The bulk parameterizations of turbulent air-sea fluxes in NEMO4: the origin of Sea Surface Temperature differences in a global model study

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Abstract.

Wind stress and turbulent heat fluxes are the major driving forces which that modify the ocean dynamics and thermodynamics. In the Nucleus for European Modelling of the Ocean (NEMO) ocean general circulation model, these turbulent air-sea fluxes (TASFs) can critically impact the simulated ocean characteristics. This paper investigates how the different various bulk parameterizations to calculate turbulent air-sea fluxes in NEMOv4 drives can lead to substantial differences in sea surface temperature the estimation of sea surface temperatures (SST). Specifically, we study the contribution of different aspects and assumptions of the bulk parameterizations in driving the SST differences in NEMO global model configuration at 1/4 degree of horizontal resolution. These aspects include the use of the skin temperature instead of the bulk SST in the computation of turbulent heat flux components and the estimation of wind stress and of turbulent heat flux components, which vary in each parameterization due to different bulk transfer coefficients. The analysis of a set of short-term sensitivity experiments, where the only change is related to one of the aspects of the bulk parameterizations, shows that parameterization-related SST differences are primarily sensitive to the wind stress differences and to the implementation of skin temperature in the computation of turbulent heat flux components. Moreover In addition, in order to highlight the role of SST-turbulent heat flux negative feedback at play in ocean simulations, we compare the TASFs TASF differences obtained using the NEMO ocean model with the estimations from by Brodeau et al. (2017), who compared the different bulk parameterizations using prescribed SST. Our estimations of turbulent heat flux differences between bulk parameterizations is weaker than that are weaker than those found by Brodeau et al. (2017).

1 Introduction

Ocean and atmosphere circulations are highly influenced by the transfer of momentum and heat at the air-sea interface (e.g., Gill, 1982; Siedler et al., 2013). These transfers of energy are primarily driven by surface radiative flux and turbulent air-sea air-sea fluxes (TASFs), which include wind stress and the turbulent heat flux components (THFs, latent and sensible heat fluxes). In the upper ocean, the wind stress is a major driving force for of basin-scale circulation (e.g., Chen et al., 1994; Shriver and Hurlburt, 1997), and the THFs are important for determining its thermal properties (e.g., Yuen et al., 1992; Swenson and

Hansen, 1999). Therefore, both wind stress and THFs are important for the evolution of sea surface temperature (SST), because of their contribution to turbulent mixing within the ocean surface mixed layer (e.g., Barnier, 1998).

Since direct observations of TASFs are sparse in space and time, the estimates of TASFs are derived using bulk formulas, which relate each component of turbulent air-sea flux to more easily measurable and widely available meteorological surface atmospheric variables (e.g. wind speed, air temperature, air specific humidity) through bulk transfer coefficients. These coefficients are estimated using bulk parameterizations. Different bulk parameterizations are currently used and they which are traditionally developed statistically, comparing in situ meteorological observations of surface atmospheric variables with TASFs derived from ship and buoy measurements (Large and Pond, 1981, 1982; Smith, 1988; Fairall et al., 1996, 2003; Bradley and Fairall, 2007; Edson et al., 2013).

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In the NEMO ocean general circulation model (OGCM), TASFs are computed by means of bulk formulas using prescribed surface atmospheric variables (air temperature, air humidity, wind) and the prognostic SST of the model (hereinafter online prognostic SST approach). The online prognostic SST approach allows to incorporate This approach incorporates the response of the ocean (i.e. SST) to atmospheric events into the estimation of the THFs and of longwave radiation (i.e. non solar heat flux components, NSHFs) at every each time step of the numerical experiment. The possibility of feedback mechanisms feedback between the ocean and the atmosphere partially simulates simulate the energy exchange between them (Kara et al., 2000). The approach requires the choice of OGCM entails the selecting a given bulk parameterization, which influences the magnitude of the wind stress and of the THFs (Kara et al., 2000). The TASFs affect the simulated ocean characteristics and in particular the evolution of the SST (Torres et al., 2019). It is worth mentioning that the The online prognostic approach does only partially close only partially closes the air-sea feedback. Surface winds and clouds are affected by the SST structure on daily time-scale time-scales which, in turn, affect the SST and the TASFs (Desbiolles et al., 2021; de Szoeke et al., 2021; Gaube et al., 2019; Li and Carbone, 2012; Small et al., 2008). The closed air-sea feedback (hereinafter coupled approach) in the system might could substantially impact the turbulent fluxes (Lemarié et al., 2021; Small et al., 2008), but however the coupled approach is still not yet mature in the ocean model community. Recently Lemarié et al. (2021) implemented a first attempt of a exploited a simplified atmospheric boundary layer model (ABL) to improve the representation of air-sea interactions in NEMOv4.2. However, the online prognostic SST approach is still largely-widely used by the ocean modeling community in a variety of applications.

Brodeau et al. (2017) compared a set of bulk parameterizations which compute TASFs using prescribed SST (hereinafter offline prescribed SST approach) rather than the prognostic SST of the model. Based on their approach Brodeau et al. (2017) They reported that the use of different bulk parameterizations to estimate TASFs can typically produce differences in total turbulent heat flux (Q_T) , i.e. the sum of the THFs, latent and sensible heat fluxes) of about $10W/m^2$ and in wind stress of about $20mN/m^2$. The online prognostic SST approach, used by in the NEMO experiments performed for this in our study, can substantially modify these estimations estimates through the negative SST feedback on Q_T , likely dampening which likely dampens the Q_T discrepancies across the different various bulk parameterizations (Seager et al., 1995).

The purpose aim of this work is to better understand the response of the prognostic SST to the TASFs and to their parameterization in NEMO version 4.0 at $1/4^{\circ}$ of horizontal resolution, and to. We also discuss the role of the SST- Q_T negative

feedback at play in the online prognostic SST approach. We address the sensitivity of the SST to various aspects of the different bulk parameterizations, such as the inclusion of the skin temperature in the computation of the THFs and the role of the bulk transfer coefficients in the estimation of the wind stress and the THFs. In order to do that, we THFs. We thus analysed differences between short-term sensitivity experiments where bulk assumptions are excluded (e.g. skin temperature) or where bulk transfer coefficients are computed mixing the different bulk parameterizations. Lastly, in order to highlight the role of the SST- Q_T negative feedback at play in our online prognostic SST approach, we compare the TASFs with the estimations from Brodeau et al. (2017). We also provide a simple validation of the different experiments against a various experiments against an SST observed dataset, but however the main objective of the work is was to investigate the impact of a set of bulk parameterizations on the SST generated by NEMO rather than evaluate evaluating their accuracy in reproducing it.

This paper is organized as follows: in section. Section 2, we present presents the model used for this study, a short overview of the bulk formulas implemented in NEMOv4, the experimental set-up and the modifications introduced in the bulk parameterizations to performed used for the sensitivity experiments. In section Section 3 we present the parameterization-related SST discrepancies, we quantify SST discrepancies related to various aspects of the different bulk parameterizations and we compare and discuss our finding in relation to existing worksfindings with the literature. Our conclusions are summarized in section drawn in Section 4.

