An inverse method to derive surface fluxes from the closure of oceanic heat and water budgets: application to the north-western Mediterranean Sea

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Key Points:

- Hourly surface fluxes are produced with an inverse method over the north-western Mediterranean, during one year at a fine spatial scale
- With the fluxes deduced from the inverse method, the annual heat and water budgets are closed within some W m^{-2} and some mm yr^{-1}
- Compared with the adjusted fluxes, numerical prediction models are evaluated : they fail to retrieve the mean annual patterns and values

Abstract

The large amount of data collected during DeWEX, MOOSE and HyMeX campaigns in the north-western Mediterranean in 2012-2013 allowed to implement an inverse method to solve the difficult problem of heat and water budget closure. The inverse method is based on the simulation of the observed heat and water budgets, strongly constrained by observations collected during the campaigns and on the deduction of adjusted surface fluxes. The inverse method uses a genetic algorithm that generates 50.000 simulations of a single-column model and optimizes some adjustable coefficients introduced in the surface fluxes. Finally, the single-column model forced by the adjusted fluxes during one year and over a test area of about 300 x 300 km² simulates the daily mean satellite SST with an accuracy of 0.011°C, as well as daily mean SSS and residual buoyancy series deduced from wintertime analyses with an accuracy of 0.011 and 0.03 $m^2 s^{-2}$ respectively. The adjusted fluxes close the annual heat and rescaled water budgets by less than 5 W m^{-2}. To our knowledge, this is the first time that such a flux dataset is produced. It can thus be considered as a reference for the north-western Mediterranean and be used for estimating other flux datasets, for forcing regional models and for process studies. Compared with the adjusted fluxes, some operational numerical weather prediction models (ARPEGE, NCEP, ERA-INTERIM, ECMWF and AROME), often used to force oceanic models, were evaluated: they are unable to retrieve the mean annual patterns and values.

Keywords

Heat and water surface fluxes, Budget closure, North-western Mediterranean Sea, Air-sea interactions, Inverse method

Short title

An inverse method for oceanic surface fluxes

1. Introduction

The knowledge of surface fluxes exchanged between the ocean and the atmosphere has important issues: forcing oceanic models, studying the processes by which the ocean and the atmosphere exchange energy and mass, getting climatological estimates of the variability of ocean surface forcings, and evaluating their role in the Earth's climate system. In the last twenty years, lots of gridded air-sea flux fields, derived from in-situ observation analyses, from numerical model reanalyses, from satellite retrievals or from merging satellite and numerical model outputs were produced [e.g., *Large and Yeager*, 2009; *Valdivieseo et al.*, 2015; *Jordà et al.*, 2016 for the Mediterranean]. However, surface flux fields are difficult to estimate because they are highly dependent (1) of the biases which affect empirical bulk formulae, (2) of uncertainties in exchange coefficients (especially at low and high winds), (3) of imperfect boundary layer parameterizations (see the review by *Cronin et al*., 2014), and (4) of the spatial and temporal resolutions of flux-related variables [*Artale et al.*, 2002; *Ruti et al.*, 2008]. In consequence, few flux datasets are able to close budgets for the global ocean [*Valdivieso et al.*, 2015] or at basin-scale [*Castellari et al.*, 1998; *Sanchez-Gomez et al.*, 2011]. Urgent improvements are also needed for radiative [*Liu et al.*, 2015] and water budgets [*Bowman et al.*, 2009; *Romanou et al.*, 2010 for the Mediterranean].

Moreover, errors and uncertainties affecting fluxes lead forced oceanic models or coupled models to diverge [*Rosati and Miyakoda*, 1988]. Generally modelers use restoring terms in the scalar equations to prevent the model solution to drift from prescribed values or from the mean climatological state [*Barnier et al.*, 1995]. However, relaxation techniques alter and modify the model thermodynamics and may produce distortions in annual cycles [*Killworth et al.*, 2000], and over longer time scales, may alter or even suppress some internal modes of variability [*Simmons and Poyakov*, 2004]. Another expedient consists in correcting surface fluxes [*Large and Yeager*, 2009; *Pettenuzzo et al.*, 2010]. For that, many techniques have been used in different regions of the world ocean in order to close heat and water budgets or at least to be consistent with some constraints [see the review by *Large and Yeager*, 2009]. Some include inverse methods by imposing oceanic constraints, like observed transports [*Isemer et al.*, 1989; *MacDonald and Wunsch*, 1996], and mixed layer heat contents [*Gaspar et al.*, 1990b] or atmospheric constraints, i.e., mass, moisture and energy budgets [*Trenberth*, 1997], temperature

