametrisations and the ability of the model to reproduce the diurnal signals seen from the in situ measurements. In addition, special focus is given to testing and validation of different model set-up combinations using experimental data from different campaigns in the Atlantic Ocean, in order to establish a model set-up that can be applied to different regions.

Key words: SST; diurnal variability; GOTM.

1. INTRODUCTION

During day time and under favourable conditions of low winds and solar heating, the upper few meters of the oceanic layer may experience an increase of temperature that can reach up to several degrees. This mechanism can be further supported by parameters than limit the penetration of light into the water column. Studies have shown that the diurnal amplitude is higher closer to the surface, since heat is largely trapped there, thus the diurnal variability is captured best by radiometers that provide skin and sub-skin measurements. Diurnal SST variability has been observed in different areas of the global ocean including the Mediterranean [11], western North Atlantic [12], and the Gulf of California [17] using combinations of in situ and satellite observations. Recently, a preliminary study has revealed large diurnal warming signals when compared to drifting buoys in the inter-tropical Atlantic, when in other regions of the SEVIRI disc the agreement between drifters and the satellite diurnal signal was found to be around 0.5 K [10]. Most of the studies mentioned above were limited in the Tropics and mid-latitude regions but recently diurnal warming has been reported at higher

latitudes [4, 6].

Atmospheric, oceanic and climate models are currently not adequately resolving the daily SST cycle, resulting in biases of the total heat budget estimates [16, 17, 2, 1] and therefore, demised model accuracies. In addition, strong SST diurnal signals can complicate the assimilation of SST fields in ocean and atmospheric models, the derivation of atmospheric correction algorithms for satellite radiometers and the merging of satellite SST from different sensors [3]. Not accounting for the daily SST signal can cause biases in the scatterometer derived ocean wind fields and biases in the estimated net flux of CO₂, as the out flux of oceanic CO₂ is positively correlated with the increase of SST. Ongoing efforts to understand the diurnal variability of SST have been greatly promoted by the availability of SST retrievals from infra-red radiometers in geostationary orbit, thus allowing the hourly monitoring of the diurnal signal's evolution.

Thus, there is an increased need to understand and quantify the diurnal SST variability at different regions and resolve the vertical extend of the diurnal signal, in order to relate observations from different instruments and to remove trends from climate records. Part of the effort to create a long time series of stable SST fields consists of successfully modelling the diurnal cycle at a given location in order to correct for the inconsistent satellite overpass times. This can be achieved using either observational evidence from in situ and satellite-derived SSTs or, models able to resolve the daily SST cycle and its vertical extend. A comparison of diurnal variability from SEVIRI and three models of different background, [7] highlighted the dependence of such models on the input fields, in particular the wind (typically obtained from atmospheric models). Consequently, there is a need to evaluate the impact of properly resolving the daily variability of SST in atmospheric models, in terms of momentum and heat fluxes.

Financed by the European Space Agency's Support To Science Element (STSE), the "SSTDV: R.EX. - IM.A.M." project focuses on studying the regional extent of diurnal warming and its implications for mesoscale atmospheric modelling. The 6-year long archive of the Meteosat Second Generation Spinning Enhanced Visible/Infra-Red Imager (SEVIRI) hourly SST fields was used for a low, mid and high latitude evaluation of the diurnal cycle and identify regional patterns [8]. Identifying areas where common diurnal warming patterns occur is important to better understand the conditions under which the diurnal cycle is formed. The implementation of the 1 dimensional General Ocean Turbulence Model (GOTM) took place, in order to model the diurnal signals identified from SEVIRI SST fields and in situ measurements. This will serve as the link between the surface signals of the diurnal cycle, available by satellites, and the observational evidence from drift-

ing and moored buoys. The model is tested using experimental data consisting of measured meteorological (air pressure and temperature, wind speed, humidity, long- and short-wave radiation) and oceanographic parameters (water temperature and salinity), with which the model can be initialised. The final aim is to produce modelled SST fields comparable with hourly SEVIRI SSTs, and consistent with in situ measurements thus establishing the validity of the GOTM model to be used as a proxy for removing diurnal signals from SST time-series, adding diurnal variability on bulk SST and other relevant topics.