2 Model configuration, bulk forcing and experimental set-up

2.1 NEMOv4 model configuration

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The sensitivity of prognostic SST to bulk parameterizations is investigated in a numerical study using the Nucleus for European Modelling of the Ocean¹ (NEMO, version 4.0, revision 12957). NEMO is a three-dimensional, free-surface, hydrostatic, primitive-equation global ocean general circulation model (Madec G. and NEMO System Team, 2019) coupled to the Sea Ice modelling Integrated Initiative (SI³, NEMO Sea Ice Working Group, 2020). Our configuration uses the global ORCA025 tripolar grid (Madec and Imbard, 1996) with $1/4^{\circ}$ horizontal resolution (27.75km) at the Equator, which increases with latitudes, e.g. 14km at 60 °. The vertical grid has 75 levels, whose spacing increases with a double hyperbolic tangent function of depth from 1 m near the surface to 200 m at the bottom, with partial steps representing the bottom topography topography of the bottom (Bernard et al., 2006). The model bathymetry-bathymetry of the model is based on the combination of the ETOPO1 data set (Amante and Eakins, 2009) in the open ocean and GEBCO (IOC, 2003) in coastal regions. The horizontal turbulent viscosity is parameterized by means of a biharmonic function with a value of $1.8 \times 10^{11} m^4 s^{-1}$ at the Equator, reducing poleward as the cube of the maximum grid cell size. The advection of the tracers uses a total variance dissipation (TVD) scheme (Zalesak, 1979). The Laplacian lateral tracer mixing is along isoneutral surfaces with a coefficient of $300m^2s^{-1}$. The vertical mixing of tracers and momentum is parameterised using the turbulent kinetic energy (TKE) scheme (Blanke and Delecluse, 1993). Subgrid-scale vertical mixing processes are represented by a background vertical eddy diffusivity of $1.2 \times 10^{-5}m^2s^{-1}$

¹https://www.nemo-ocean.eu/

and a globally constant background viscosity of $1.2 \times 10^{-4} m^2 s^{-1}$. The bottom friction is quadratic friction at the bottom is quadratic, and a diffusive bottom boundary layer scheme is included. The continental runoff data are a monthly climatology derived from the global river flow and continental discharge data set dataset for the major rivers (Dai and Trenberth, 2002; Dai et al., 2009), and estimates by Jacobs et al. (1996) for the Antarctic coastal freshwater discharge. The initial conditions for temperature and salinity are provided by the World Ocean Atlas 2013 (Levitus et al., 2013). All the experiments are forced with the hourly ERA5 Reanalysis of the ECWMWF (Hersbach et al., 2020).

2.2 The bulk formulas and their parameterization in NEMO4.0

As stated in the introduction, NEMO uses the online prognostic SST approach to compute TASFs, which are estimated using the prognostic SST and prescribed atmospheric surface variables by means of aerodynamic bulk formulas:

$$\tau = \rho C_D \mathbf{u} U \mathbf{u}_{\mathbf{z}} \tag{1a}$$

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$$Q_H = \rho C_p C_H (\theta_z - T_s) U \tag{1b}$$

$$E = \rho C_E(q_0 - q_z)U \tag{1c}$$

$$105 \quad Q_L = -L_v E \tag{1d}$$

where τ is the wind stress, Q_H is the turbulent flux of sensible heat, E is the evaporation, and Q_L is the turbulent flux of latent heat. Throughout this paper, we use the convention that a positive sign of τ , of THFs (Q_H and Q_L), and of the total turbulent heat flux Q_T ($Q_T = Q_H + Q_L$) means a gain of in the relevant quantity for the ocean. The term ρ is the density of air; C_p is the heat capacity of moist air, and L_v is the latent heat of vaporization. $\mathbf{u_z}$ is the wind speed vector at height \mathbf{z} , which may be referred absolute or relative to the ocean currents. The bulk scalar wind speed U is the scalar wind speed $|\mathbf{u_z}|$ with the potential inclusion of a gustiness contribution. The convective gustiness. Convective gustiness is a temporary increase of in the wind speed due to the friction and the free convection and it, and is active and significant in very calm wind conditions with an unstable near-surface atmosphere. It is added to the wind speed and it avoids zero wind singularity. θ_z and q_z are the potential temperature and specific humidity of air at height \mathbf{z} , while T_s , T_s can be the temperature and specific humidity at the surface. Depending on the bulk parameterization used, T_s can be the temperature at the air-sea interface (sea surface skin temperature, SSTskin) or at typically 1 meter deep typically at a depth of one meter (bulk sea surface temperature, SST). The SSTskin differs from the SST due to the contributions of two effects of opposite signtwo effects with opposite signs: the cool skin and warm layer (CSWL). The cool skin is the cooling of the millimeter-scale uppermost layer of the oceanto-ensure

which ensures a steep vertical gradient of temperature which that sustains the heat flux continuity between the ocean and atmosphere. The warm layer is the warming of the upper few meters of the ocean under day in daytime and sunny conditions. C_D , C_H , and C_E are the Bulk Transfer Coefficients (BTCs) for wind stress, sensible heat, and moisture, respectively. Therefore, the main differences among The main differences between bulk parameterizations are therefore usually related to:

- 1. The use of the skin temperature (hereinafter SSTskin) rather than the bulk SST in the estimation of near surface atmospheric stability and bulk formulas.
- 2. The form dependence of the exchange coefficients on the wind speed
- 3. The inclusion of convective gustiness in the wind calculation

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4. The effect of including ocean current in currents in wind stress

In this study, we attempt to disentangle the effects of the first two aspects on SST (section Sections 3.2, 3.3 and 3.4), and we discuss the effect of the inclusion of convective gustiness in the wind stress computation (section Section 3.4). The effect effects of the ocean current interaction/feedback in the bulk formulation has been widely explored in the literature (e.g. Renault et al., 2019a, b; Sun et al., 2019). Although many previous studies studies have highlighted the substantial difference in the surface input to the ocean between calculations that use absolute vs. relative wind, we have preferred decided to leave this aspect to further future work since the implementation of this correction does substantially depend essentially depends on the characteristics of the forcing fields (Renault et al., 2020).

The online prognostic SST approach of NEMO uses the modelled SST at each time step to estimate NSHFs (i.e. THFs + long wave radiation). In our experiments, we only focus on the NSHFs computed by bulk formulas, namely the THFs. The SST is responding responds to the total turbulent heat flux Q_T at each time step: the Q_T generate SST anomalies, and SST anomalies, in turn, ean-modulate Q_T . Specifically, SST and Q_T feedback negatively: when the SST gets-becomes anomalously cold, then Q_T increases, and that means that Q_T increases in response, the SSTwill tend to increase and the Q_T to decrease which increases SST, then QT will decrease, and so on. This negative feedback of the online prognostic SST works to reduce the heat fluxes difference reduces the differences in heat fluxes across the different bulk parameterizations. On the other hand, the wind stress is not affected by the this type of first-order feedback at play for the Q_T .