Q1 and humidity Q2 budgets [*Curry et al.*, 1999]. Other studies propose linear inverse analyses by using heat flux constraints [*Grist and Josey*, 2003], or assimilation of observations in numerical models with the adjoint equation formalism of a one-dimensional [*Roquet et al.*, 1993] or three-dimensional modeling approach [*Stammer et al.*, 2004; *Yuan and Rienecker*, 2003]. Variational objective analyses are another alternative to obtain best estimates of meteorological variables needed to estimates surface fluxes [e.g., *Yu et al.*, 2004; *Yu and Weller*, 2007].

Caniaux et al. [2005b] tested an inverse method based on the optimization of numerous model runs by a genetic algorithm to produce adjusted fluxes at a rather fine scale, in order to study subduction in the north-eastern Atlantic. They showed that, if the region of study was well sampled during a relatively long period of time (the POMME experiment in 2000-2001, *Mémery et al.*, 2005), the inverse method was particularly suitable to produce surface fluxes and to simulate realistically the oceanic upper layers without any correction or restoring term [*Paci et al.*, 2005; *Giordani et al.*, 2005] and to deduce reliable seasonal and annual subduction rates [*Paci et al.*, 2007]. Here, we address the same question in a different context and region, i.e., in the north-western Mediterranean (NWM).

The NWM is much more energetic than the intergyre region of the north-eastern Atlantic. The basin is characterized by the presence of the Northern Mediterranean Current (or Liguro-Provençal Current), which flows southwestward along the continental margin [*Millot*, 1987], and further south by the northeastward return flow marked by the eddying Balearic front around 40°N [*Send et al.*, 1999; *Poulain et al.*, 2012]. The NWM is also known to form dense waters, the Western Mediterranean Deep Waters (WMDW), during deep convective events [*Rhein*, 1995; *Marshall and Schott*, 1999]. Another difference is that surface fluxes are dominated by frequent continental gale force winds [*Bourassa et al.*, 2013], associated with cold and dry air masses that contrast significantly with the SSTs to generate important heat loss [*Leaman and Schott*, 1991], i.e., in conditions where the errors and uncertainties which affect the bulk formulae are the largest. Moreover, fine temporal and spatial resolution fluxes are crucial for simulating correctly both the intensity and timing of intense mixing and deep oceanic convection, given the low Rossby radius reached in winter and the stochastic nature of the mechanisms at play [*Castellari et al.*, 2000; *Herrmann and Somot*, 2008; *Béranger et al.*, 2010]. There is also a clear need of accurate surface fluxes at fine temporal and spatial scales to produce realistic estimates of dense water formation rates in the NWM [*Durrieu de Madron et al.*, 2013; *Waldman et al.*, 2016].

As the NWM was extensively sampled from summer 2012 to summer 2013, with still more numerous in-situ data than during the POMME campaigns, mostly due to gliders (nonexistent in 2000-2001) and to an increased number of ARGO floats, an attempt to test *Caniaux et al.* [2005b]'s inverse method is exposed in the present paper. During one annual cycle, the NWM was investigated in the frame of three scientific programs: the Mediterranean Ocean Observing System for the Environment (MOOSE) [*Testor et al.*, 2012, 2013a], the Mediterranean Pelagic Ecosystems Experiment (DeWEX) [*Testor*, 2013b; *Conan*, 2013] and the Hydrological Cycle of the Mediterranean Experiment (HyMeX) [*Drobinski et al.*, 2014].

The paper is organized as follows: section 2 provides a description of the inverse method and single-column model (SCM) approach. Results including the optimized corrections and simulations are presented in section 3. In section 4, a local evaluation of the adjusted fluxes against in-situ data, an evaluation of some numerical weather prediction models (NWPM) fields and an estimate of the heat and water budget closure are provided. Conclusions are drawn in section 5. Note that the SCM presented in section (2) can be used not only to optimize surface forcings but also to study the physics of the near surface layers; for instance to investigate the different processes at play in the evolution of SSTs, SSSs, of temperature and salinity profiles, stratification and so on. A brief outline of this use of the SCM can be found in subsection 3.2 or in *Caniaux et al.* [2015].