2. DATA

2.1. In Situ and Model Data

The locations of the three moorings are shown in Fig. 1. The Marine Light-Mixed Layer 1991 (MLML91) experiment took place from April to September 1991; data are available from the Upper Ocean Processes Group of the Woods Hole Oceanographic Institute (<http://uop.whoi.edu/archives/dataarchives.html>). The mooring, positioned at 59.489 °N, 20.826 °W, was equipped with instruments to measure east/north wind components, air temperature, barometric pressure, relative humidity, incident long-wave and short-wave radiation at 3 m every 15 minutes. Water temperature at depths of 2, 10, 30, 50, 70, 80, 102, 118 and 150 m were obtained every 15 minutes [14].

The Prediction and Researched Moored Array in the Atlantic (PIRATA) mooring at 15 °N, 38 °W is equipped with temperature sensors, the upper most of which are at 1, 5, 10, 13, 20, 40, 60, 80, 100, 120 and 140 m. Meteorological observations of wind speed and direction, air temperature and relative humidity at 4 m were obtained every 10 minutes, air pressure at 3 m was obtained hourly, while measurements of down-welling short-wave and long-wave radiation at 3.5 m were obtained every 2 minutes. Data used in the present study are obtained from the Tropical Atmosphere Ocean (TAO)/TRITON project through http://www.pmel.noaa.gov/tao/data_deliv/deliv.html, for the period 2006-2007, when long-wave radiation was available.

The Arkona Becken platform is part of the MARNET network (http://www.bsh.de/en/Marine_data/Observations/MARNET_monitoring_network), maintained by the Bundesamt für Seeschifffahrt und Hydrographie (BSH). The platform is located in the Baltic Sea (54.88 °N, 13.87 °E), at a depth 45 m. Temperature sensors are placed at 2, 5, 7, 16, 25, 33, 40, 43 and 45 m, obtaining hourly measurements. Meteorological observations of wind speed and direction, air pressure and temperature, relative humidity and down-welling short-wave radiation are obtained hourly at a height of 10 m.

Climatological temperature and salinity profiles are obtained from the World Ocean Atlas 13 (WOA13) through the National Oceanographic Data Centre (http://www.nodc.noaa.gov/OC5/WOA13/pr_woa13.html). Profiles from the EN4.0.2 dataset available from the UK Met Office are obtained through the Hadley Centre (http://www.metoffice.gov.uk/hadobs/en3/data/EN3_v2a/download_EN3_v2a.html). The Baltic Sea Physics Analysis dataset from the Danish Meteorological Institute (DMI) is available through the MyOcean project (<http://www.myocean.eu/>). Hourly temperature is available every 5 m from 0 to 100 m, 150, 200, 300 and 400 m with a spatial resolution of 1.9 km.

Atmospheric variables such the u -, v - wind components at 10 m, surface pressure, dry air temperature, dew point temperature and cloud cover are obtained from the European Centre for Medium-range Weather Forecasting (ECMWF) using the global atmospheric model operational archive (experiment version 1), at 0.125° spatial and 3-hour temporal resolution.

2.2. SEVIRI SST

SEVIRI hourly SST on a 0.05° grid were obtained from the Centre Météorologie Spatiale (CMS), Météo France to be used for comparisons with the GOTM model estimates. MSG/SEVIRI SST retrievals are classified using a quality flag index that ranges from 0 (unprocessed) to 5 (excellent). SEVIRI SSTs are corrected for the cool skin bias by an addition of 0.2 K at CMS, before they are released. Two different SEVIRI products are used, i.e. the 6-year long experimental product to derive long-term estimates of diurnal warming and the newly processed SEVIRI product which includes a bias correction [9], is used for 2013 to compare with GOTM modelled temperatures.

3. METHODS

3.1. Diurnal Warming

Diurnal warming is defined as the increase of day-time temperature from the night-time foundation temperature, representative of well-mixed conditions. The latter is assumed to be the average SST from midnight to 4 a.m. local time (LT) and is constructed separately for each day. The day-time increase is then calculated as the hourly day-time SST value minus the previous night's foundation SST.