In this study we focus on three of bulk parameterizations implemented in NEMOv4: NCAR (Large and Yeager, 2009), COARE 3.6 (Edson et al. (2013) + Chris Fairall, private communication, hereinafter referred to as "COARE"), and ECMWF as coded in the Aereobulk package (Brodeau et al., 2017). All the codes to estimate TASFs in the NEMOv4.0 framework, originates originate from this AeroBulk package, which is completely open source and available at (Brodeau et al., 2017). COARE and ECMWF parameterizations are meant designed to be used with the SSTskin, so that the two algorithms include a CSWL parameterization to estimate $\frac{\text{SSTskinit}}{\text{SSTskinit}}$. NCAR uses the bulk SST in heat fluxes the heat flux calculation and the zero-wind singularity is avoided by simply setting a minimum value for the scalar wind speed to at 0.5m/s. To calculate the BTCs, the bulk parameterizations rely on an empirical closure. More specifically, in COARE and ECMWF

parameterizations, the computation of BTCs relies on uses the Monin-Obukhov similarity theory (MOST, Monin and Obukhov, 1954). As such, BTCs are a function of the roughness lengths and of the stability of the atmospheric surface layer. The NCAR parameterization uses a combination of the MOST theory with a semi-empirical form of the drag coefficient in which the BTCs are computed as a function of neutral wind speed (e.g. the wind speed at neutral stability condition in neutral stability conditions and at 10m reference level, U_{N10}). Then, the The BTCs are shifted to the current atmospheric stability. Figure 1 shows the

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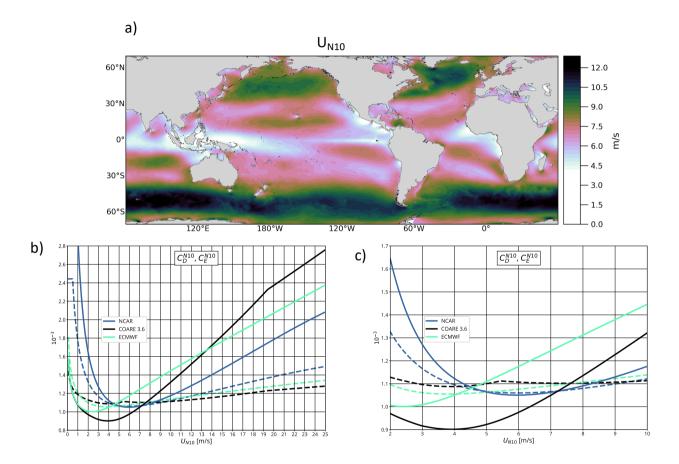


Figure 1. a) Annual mean of U_{N10} from NCAR parameterization b) Neutral drag and moisture transfer coefficients (C_D^{N10} and C_E^{N10}) for COARE (black), NCAR (blue), and ECMWF (green) bulk parameterizations (solid and dashed lines, respectively), as functions of the neutral wind speed at 10 m; c) zoom of pannel panel b) for the wind range 2 - 10m/s

 U_{N10} annual mean and the neutral BTCs as a function of U_{N10} for the selected bulk formula parameterizations. Due to the stronger neutral drag coefficient C_D^{N10} , the NCAR parameterization tends to enhance wind stress with respect to COARE and to lower extend to ECMWF under light wind condition conditions (u < 5m/s). On the other hand, the ECMWF parameterization enhances wind stress with respect to NCAR and COARE for wind speed speeds above 5m/s, while COARE enhances it for wind speed speeds above 13m/s. For the discussion of the following results, it is important to highlight the wind speed range

where the NCAR C_D^{N10} function intersects ECMWF and COARE C_D^{N10} functions (Figure 1c). In the range of 7-9 m/s, the C_D^{N10} of COARE is smaller than ECMWF, but slightly higher or approximately equal (around 7 m/s) than NCAR C_D^{N10} . In the range of 4-5 m/s, the C_D^{N10} of ECMWF is slightly smaller or approximately equal than NCAR, but higher than COARE C_D^{N10} .

165 Under weak conditions, Under weak-wind conditions, the NCAR parameterization tends to enhance evaporation with respect to COARE and ECMWF due to the stronger C_E^{N10} (see Figure 1). For a detailed explanation of BTCs-the BTC derivation for each bulk parameterization, please refer to the technical report by Bonino et al. (2020).

2.3 Experimental set-up

In order to investigate the role of different aspects of bulk parameterizations in driving prognostic SST, we performed six numerical experiments (Table 1). All the experiments are 1-year long experiments lasted one year, starting from January 2016 170 after 1-year of spinup a one-year spin-up. There is no intent to analyze this year in relation to a specific climatic mode. The simulation simulations are forced by the hourly surface atmospheric variables of the ERA5 Reanalysis (Hersbach et al., 2020). We first performed three experiments (hereinafter 'control experiments') in order to quantify the bulk parameterization-related SST discrepancies. In particular, we performed ECMWF S, COARE S and NCAR experiments, which use the ECMWF, COARE 175 and NCAR parameterizations, respectively. ECMWF_S and COARE_S experiments use the SSTskin (through their respective CSWL scheme) and consider convective gustiness in the wind speed calculation. As opposed. In contrast, the NCAR experiment computes THFs using bulk SST and the convective gustiness is not considered in the wind speed computation. In order to disentangle the contribution of the skin temperature and the contribution of the different wind stress and THFs in driving sea surface temperature differences, we performed two three sensitivity experiments (hereinafter 'mixed experi-180 ments'). First, we performed the ECMWF NS experiment, which uses the ECMWF parameterization, and THFs are computed using bulk SST rather than SSTskin. Second, we run-performed the CdNC CeEC NS experiment, which uses the ECMWF parameterization to calculate C_H and C_E BTCs and the NCAR bulk formula to calculate C_D BTC. THFs are computed using bulk SST. Moreover, we We also performed an additional experiment, called ECMWF_NS_NG, which differs from ECMWF_NS only for in terms of the exclusion of the convective gustiness in the wind speed calculation. The comparison between and is used to determine the Skin Temperature contribution in driving THFs differences and in turn SST differences. The comparison between and, which differ only for the C_D BTC computation, and between and, which differ only for the C_H and C_E BTCs computation, teach us about the wind stress and the THFs differences contribution in driving SST differences, respectively. Moreover, we compare and experiments to show the effect of the inclusion of convective gustiness in the wind speed calculation on wind stress computation (shown in the supplementary material). We analyze annual mean differences between experiments. We use the We used the absolute wind, e.g. which means that the parameterizations do not include the ocean eurrents current feedback to calculate the wind in equation 1a.

Experiment name	sea surface temperature used (T_s)	computation of C_D	computation of C_E and C_H	convective gustiness
COARE_S	SSTskin	COARE3.6	COARE3.6	Yes
ECMWF_S	SSTskin	ECMWF	ECMWF	Yes
NCAR	SST	NCAR	NCAR	No
ECMWF_NS	SST	ECMWF	ECMWF	Yes
CdNC_CeEC_NS	SST	NCAR	ECMWF	No
ECMWF_NS_NG	SST	ECMWF	ECMWF	No

Table 1. Summary of the numerical experiments.

3 Results

We here Here we discuss the parameterization-related discrepancies in the control experiments in terms of TASFs,—(i.e. Q_T and τ). WSC, SST and meridional heat transport (section 3.1), and we describe the sensitivity of the prognostic SST of the model to. Then, we try to analyze the contribution of various aspects of the bulk parameterizations parameterizations in driving these SST and meridional transport discrepancies. In particular, the comparison between ECMWF_S and ECMWF_NS is used to determine the Skin Temperature contribution (section 3.2—), while the comparisons between CdNC_CeEC_NS and NCAR (section 3.3). Except for sections 3.1 and 3.2, we consider only experiments which estimate the NSHFs using $T_s = SST$ in order to disentangle the THFs and wind stress differences contribution to and between CdNC_CeEC_NS and ECMWF_NS (section 3.4) teach us about the Bulk Transfer Coefficients contribution. In section 3.4, we also compare ECMWF_NS_NG and ECMWF_NS experiments to show the effect of the inclusion of convective gustiness in the prognostic SST without the effect of the CSWL implementation, wind speed calculation on wind stress computation (shown in the supplementary material). For each pair of experiments, we only show the differences in TASFs and their components (e.g. U,C_D,C_E) which are relevant to understand the SST or meridional heat transport discrepancies. The complementary TASFs differences are reported in the supplementary material. We analyze annual mean differences between experiments and assess their statistical significance using t-test.