2. Methodology

2.1. The Inverse Method

The purpose of the inverse method is to perform many sensitivity tests with a numerical tool forced at the surface with different sets of heat, water and momentum fluxes and to select the best fluxes that allow to simulate realistically the evolution of a water column. For obvious computer time reasons, it is impossible to use a three-dimensional (3D) model but rather a simplified model, i.e., a SCM specially adapted to simulate a given area of the NWM (hereafter the test area). From an initial estimate of the surface fluxes (hereafter the guess fluxes), and by varying some adjustment coefficients for correcting the fluxes, an optimal set of these coefficients is derived from the minimization of the distance between observed and modeled quantities (SSTs, SSSs, residual buoyancies, temperature and salinity profiles). We therefore impose a very strong constraint on the modeled evolution of the heat and water budgets, which results from the balance between lateral advective forces and surface fluxes. The choice of the best set of adjusted coefficients is done through the use of a genetic algorithm, an effective statistical tool for finding the minimum of particularly complex functions. Finally, thanks to the optimized coefficients, the guess fluxes can be corrected at any time step and any grid point of the test area, or of a somewhat larger surface area.

The SCM used is derived from the one-dimensional (1D) numerical model of vertical mixing developed by *Gaspar et al.* [1990a] and updated *Wade et al.* [2011]. It solves the heat, salt and momentum equations and is closed by a 1.5 turbulent scheme solving a turbulent kinetic energy equation. It includes a parameterization of the diapycnal mixing [*Large et al.*, 1994; *Kantha and Clayson*, 1994] to better represent non local sources of vertical mixing under the mixed layer depth. For the present study, the model was modified to take into account advection terms considered as external forcings, and added at each time step in the temperature and salinity equations. The model includes 450 regularly spaced levels of five meters and solves vertical turbulent mixing with a semi-implicit numerical scheme and a time step of one hour.

2.2. Equations Solved

The problem is to solve a set of equations fitted to describe an extended area, i.e., the equations of the temperature and salinity averaged over the test area itself, as well as their subgrid scale fluctuations. We start from the 3D temperature (or salinity) equation:

$$\partial_t T = \frac{F_{sol}\partial_z I}{\rho_0 C_p} - \vec{u}.\vec{\nabla}_h T - w\partial_z T - \partial_z\left(\overline{T'w'}\right) - \nabla_h.\left(\overline{T'.\vec{u}'}\right) \quad (1)$$

where the temperature tendency results from net solar radiation input F_{sol}, horizontal and vertical advections, vertical turbulent mixing (with the non-solar heat flux specified at the surface boundary, i.e., the sum of latent, sensible and net infra-red heat fluxes) and horizontal diffusion respectively. In equation (1), the single primes refer to the unresolved turbulent scales involved; $\partial_z I$ is the fraction of F_{sol} that penetrates at depth *z;* ρ_0 and C_p are a reference surface density and the specific heat capacity of sea water respectively. The horizontal and vertical advection terms $-\vec{u}.\vec{\nabla}_h T$ and $-w\partial_z T$ were partitioned into Ekman (the horizontal Ekman current is denoted $\vec{u}_e$ and the vertical Ekman velocity w_e) and non-Ekman components ($\vec{u}_{ne}$ and w_{ne} respectively) so that (1) is rewritten as:

$$\partial_t T = \frac{F_{sol}\partial_z I}{\rho_0 C_p} - \vec{u}_e.\vec{\nabla}_h T - \vec{u}_{ne}.\vec{\nabla}_h T - w_e\partial_z T - w_{ne}\nabla_z T + \partial_z\left(K\partial_z T\right) - \nabla_h.\left(\overline{T'.\vec{u}'}\right) \quad (2)$$

in which the vertical turbulent fluxes ($-\overline{w'T'}$) in equation (1) were parameterized using the classical concept of eddy diffusivity ($K\partial_z T$). In *Caniaux et al.* [2005b], the horizontal and vertical non-Ekman advection terms were altogether derived from the evolution of mean temperature and salinity profiles deduced from four hydrological surveys performed during the one year of the POMME experiment. This hypothesis was valid as long as advection was a weak term in comparison with the other processes, not only near the surface but also at depth. This technique could not be used any more, since horizontal advection is highly depth dependent in the NWM and plays a much more important role in the top layers than at deeper levels (see subsections 2.4.3 and 3.2). This led us to hypothesize that the horizontal non-Ekman advection term could be represented by geostrophic advection, a term that could easily be deduced from the outputs of a 3D model run (see subsection 2.4.3).