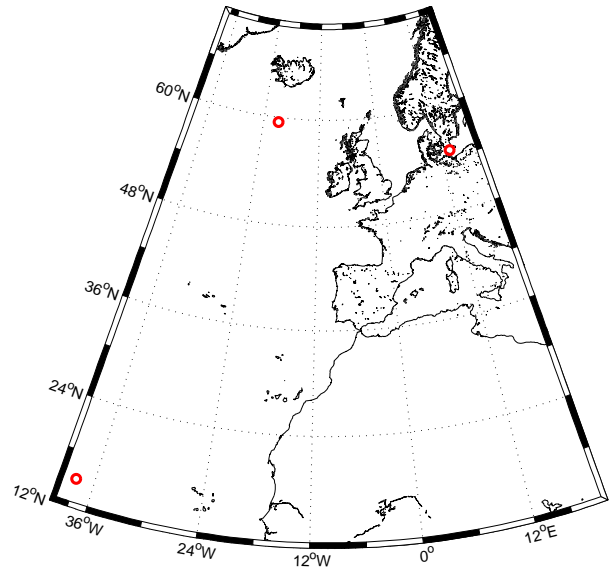


Figure 1. Map with the locations of the three sites with measured oceanographic and meteorological variables used for the GOTM set-up.

3.2. Modelling

GOTM is a 1 dimensional turbulence model that describes the basic thermodynamic and hydrodynamic processes related to the vertical mixing by solving the 1-d equations for the transportation of heat, salt and momentum [15]. Surface fluxes can be either prescribed from NWP models or calculated internally in GOTM using bulk flux algorithms requiring the input of the 10-m wind components, the air temperature, pressure, humidity and cloud cover. The model includes a 2-band parametrisation for the light extinction in the water column. An additional 9-band parametrisation has been included. Additional options have been included for i) the calculation of the net long-wave radiation by means of a Brunt type formula and ii) the prescription of the down-welling long wave radiation from measurements. New stability functions, i.e. dimensionless quantities involved in the expressions for the diffusivity of heat and momentum, have also been added. In this study, the options examined include the parametrisation for the calculation of the long-wave radiation, the method to compute the typical length scale of the turbulence quantities and the light extinction parametrisation (see Tab. 1).

The vertical grid is calculation according to Eq. 1 as in [13]

$$h(i) = D * \frac{\tanh \frac{i}{D/3} - \tanh \frac{i-1}{D/3}}{\tanh 3} \quad (1)$$

where i is the layer number, h is the layer height and D the depth of the water column. The number of vertical layers versus depth, for a 150 m depth, are

shown in Fig. 2. The model time-step is 1 minute with outputs saved every hour.

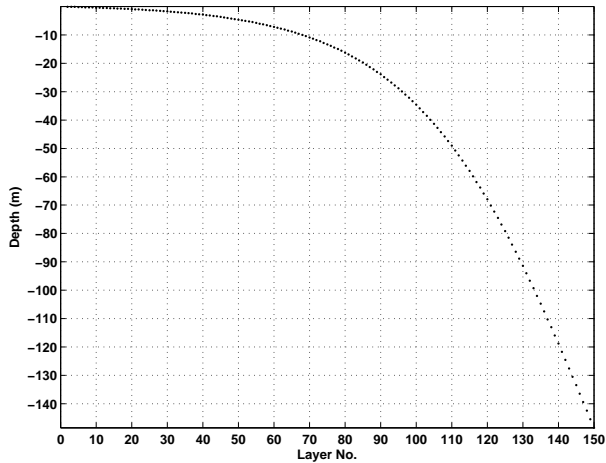


Figure 2. Number of layers as a function of depth for a vertical grid down to 150 m depth.