3.1 Parameterization-related discrepancies

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We compare compared the SST simulated by the ECMWF_S, COARE_S and NCAR control experiments with the European Space Agency (ESA) Climate Change Initiative (CCI) SST dataset v2.0 (hereinafter ESA CCI SST dataset) which consists of daily-averaged global maps of SST on a 0.05° x 0.05° regular grid, covering the period from September 1981 to December 2016 (Merchant et al., 2019). All the control experiments present a warm bias in the Eastern Pacific, in the Eastern Boundary Upwelling systems (EBUS), in the Western Boundary Currents (WBCs) and in the Antarctic Circumpolar Current (ACC) region. The SST reproduced by COARE_S and ECMWF_S shows a cold bias of about -1°C in the North Atlantic open ocean at mid-latitudes, and a warm bias of about 0.5°C in the Indian Ocean and the Western Pacific (Figure 2a,b); The NCAR SST is also colder than observations, with a larger bias of about -2°Cin the North Atlantic (Figure 2c). The bias is generally higher compared with the other two experiments and covers wider areas.

Figure 3 shows the differences in total turbulent heat fluxes, wind stress and wind stress curl, from ECMWF_S and COARE_S with respect to NCAR. ECMWF_S wind stress is slightly weaker with respect to NCAR over the equatorial band and it is stronger elsewhere (Figure 3a). In COARE_S the wind stress is weaker than NCAR over a broader region with respect to ECMWF_S, namely over the areas characterized by calm wind conditions (see Figure 1). The wind stress curl (WSC) patterns are similar for the two pairs of differences (Figure 3c), they differ only for and differ only in terms of their magnitude. As regards the Q_T differences (Figure 3b), a gain of heat for ECMWF_S is a clear feature over the Pacific and Atlantic equatorial regions and over EBUS with respect to NCAR.

These TASFs likely drive probably cause substantial SST differences between experiments (Figure 4). While the SST in COARE_S is warmer than in NCAR everywhere, overall the SST in ECMWF_S is overall warmer than in NCAR, but with a colder area (down to -0.6°C) over EBUS and over the Pacific and Atlantic equatorial regions. This spatial pattern of SST differences persists when extending the simulations for up to 5 years (not shown). In these experiments, which differ only in terms of the bulk parameterization, the SST differences can arise from the differences in the wind stress and in the THFs as computed by the chosen bulk parameterization (Figure 3). In particular, the wind stress discrepancies, due to the computation of C_D and to the inclusion of the convective gustiness, the wind stress discrepancies may impact on the ocean dynamics by modifying the 3D ocean circulation and mixing and hence the pattern of the SST. The differences in THFs, due to the C_E and C_H computation and to the cool-skin/warm layer the CSWL scheme, may affect the SST through modification modifications of the heat loss to the atmosphere (dominated by evaporation in this region). Furthermore, differences in the wind stress and in THFs may also act together by amplifying or damping their single effect individual effects on the SST.

Changes on in the simulated SST can reflect on the temperature profile in the upper ocean and the distribution of heat on global scales. We have a global scale. We computed the global ocean heat transport in the upper 100 meters and compared it among our various experiments. Figure 4 (c,d) presents the meridional heat transport (MHT) as a function of latitude. The MHT is larger in ECMWF_S compared to NCAR mostly at all latitudes (Figure 4c), with the largest differences (about 0.8 PW, 20% of NCAR absolute value) in the tropical band where the ECMWF_S wind stress is stronger than NCAR one (Figure 3a). COARE_S and NCAR compare well, with differences lower than 0.3 PW (Figure 4d). Then, we will We thus focus only on

the differences between ECMWF_S and NCAR to analyze in detail in order to analyze the relationship between TASFs and SST. We show differences in MHT only when relevant. It is worth mentioning that the annual mean differences (i.e. SST, τ , WSC and Q_T) of each pair of experiments discussed in the following sections sum up linearly to give the annual mean difference between ECMWF_S and NCAR (not shown).

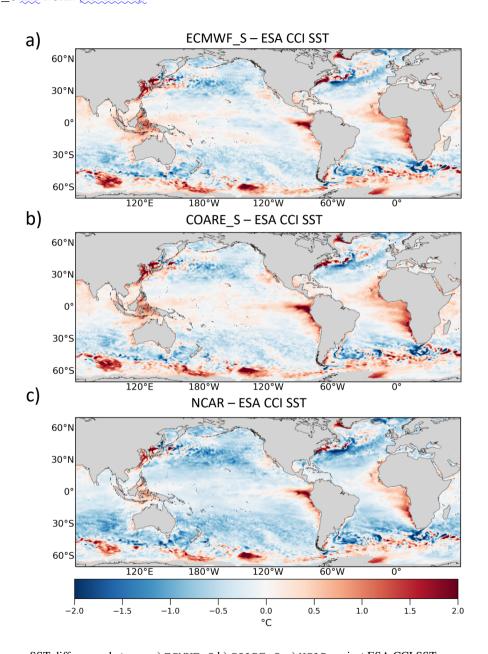


Figure 2. Annual mean SST differences between a) ECMWF_S b) COARE_S, c) NCAR against ESA CCI SST.

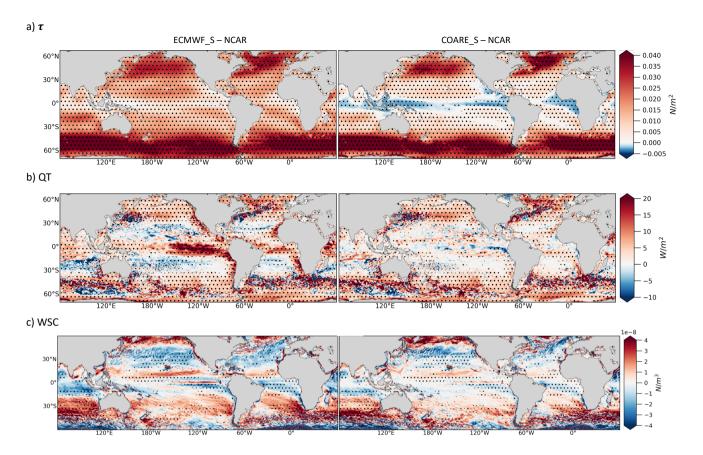


Figure 3. Annual mean differences between experiments of on a) wind stress (τ) and b) total turbulent heat fluxes (QT) and c) wind stress curl (WSC) between ECMWF_S and NCAR experiments (left) and COARE_S and NCAR experiments (right). Hatching indicates significant values (95% confidence level)

3.2 Skin temperature

The ECMWF and COARE parameterizations, in contrast to NCAR, expect SSTskin as the surface temperature input in order to estimate the near surface atmospheric stability and to compute the THFs. The SSTskin is also used to estimate the upward long wave flux, needed_which is required by the CSWL scheme as a component of the NSHFs. Here, we We now compare the results between ECMWF_S and ECMWF_NS to understand the impact of the CSWL implementation in driving causing the differences in the THFs and by consequence thus in the SST shown in Figure 4 (see Table 1 for experiments experiment details). We discuss the impact of the use of skin temperature for on the ECMWF parameterization, but however similar results are found using COARE (not shown). The ECMWF_S experiment uses the CSWL scheme, so that $T_s \equiv SSTskin$ is used to compute THFs, as opposed to ECMWF_NS in which $T_s \equiv SST$. Consideration of the CSWL effect yields a an SST global mean warming of 0.2°C (Figure 5c), with a maximum of 0.3°C over the western equatorial Pacific Ocean, in the Indo-Pacific Warm Pool. In the tropical eastern and Northern Pacific Ocean, and over ACC, the differences are below 0.1°C. The the global-mean

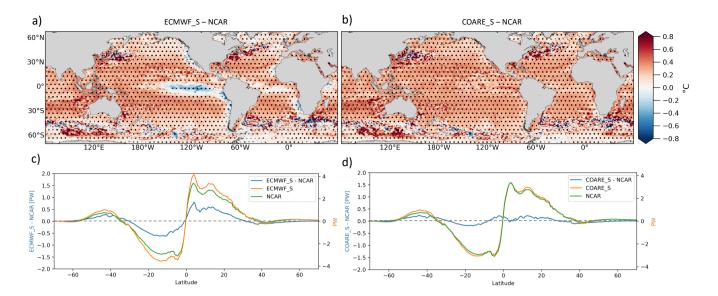


Figure 4. Annual mean SST differences between a) ECMWF_S-NCAR and b) COARE_S - NCAR; Global Meridional Heat Transport values on the right y axis) and differences (values on the left y axis) in the upper 100m ocean between c) ECMWF_S and NCAR and d) COARE_S and NCAR. Hatching indicates significant values (95% confidence level).

SSTskin tends to be about 0.1°C colder than the SST (Figure 5a). On a global average basis, the cool skin process dominates over to predominates over the warm layer effect. Specifically, evaporation occurs almost everywhere and most of the time, while the warm layer builds up only under sunny and low wind conditions.

The colder T_s in ECMWF_S with respect to ECMWF_NS yields a slightly weaker heat loss to the atmosphere due to the decreased NSHFs (mostly evaporation). In ECMWF_S the weaker heat loss to the atmosphere implies a gain of heat heat gain by the ocean (positive regions in Figure 5b) of approximately $1W/m^2$ on global average compared to ECMWF_NS. We can conclude that the negative SST discrepancies between parameterizations noted in Section 3.1 (Figure 4a) are not explained by the use of the CSWL scheme in the ECMWF parameterization. Nevertheless, the CSWL scheme has a large impact on the positive SST difference between ECMWF_S and NCAR. The SST differences between ECMWF_NS and NCAR (Figure 6a) with respect to the SST differences between ECMWF_S and NCAR (Figure 4) present a reduction of in the overall warm temperature differences, but the cold temperature difference over the tropical Pacific and Atlantic and over the EBUS are still present. τ and WSC differences are shown in Figure S1.

3.3 Turbulent Heat fluxes

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In order to investigate the effect of the different computations of the THFs between ECMWF_S and NCAR in driving SST differences (Figure 4a), we compare compared the results between CdNC_CeEC_NS and NCAR (see Table 1 for experiments details).

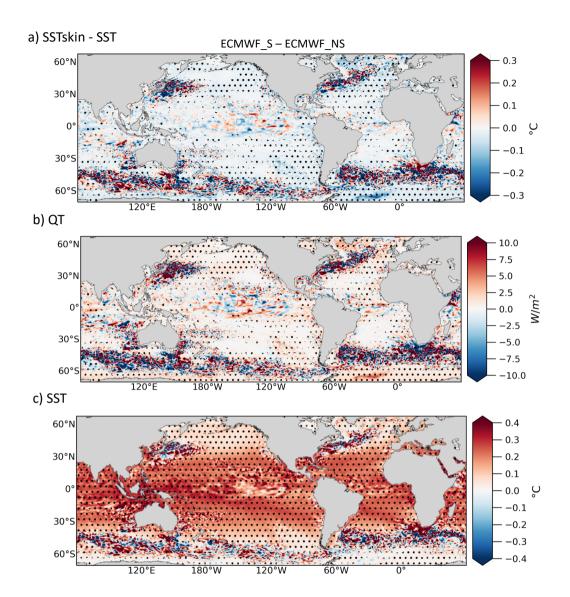


Figure 5. Annual mean differences of a) SSTskin-SST, b) total turbulent heat fluxes (Q_T) and c) SST between ECMWF_S- ECMWF_NS. Hatching indicates significant values (95% confidence level).

The SST differences difference between CdNC_CeEC_NS and NCAR does not show the cold bias over EBUS and over the equatorial Atlantic and Pacific as we found for between experiments ECMWF_S and NCAR (compare Figure 4a with Figure 6c). Over those areas, the SST in CdNC_CeEC_NS is warmer than in NCAR of about 0.3°C on average.

As shown in Figure 7a, CdNC_CeEC_NS receives an excess of Q_T of about $1W/m^2$ on average with respect to NCAR. The main contributor to this difference is the latent heat (Figure 7a and Figure 8b), resulting from the use of a different C_E in the two experiments. Indeed, the The C_E of CdNC_CeEC_NS, which is smaller than C_E of NCAR (Figure 8a), induces weak

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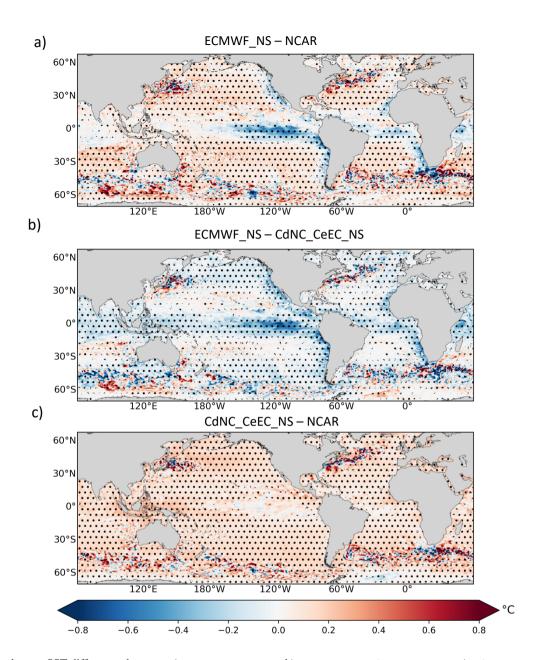


Figure 6. Annual mean SST differences between a) ECMWF_NS - NCAR, b) ECMWF_NS - CdNC_CeEC_NS, c) CdNC_CeEC_NS - NCAR. Hatching indicates significant values (95% confidence level).

evaporation. The resulting weaker heat loss to the atmosphere in CdNC_CeEC_NS with respect to NCAR implies a gain of heat by the ocean (positive regions in Figure 7a) of about $2W/m^2$ over low-latitudes and up to $6W/m^2$ over mid-latitudes (Figure 7b). A similar process is acting also also occurs in areas where the annual mean pattern of QT is patchy due to the mesoscale

activities in both in summer and winter seasons (e.g. in the Western Boundary Currents, Figure \$1\$\, \$2\$). In CdNC_CeEC_NS, the negative virtual temperature differences at the air-sea interface are smaller than NCAR, inducing weaker heat loss losses from the ocean to the atmosphere. It is worth mentioning that the one-year simulation might not be adequate to properly represent the mean state in WBCs regions due to the chaotic dynamics of these regions - this may explain some of the noise in the difference maps. However, this does not affect the robustness of the results.