4. RESULTS

The percentage of quality 5 SEVIRI SST retrievals that show an increase in day-time temperature of 1° or more compared to the night-time, foundation SST is shown in Fig. 3. The high percentage appearing on the left part of the SEVIRI disk is due to few available retrievals that may also be anomalously high because of higher retrieval errors caused by the longer atmospheric path. Grid cells with less than 10 retrievals have been excluded for this reason; nonetheless large areas still remain “observable” but highly uncertain. However, the remaining part of the SEVIRI disk also shows relatively high percentages of increased day-time warming not only in enclosed basins and coastal areas but in the open ocean. Such findings demonstrate the importance of properly modelling the diurnal variability of the upper water temperature structure and justifies the use of the three different locations where diurnal warming occurs.

Given the extent of diurnal warming identified from the SEVIRI data, the GOTM model was evaluated at three different locations characteristic of open ocean tropical and mid/high latitude waters and coastal, enclosed basins. Forcing fields are expected to play an important role to the model’s ability to reproduce observed temperature and sensitivity tests performed at the MLML91 location showed that the parametrisation used by GOTM to calculate the net short-wave radiation is accurate despite the lack of necessary cloud cover information. Fig. 4 shows the measured down-welling short-wave radiation at the MLML91 buoy for 6-10 June 1991 (black stars). When prescribing the short-wave radiation from measurements, GOTM interpolates it to match

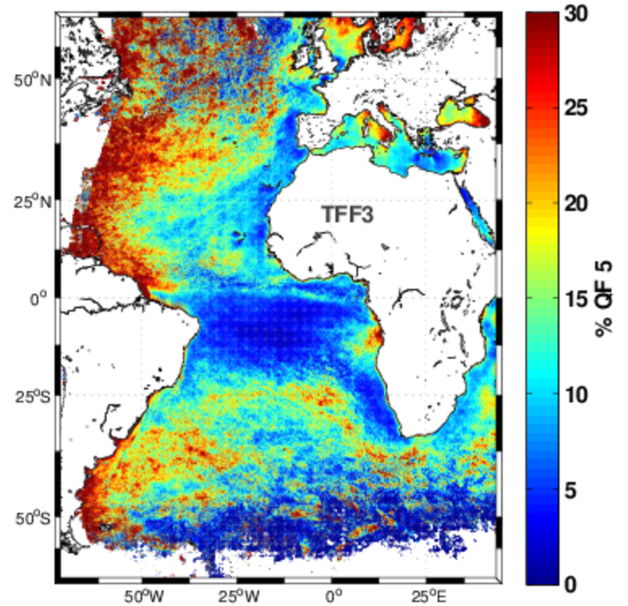


Figure 3. SEVIRI estimated diurnal warming exceeding 1° as a percentage of the available quality 5 SST retrievals.

the model time-step and this parameter, as used in GOTM, is shown as the black solid line while the internally calculated short-wave radiation is shown as the black dashed line. The short-wave radiation at the buoy is down-welling while GOTM computes the net short-wave radiation and thus the former is expected to be higher, but as no cloud information is available the GOTM calculated parameter can be overestimated.

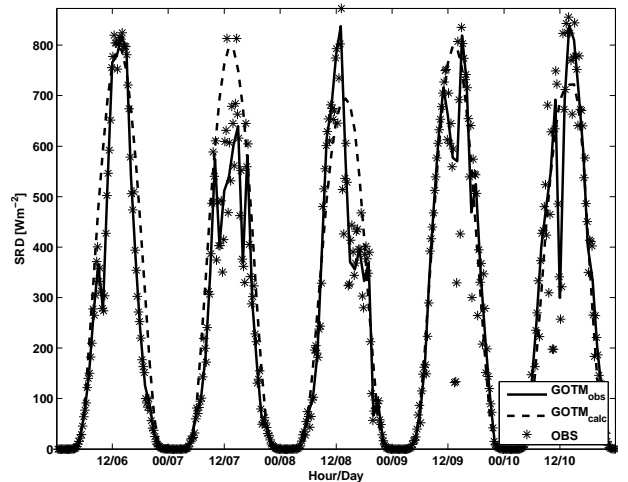


Figure 4. Short-wave radiation measured at the buoy, prescribed in GOTM and calculated internally.

Fig. 5 shows the impact of the length scale method and the light extinction schemes, as a function of the error statistics between the 2 m temperature as modelled by GOTM and measured at the buoy location.

Table 1. GOTM set-up options.

| Code | Option | Code | Option |
|------|---|------|--|
| | 1. Long-Wave Radiation | | 3. Light Extinction |
| 1 | Clark et.al (1974) | 1 | 2-band Jerlov-I |
| 2 | Hastenrath and Lamb (1978) | 2 | 2-band Jerlov-I (upper 50 m) |
| 3 | Bignami et al. (1995) | 3 | 2-band Jerlov-IA |
| 4 | Berliand and Berliand (1952) | 4 | 2-band Jerlov-IB |
| 5 | Brunt formula, coef Grant & Hignett (1998) | 5 | 2-band Jerlov-II |
| 6 | Prescribed by user | 6 | 9-band with attenuation lengths, proportional coeff. Paulson & Simpson (1981) |
| | 2. Length Scale Method | 7 | 9-band att. length Paulson & Simpson (1981), coeff. COART model |
| 1 | Dynamic dissipation | 8 | 9-band att. length Paulson & Simpson (1981), coeff. MODTRAN model |
| 2 | Dynamic Mellor-Yamada q ² 1 | | |
| 3 | Generic Length Scale | | |

With the help of this plot, certain GOTM parameters can be tuned, as for example the biases using the 2nd length-scale option are the largest, thus leading to the exclusion of this option. The 1st and 3rd length scale methods result in almost similar statistics but the 1st option has slightly lower standard deviations and it is going to be used from now on. For a given length-scale method it is seen than the 5th light extinction scheme results in the smallest bias and highest correlation, which makes it a candidate selection. As the light extinction parametrisation depends on the local conditions this option will be investigated at the other locations as well.

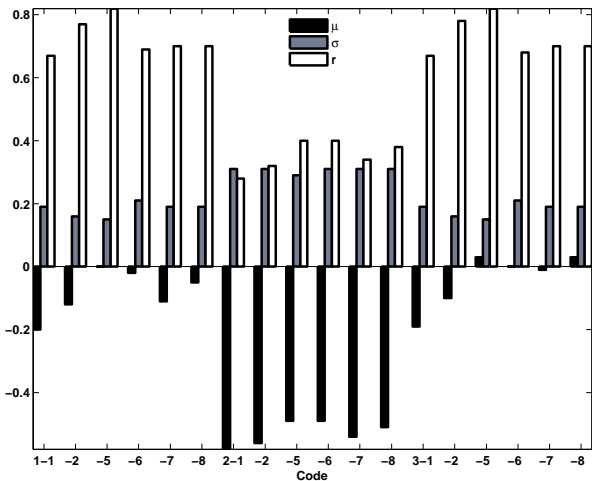


Figure 5. Statistics of the GOTM-Buoy 2 m temperature for different length scale methods and light extinction schemes.

Using certain options for some of the GOTM tunable parameters, the 2 m buoy (black crosses) and GOTM temperatures for different light extinction schemes are shown in Fig. 6. GOTM successfully reproduces

the daily variability at the buoy despite the use of only one initial temperature profile. Peak warming and cooling is generally resolved by GOTM and the different light extinction schemes result in temperature differences ranging between 0 and 0.5° for this specific case. The 2-band model (LE 1-5, red to cyan) generally results in lower modelled temperature compared to the 9-band model.

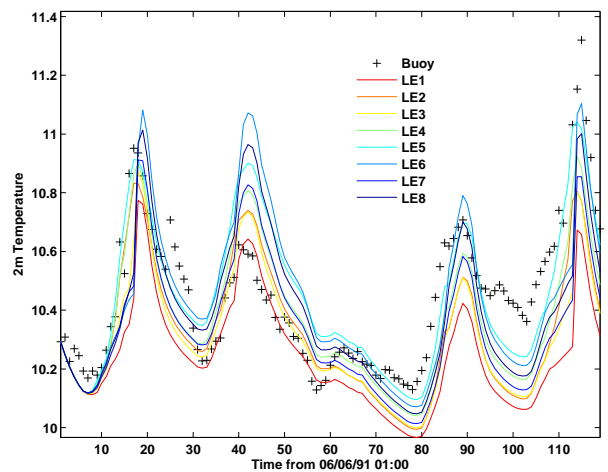


Figure 6. 2-m buoy and GOTM temperatures at MLML91 from the 6-10/06/91 with the short-wave radiation prescribed and remaining fluxes calculated from the meteo-data.