The differences in Q_T and SST have the same sign, which suggests that the Q_T drive drives the SST differences. As it is clearly shown by the annual zonal-mean differences time-series zonally-averaged differences (Figure 7b): the weaker the heat loss from the ocean in CdNC_CeEC_NS along the latitude, the warmer the ocean modeled by the CdNC_CeEC_NS experiment with respect to NCAR. τ and WSC differences are shown in Figure S3.

In summary, weak evaporation and , by consequence, thus the weaker heat loss in CdNC_CeEC_NS generates an ocean surface temperature that is warmer than NCAR.

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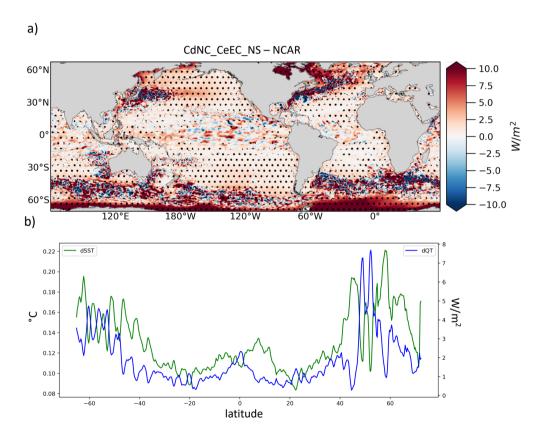


Figure 7. a) Annual mean differences of total turbulent heat fluxes QT between CdNC_CeEC_NS and NCAR experiments. b) zonally-averaged differences of in SST (green) and of Q_T (blue) annual means between the same experiments. Hatching indicates significant values (95% confidence level).

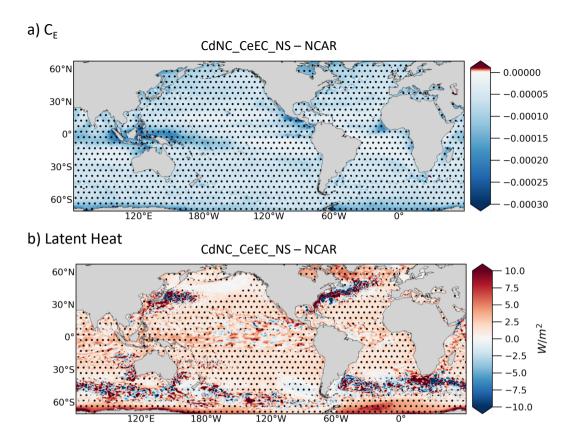


Figure 8. Annual mean differences of a) specific humidity transfer coefficient (C_E) , b) latent heat between CdNC_CeEC_NS and NCAR

3.4 Drag coefficient and Wind stress

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The We investigated the impact of the wind stress in driving the SST differences between ECMWF_S and NCAR bulk parameterizations is here investigated by comparing results from ECMWF_NS and CdNC_CeEC_NS simulations (see Table 1 for experiments details). CdNC_CeEC_NS differs from ECMWF_NS for the use of a different algorithm to compute C_D and for the inclusion of gustiness in the stress computation.

The SST simulated by ECMWF_NS is colder than CdNC_CeEC_NS over EBUS and the tropical Pacific and Atlantic oceans (Figure 6b), regions characterized by wind driven which are characterized by wind-driven upwelling. This suggests that wind stress is a major driver of the SST differences (Figure 4a). Referring to Equation 1a, the wind stress is proportional to the wind speed vector at height z ($\mathbf{u_z}$), the bulk scalar wind speed $|\mathbf{u_z}|U$ (with the potential inclusion of a gustiness contribution U), and the drag coefficient (C_D). Including Since U does not depend on SST and on C_D , including gustiness in the ECMWF calculation produces the scalar wind speed differences in Figure 9a. As expected, the differences caused by the gustiness correction, which do not exceed 0.3m/s, emerge in regions with calm and unstable conditions. They are indeed These areas

are in fact located in the 5° N - 10° N latitude band, in the eastern Pacific and Atlantic oceans, in the tropical western Pacific including the southern China Sea, and the tropical Indian Ocean. These differences do not exceed 0.3m/s. Differences of Differences in C_D and C_D^{N10} fields between experiments show similar patterns (Figure 9b-c), suggesting that the differences in C_D between parameterizations are related to the neutral coefficient (C_D^{N10}) calculation rather than to its stability correction (term to add to C_D^{N10} to get obtain C_D coefficients). IndeedIn fact, as discussed in section Section 2.2 for C_D^{N10} , the ECMWF C_D is larger than NCAR for wind speeds above 5 m/s, and smaller than NCAR for calm up to light breeze conditions (U < 5 m/s). In the areas where U is approximately 4-5 m/s, such as in the north-west Pacific and Atlantic ocean (between 20° N and 30° N) and in the south-east Pacific and Atlantic ocean (between 20° S and 30° S), the ECMWF C_D is similar or slightly smaller than NCAR.

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Since the wind stress is not affected by the type of first-order feedback at play for the NSHFs (SST- Q_T negative feedback, see section Section 2.2), differences of in U and C_D between experiments are reflected onto in the resulting different fields after bulk calculation (i.e. τ and WSC, Figure 10). In particular, over Over the ACC, the northern and southern mid-latitudes (e.g. EBUS), and the Atlantic storm track (i.e. regions characterized by wind speeds above 5m/s and ECMWF_NS C_D larger than CdNC_CeEC_NS C_D , see Figure 10), the ECMWF_NS wind stress is stronger by an average value of $0.035N/m^2$ (about 20% of NCAR absolute value) with respect to NCAR. In the 5°N - 10°N region, which is a latitudinal band characterized by mean winds below 5m/s and C_D larger in CdNC_CeEC_NS than ECMWF_NS (Figure 10), ECMWF_NS shows a wind stress reduction of $-0.003N/m^2$ (about 3% of NCAR absolute value) with respect to NCAR. In regions where the differences in C_D and wind stress are opposite (e.g. the north-west and south-west Pacific and Atlantic ocean, Indian ocean, Baja California, Equatorial warm pool), the inclusion of convective gustiness in the U calculation may play a role in strengthening the wind stress in ECMWF_NS (9a). In addition, the high time-variability of the C_D differences (not shown) could hide the relation between C_D and τ . In addition, including the convective gustiness in U calculation strengthens the wind stress in . Both hypotheses are verified, the ECMWF_NS experiment presents a stronger wind stress almost everywhere over the global ocean compared to a twin experiment (i.e. ECMWF NS NG) where the convective gustiness is not used in the computation (Figure \$2S4) and the correlation between C_D differences and wind stress differences is always significant and positive (not shown). The higher the difference in C_D , the stronger the differences in wind stress.

The SST differences between ECMWF_NS and CdNC_CeEC_NS over the tropical Pacific and Atlantic Oceans (Figure 6b) are likely probably related to Ekman suction, which is driven by the positive (negative) wind stress curl in the northern (southern) hemisphere. Substantial differences are were found in ECMWF_NS compared to CdNC_CeEC_NS, characterized by greater mean wind stress both north and south of the tropical band and weaker wind stress along the equator (Figure 10a). These latitudinal differences of the in wind stress between experiments reflect are reflected in the differences in the wind stress curl patterns (Figure 10b). Indeed, a stronger acceleration (deceleration) of southeast trades north (south) of the equator in ECMWF_NS may lead to a stronger positive (negative) curl north (south) of the Equator (Chelton et al., 2001). We found this relation. This relation was found to be significant north of the equator: the stronger positive wind stress curl in ECMWF_NS than CdNC_CeEC_NS results resulted in a colder SST in ECMWF_NS compared to CdNC_CeEC_NS (see correlation map in Figure \$3355).