Performing similar analysis at the tropical location of the PIRATA buoy, the statistics between the 1 m GOTM minus buoy temperature for the period 22-25 August 2006 are presented in Fig. 7, for in situ measured forcing fields (top) and ECMWF forcing fields (bottom). The different coloured bars show the mean bias μ (black), standard deviation σ (grey) and correlation coefficient r (white) for the various

combinations of the long-wave radiation parametrisation (first digit) and light extinction scheme (second digit). No significant differences between the two types of forcing is found, with generally μ and σ lower than 0.1° and correlation r higher than 0.9 for the long-wave radiation parametrisations 1-4. The 1st and 7th option for the light extinction scheme are the ones with lowest biases and σ values.

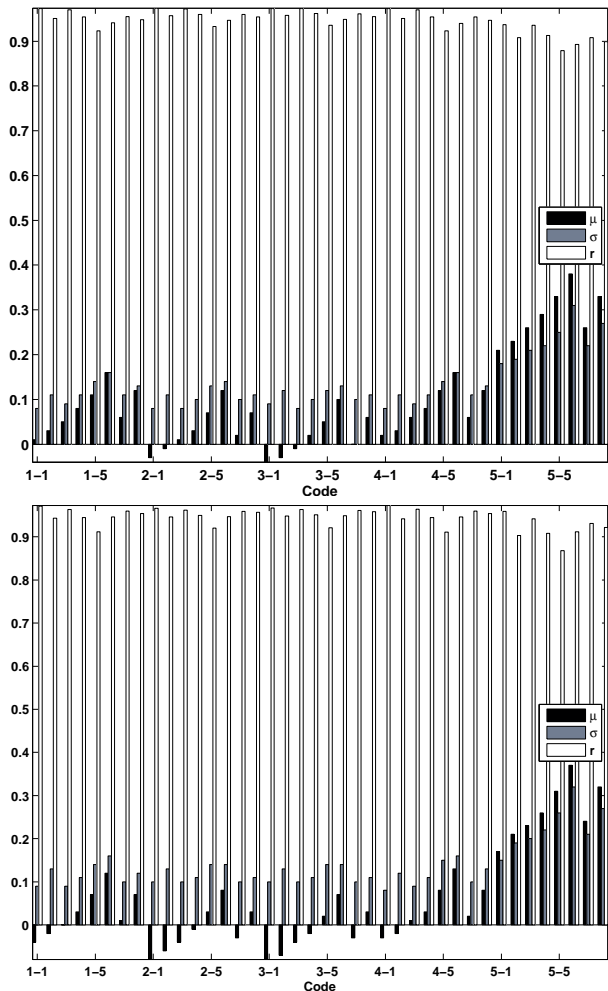


Figure 7. 1 m GOTM minus buoy temperature for different combinations of the parametrisation for the long-wave radiation (1st digit) and the light extinction scheme (2nd digit). GOTM uses in situ measured forcing fields (top panel) or ECMWF fields (bottom).

The observed and modelled 1 m temperature at the PIRATA location for the period 22-25 August 2008 is shown in Fig. 8. GOTM using in situ measured forcing fields (blue) reproduces the temperature measured at the buoy using only one initial vertical profile. It shows slightly higher peak warming in the first 2 days, but lower peak values during days 3 and 4; nonetheless the difference between measurements and GOTM does not exceed 0.2°C . When GOTM uses the ECMWF forcing fields and one initial pro-

file (cyan), the peak warming is reproduced in the 1st and last days but it is overestimated in day 2 and underestimated in day 3 by no more than 0.3°C . Moreover, a time mismatch is identified related to different time formats between ECMWF and the in situ measurements.

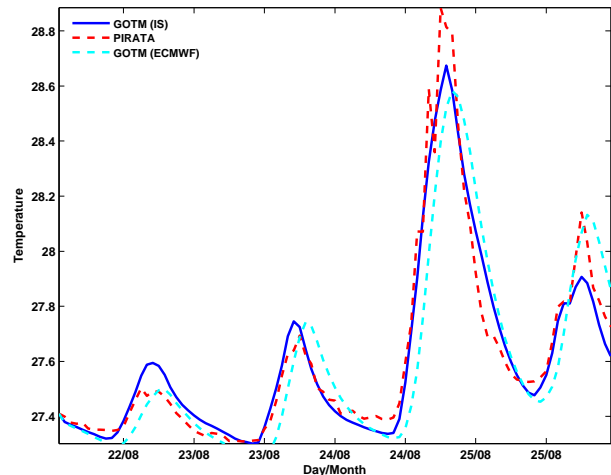


Figure 8. Measured (red dashed) and GOTM modelled 1 m temperature using in situ measured meteorological variables and profile (blue solid) with BRM 3 and LE 3 and ECMWF forcing and the in situ profile with BRM 4, LE 1 (cyan).

The comparison between the GOTM top layer temperature and the SEVIRI sub-skin SST at the Arkona Becken location from the 9th to the 14th of July 2013 is shown in Fig. 9. The black lines represent GOTM temperatures using ECMWF forcing fields, the short-wave radiation directly prescribed from ECMWF and different initial temperature profiles; grey lines are similar but with the short-wave radiation calculated using the ECMWF cloud cover. It is evident that when possible, prescribing the short-wave radiation is preferable due to the uncertainty of the cloud cover field. GOTM matches SEVIRI observations but the peak warming on the 12th of June is overestimated by GOTM. Small differences due to the different profiles are identified particularly during cooling phases but they are typically less than 0.5°C .

5. DISCUSSION

This study summarises the findings of the ESA STSE project SSTDV: R.EX.-IM.A.M. related to the modelling of the diurnal variability of SST using the 1-dimensional GOTM model. Tests were conducted in order to evaluate the model's sensitivity to the forcing fields and the initial temperature profiles. It was shown that the method to compute the short-wave radiation is highly accurate but requires the cloud cover information which can only be obtained

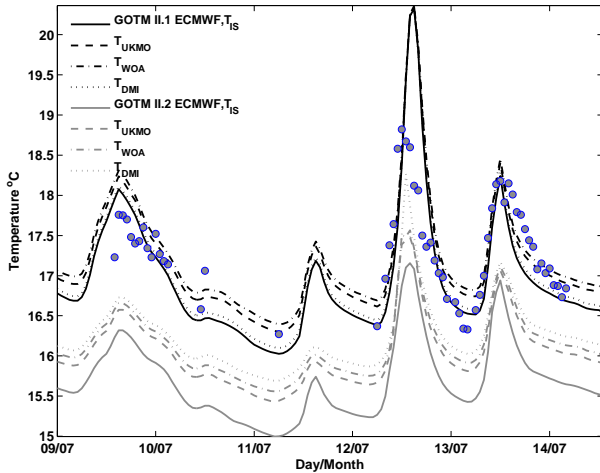


Figure 9. Top layer temperature from GOTM using ECMWF forcing fields and different temperature profiles and sub-skin SST from SEVIRI (circles) from July 4th to 14th, 2013.

from NWP models. When diurnal warming events were modelled and the cloud cover was assumed to be zero, the GOTM temperature matched well with the buoy measurements. When NWP forcing fields were used, better statistics resulted from prescribing the short-wave radiation directly from the NWP field rather than calculating it using the cloud cover field, due to its higher uncertainty.

Comparing the use of in situ versus ECMWF forcing fields in one location, GOTM minus buoy temperature differences did not exceed 0.1°C with standard deviations lower than 0.2°C independent of the forcing fields. Such low error statistics are not to be expected always, as in some cases ECMWF forcing fields may deviate from the in situ measurements because of restrictions in the NWP model's ability to represent the small scale processes but it should be kept in mind that in situ instruments are also subject to operational failure and some uncertainty in the measurements. Nonetheless, such findings are promising if one aims at using GOTM to evaluate diurnal warming at larger spatial scales.