The stronger wind stress along EBUS in ECMWF_NS compared to CdNC_CeEC_NS, instead, likely-probably enhances coastal upwelling, explaining most of the SST differences over these regions. Part of the SST difference could be also also be related to Ekman suction. ECMWF_NS shows stronger positive (negative) wind stress curl in the northern (southern) hemisphere EBUS compared to CdNC_CeEC_NS (Figure 10b). The vertical velocity, and in turn, the coastal SST along EBUS are, indeed, extremely sensitive to wind forcing changes (Bonino et al., 2019; Small et al., 2015; Capet et al., 2004; Desbiolles et al., 2014). These relations are were confirmed along the coast of the Benguela Upwelling System (Figures \$4 and \$5\$6 and \$6\$). During the Benguela upwelling season (ONDJ), the enhanced wind stress and negative wind stress curl in ECMWF_NS reinforce the vertical velocity with respect to CdNC_CeEC_NS (Figure \$4\$6), resulting in a colder surface temperature (see correlation maps Figure \$5\$7).

It is important to highlight that the The differences in the wind stress are also responsible for the changes in the meridional heat transport. MHT differences between ECMWF_NS and CdNC_CeEC_NS resemble the differences between ECMWF_S and NCAR (compare Figure 4c and Figure 11c), with a higher transport in ECMWF_NS at all latitudes. The largest differences are located in the tropical region (up to 0.6 PW, about 18% of NCAR mean value), where the differences in meridional transport (linked to the equatorial upwelling) between the two experiments are likely maxima.

Even though Although the two experiments use the same C_E and C_H , the dependence of Q_L and Q_H to on the prognostic SST at each time-step generates differences in Q_T (Figure 11a). The ocean gains heat in ECMWF_NS compared to CdNC_CeEC_NS (i.e. positive Q_T differences) over the EBUS and the Equatorial region. In contrast to the previous finding, the differences in Q_T and SST have an opposite sign, indicating that SST differences drives drive the Q_T differences: the colder the temperature produced by ECMWF_NS wind stress with respect to CdNC_CeEC_NS, the higher the heat gained by ECMWF_NS along the latitudes (Figure 11b). In summary, ECMWF_NS reproduces stronger wind stress and wind stress curl along EBUS, and stronger cyclonic wind stress curl along the Equator, that generates which generate colder SST with respect to CdNC_CeEC_NS, through enhanced upwelling processes.

In light of Given the importance of the wind stress in driving the SST differences between ECMWF and NCAR parameterizations, we discuss now examine why COARE_S does not display show the cold SST differences in comparison to NCAR over EBUS and the equatorial Pacific (Figure 4b). With wind speed speeds ranging from 7 to 9 m/s (e.g. over EBUS), the C_D in the COARE_S parameterization is smaller than that of the ECMWF parameterization, but slightly higher or almost identical (around 7 m/s) than the C_D of NCAR (refer to Figure 1c). Moreover, over the northern equatorial band, the C_D of COARE_S is smaller than that of ECMWF_S and NCAR. As a consequence, the COARE_S differences in wind stress (Figure 3ba) in comparison with NCAR are characterized by a strong decrease, roughly 10%, over the northern equatorial band and a slightly increase of slight increase in the wind stress, roughly 2%, over EBUS. The increase of in wind stress over EBUS in COARE_S (2% in comparison to 25% in ECMWF_S) is not enough insufficient to promote stronger coastal upwelling in the annual mean, and in turn colder SST with respect to NCAR. As regard regards the equatorial upwelling, the weak increasing of increase in the wind stress in the north northern equatorial region (e.g. northern equatorial cold front, Figure 3b) compared to NCAR wind stress (Figure 3a), prevents the enhancement of the positive wind stress curl in COARE_S (Figure 3c). Nevertheless However,

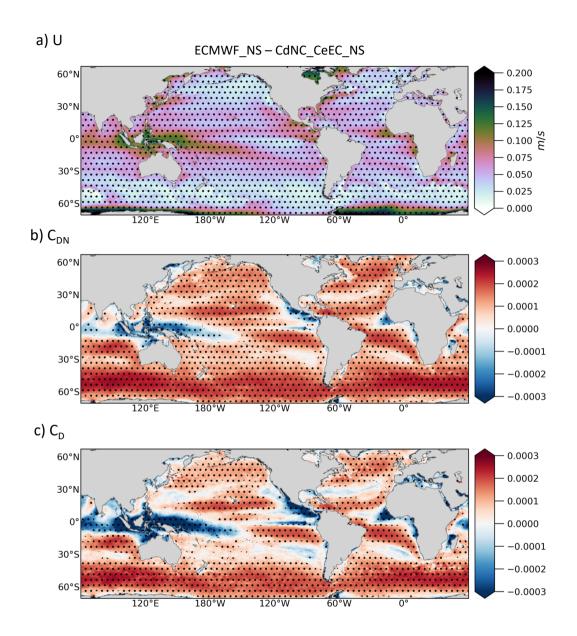


Figure 9. Annual mean differences of in a) wind speed (U), b) neutral wind stress transfer coefficient (C_{DN}) and c) wind stress transfer coefficient (C_{DN}) between ECMWF_NS and CdNC_CeEC_NS. Hatching indicates significant values (95% confidence level).

to properly identify the drivers of the pattern in the SST differences between COARE_S and NCAR extra dedicated numerical experiments should, further numerical experiments need to be performed.

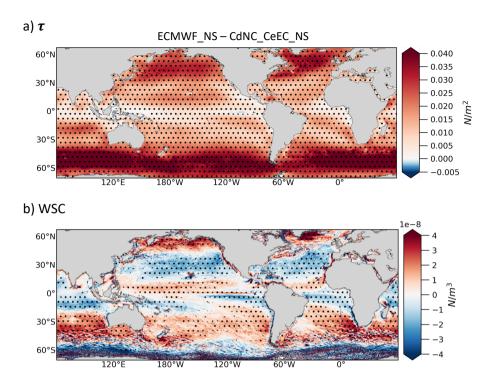


Figure 10. Annual mean differences of in a) wind stress (τ) and b) wind stress curl (WSC) between ECMWF_NS and CdNC_CeEC_NS.

3.5 Online prognostic SST approach vs offline prescribed SST approach

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In order to discuss the role of the SST- Q_T negative feedback at play in the online prognostic SST approach, we compare compared our results with Brodeau et al. (2017), who compared the different bulk parameterizations using the offline prescribed SST approach (i.e. TASFs are computed by means of bulk formulas using prescribed surface atmospheric variables and prescribed SST). It is worth mentioning that there are There are a few discrepancies in the bulk implementation between this study and Brodeau et al. (2017). They The latter authors used the COARE3.0 parameterization instead of COARE3.6 and, their simulations, which were performed for a longer (1982-2014) period, are were forced by the ERA-Interim reanalysis instead of ERA5. Therefore, our scope Our aim in this comparison is therefore only to qualitatively understand the negative feedback between the SST and the Q_T at play in our experiments.

Brodeau et al. (2017) report a mean global increase of in the wind stress of $20mN/m^2$ using ECMWF parameterization instead of NCAR parameterization. The computation of the wind stress is not affected by the SST- Q_T negative feedback (see equation 1a), so that our results of. This means that our result of the $20mN/m^2$ global mean increase of in wind stress is completely in line with the prescribed SST comparison by Brodeau et al. (2017). Our findings do not follow Brodeau et al. (2017) in terms of the Q_T differences between ECMWF_S and NCAR parameterizations. They find The latter authors found a global mean increase of in Q_T of $13W/m^2$ for ECMWF_S, while in our experiments ECMWF_S displays showed a mean global

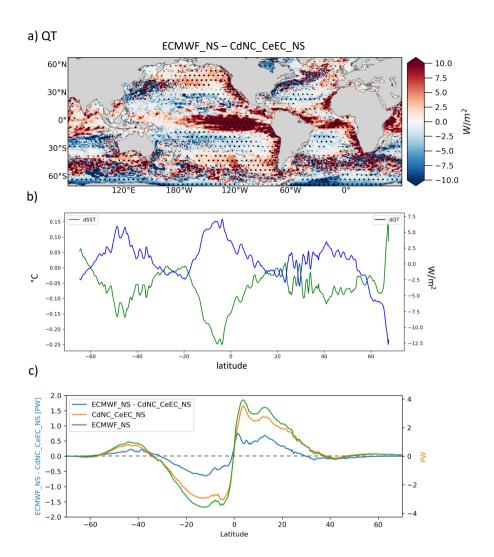


Figure 11. a) Annual mean differences of \underline{in} turbulent heat fluxes (Q_T) between ECMWF_NS - CdNC_CeEC_NS; b) Annual zonal-mean differences time-series of SST (green) and Q_T (blue) between ECMWF_NS - CdNC_CeEC_NS; c) Global Meridional Heat Transport in the upper 100m ocean (values on the right y axis) for ECMWF_NS and CdNC_CeEC_NS and differences (values on the left y axis) between them. Hatching indicates significant values (95% confidence level).

increase of $5W/m^2$ with respect to NCAR. Moreover, they report an increase of $7W/m^2$ considering SSTskin rather than SST in the COARE parameterization, while in our experiments ECMWF_S displays showed a mean global increase of $1W/m^2$ with respect to ECMWF_NS. The negative feedback between the SST and the Q_T which is active in our experiments reduced the differences in the total turbulent flux across parameterizations compared to the prescribed SST comparison.

4 Summary and conclusions

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In this work we have investigated how the implementation of different bulk parameterizations in the NEMOv4 ocean general circulation model drives substantial changes in prognostic sea surface temperature. Specifically, we studied the contribution of different aspects and assumptions of the bulk parameterizations in driving the SST differences across numerical experiments performed using the NEMO global model configuration with $1/4^{\circ}$ of horizontal resolution. In particular, we We analyzed and quantified the role of the inclusion of the skin temperature in the computation of the turbulent heat flux components, and we also studied the role of the turbulent heat flux components and of the wind stress in driving the SST changes between parameterizations. In order to do that, we analysed We analysed annual mean TASF differences between 'control experiments', short-term numerical experiments which used the bulk parameterizations implemented in NEMOv4, and 'mixed experiments', short-term sensitivity experiments where bulk assumptions are excluded (e.g. skin temperature) or bulk transfer coefficients are computed mixing the bulk parameterizations (e.g. C_D from NCAR parameterization and C_E and C_H from ECMWF parameterization). Moreover, the relevance of this work, other than In addition to highlighting the sensitivity of the sea surface temperature to the bulk parameterizations, is also to discuss the we believe that the importance of this work is also the examination of the role of the SST- Q_T negative feedback at play in the simulations. As such, we We compared the modeled turbulent air-sea fluxes with the estimations from by Brodeau et al. (2017), who analyzed the same bulk parameterizations, but using the offline prescribed SST approach. The Our findings can be summarized as follow:

- 1. The implementation of skin temperature in the bulk parameterizations reduces evaporation and decrease decreases the turbulent heat flux to the atmosphere, thus promoting ocean warming. The skin temperature is usually colder than the sea surface temperature. The skin temperature contribution in terms of turbulent heat flux is weaker with respect to than the Brodeau et al. (2017) estimations due to the negative feedback between the SST and the Q_T . In our experiments the SST is free to evolve and feeds back negatively with respect to Q_T .
 - 2. The turbulent heat flux differences between experiments are dominated by the latent heat flux contribution, which arise which arises from C_E differences between bulk parameterizations. Less evaporative ocean gains heat, which tends to promote ocean warming. The turbulent heat flux differences are weaker with respect to than the estimations of Brodeau et al. (2017) and they can be attributed to the SST- Q_T negative feedback.
 - 3. The wind stress differences between bulk parameterizations are attributable to the C_D differences, which result crucial especially in wind-driven dominantly ocean regions. In particular, experiment Experiments with enhanced wind stress or wind stress curl over EBUS and over Equatorial Pacific promote upwelling processes and consequent cooling of the sea surface temperature. Stronger wind stress results in an increase of causes an increase in the poleward heat transport in the upper ocean, which leads to a more pronounced increase in the $\neg\pm20^{\circ}N$ latitude band. The wind stress differences across the bulk parameterizations implemented in NEMOv4 is are of the same magnitude of as the wind stress differences calculated by Brodeau et al. (2017). This is due to the fact that, at first order, the wind stress computation is not affected by the SST.

It is worth underlining that we are using. We used forced ocean experiments in which the atmospheric fields (e.g. wind, air temperature, air humidity) given to the ocean model and seen in the online prognostic SST approach come from an atmospheric reanalysis, and do not respond back to the ocean variability. Introducing the air-sea feedback in the system might substantially impacts impact on the turbulent fluxes and modify our finding in findings in terms of comparing the SST response among the bulk parameterizations. In the perspective of improving the order to improve the representation of air-sea interaction in the NEMO framework, an atmospheric boundary layer (ABL) is has been integrated in the new NEMO release 4.2 (Lemarié et al., 2021). Nevertheless However, the ABL implementation is in a preliminary stage and the current online prognostic SST approach is still the favorite. Please note that most commonly used. Although the new release of NEMO, v4.2, includes some modifications to the bulk formulas of the formula version used in this study. These, these changes do not affect the presented results presented in this paper.

Appendix A: Table A1
List of Acronyms and Symbols

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Acronym	Expansion
TASFs	Turbulent Air-Sea Flux components
THFs	Turbulent Heat Flux components
NSHFs	Non Solar Heat Flux components
Q_T	Total turbulent heat flux
BTC	Bulk Transfer Coefficient
SSTSkin	Sea Surface Skin Temperature
CSWL	Cool Skin and (diurnal) Warm Layer
EBUS	Eastern Boundary Upwelling Systems
MHT	Meridional Heat Transport
WSC	Wind Stress Curl

Code availability. This version of the NEMO code is based on code release 4.0, revision number 12957 (https://forge.ipsl.jussieu.fr/nemo/ browser/NEMO/trunk?rev=12957, last access: 24 February 2022). All the codes to estimate TASFs in the NEMOv4.0 framework, originates from this AeroBulk package, which is completely open source and available at https://github.com/brodeau/aerobulk (Brodeau et al., 2017). The original code was modified in the computations of the bulk transfer coefficients applied to perform the experiments. The code and the namelists to run each experiment are available in the Zenodo archive (https://doi.org/10.5281/zenodo.6258085, DOI: 10.5281/zenodo.6258085). The model outputs used to produce the figures are also available in the Zenodo archive.

450	Author contributions. GB modified the numerical code, set up the experiment and wrote the manuscript. DI conceived and designed this study. All authors contributed to the interpretation of results and editing.
	Competing interests. The authors declare that they have no conflict of interest.
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