The choice of the light extinction is important as differences in the modelled temperature reaching up to 0.5°C were identified. As the penetration of light inside the water column depends on the water properties, which may differ between locations, no conclusive setting was found. Nonetheless, there was consistently a better performance of the 9-band model compared to the 2-band model, consistent with other studies [5, 12], and thus this option will be generally preferred.

The initial temperature profiles used as boundary conditions may provide a warmer or colder start-up compared to the in situ profile. This was investigated at the Arkona Becken location, where the cli-

matological and modelled profiles resulted in warmer temperatures by no more than 0.5°C . Nonetheless, temperature differences tended to be minimum during the peak warming and increased at the cooling phase.

GOTM was found to reproduce the temperature measured at buoy locations from in situ sensors at some depth but also retrieved by SEVIRI at the sub-skin level. Thorough sensitivity tests and statistical comparisons of modelled and measured temperatures resulted in the optimal selection of settings regarding various tunable GOTM parameters, based on the minimization of the errors between the model and observations. Nonetheless, the "universality" of some settings is questionable and more tests could be performed at different locations; a task, unfortunately, limited by the availability of concurrent meteorological and oceanographic measurements.

The work presented here is thought as part of some of the main activities of GHRSSST's Diurnal Variability Working Group. The aim is to examine the performance of different models, ranging from statistical and regression analysis parametrisations to fully physical models. The purpose of testing different models is to evaluate their performance and quantify the uncertainty when attempting to model the diurnal variability of the upper ocean temperature. If models are to be used for the operational estimation of the diurnal cycle, potentially to be included in L4 SST products, it is necessary to select those that can combine successful representation of the physical processes and minimum computational cost.

6. CONCLUSIONS

This study has focused on results within the framework of the ESA STSE project on the SST Diurnal Variability, its Regional Extent and the Implications in Atmospheric Modelling (SSTDV: R.EX. - IM.A.M.). Modelling the diurnal cycle is an ongoing aim within the satellite SST community, in order to link satellite-derived SST, representative of the upper few millimetres, with signals from in situ instruments (from 20 cm downwards). Sensitivity tests were conducted in three different locations ranging from mid/high latitude open ocean to tropical open ocean and a mid/high latitude enclosed basin, where diurnal warming exceeding 1°C was identified. In situ measurements of surface meteorological variables and water temperature profiles were used as forcing fields and the modelled temperature was compared to the observations for different model setups. Such sensitivity tests resulted in the selection of certain options for the GOTM set-up, such as the method to calculate the turbulence length scale and the down-welling long-wave radiation. In addition, forcing fields from ECMWF and climatological tem-

perature profiles were used and the errors due to the use of non measured forcing fields were quantified. More specifically, due to the uncertainty of the cloud cover fields from ECMWF, calculating the short-wave radiation was found to result in lower modelled temperature by up to 3°C during peak warming but on average the difference was not more than 1.2°C. Different initial temperature profiles were associated with smaller temperature differences, in the order of 0.3°C. Comparisons of modelled minus measured temperature using in situ versus ECMWF forcing showed practically no impact of the forcing fields to the statistics, at least for the location of the PIRATA buoy. Average biases and standard deviations were lower than 0.1-0.2°C and the correlation coefficient was higher than 0.9. The light extinction parametrisation is important if accurate modelling of the upper ocean temperature is to be achieved. From sensitivity tests it was found that while on average biases between modelled and observed temperature did not vary by more than 0.2°C due to the different light extinction schemes, instantaneous differences during peak warming reached 0.8°C. GOTM upper layer temperature, modelled using ECMWF forcing fields, matched with SEVIRI SST for a period of 10 days at a location in the Baltic Sea. The next step is to implement GOTM at many points, also accounting for horizontal advection, and compare its performance with SEVIRI observed diurnal variability estimates.

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