As some non-linear terms in equation (2) can not be explicitly calculated at any point of the test area, they were split into spatial mean and deviation from this mean; this is the case for solar radiation, vertical Ekman advection and turbulent vertical mixing (respectively the 1st , 4th and 6th terms on the right hand side of equation (2)). After decomposing these terms into their spatial mean (angle brackets) and deviation (double prime) and after averaging each term over the test area (again with angle brackets), equation (2) becomes:

$$\begin{aligned}\langle\partial_t T\rangle = {} & \frac{\langle F_{sol}\rangle\partial_z\langle I\rangle}{\rho_0 C_p} + \frac{\langle F''_{sol}\partial_z I''\rangle}{\rho_0 C_p} - \langle\vec{u}_e.\vec{\nabla}_h T\rangle - \langle\vec{u}_{ne}.\vec{\nabla}_h T\rangle \\ & - \langle w_e\rangle\partial_z\langle T\rangle - \langle w''_e\partial_z T''\rangle - \langle w_{ne}\partial_z T\rangle \\ & + \partial_z\langle K\rangle\partial_z\langle T\rangle + \partial_z\langle K''\partial_z T''\rangle - \left\langle\nabla_h.\left(\overline{T'\vec{u}'}\right)\right\rangle\end{aligned} \quad (3)$$

Finally, mean solar radiation input, horizontal Ekman advection and horizontal non-Ekman advection were evaluated explicitly from data available at each grid point of the test area (see subsections 2.4.1, 2.4.2, 2.4.3 respectively). Similarly, the mean vertical Ekman advection could be estimated by evaluating a vertical Ekman velocity w_e from the wind-stress curl at each grid point and from the modeled area mean temperature $\langle T \rangle$ (see subsection 2.4.4). The mean vertical diffusion term $\partial_z \langle K \rangle \partial_z \langle T \rangle$ was computed directly by the 1D model and the upper boundary conditions, i.e., the surface fluxes, at each grid point (see subsection 2.4.1). The term including correlations of vertical diffusion ($\partial_z \langle K'' \partial_z T'' \rangle$) was parameterized (see subsection 2.4.5) since no data could provide an evaluation of this term across the test area. The vertical non-Ekman advection term $-\langle w_{ne} \partial_z T \rangle$ and the three subgrid-scale terms: correlations in the solar penetration $\frac{\langle F''_{sol} \partial_z I'' \rangle}{\rho_0 C_p}$, correlations of the fluctuations of the vertical velocity and temperature $\langle w_e'' \partial_z T'' \rangle$ and horizontal tracer diffusion due to small turbulent scales $\langle \nabla_h . (\overline{T' \vec{u}'}) \rangle$ are weak and were supposed to be negligible.

2.3. Setup

To implement the inverse method, a simulation test area was chosen, large enough to minimize the impact of horizontal advection, but not too much so that the hydrology, water properties and bottom topography are not too heterogeneous. The area displayed in Figure 1 indicates an homogeneous bottom topography, and includes the wintertime NWM deep convective patch [e.g., *Herrmann et al.*, 2009; *Houpert et al.*, 2016]. The simulation domain covers a surface area of about 300 x 300 km² but the surface flux correction can be applied on a wider area, i.e., the whole domain area represented in Figure 1. As indicated in Figure 1, the LION buoy, anchored at 4.703°E 42.102°N, lies inside the test area, while the AZUR buoy anchored at 7.83°E 43.38°N lies in the outer domain. The LION and AZUR buoys have been providing atmospheric and oceanic observables since 2001 and 1999 respectively; these data were used for evaluation of the adjusted fluxes in subsection 4.1.

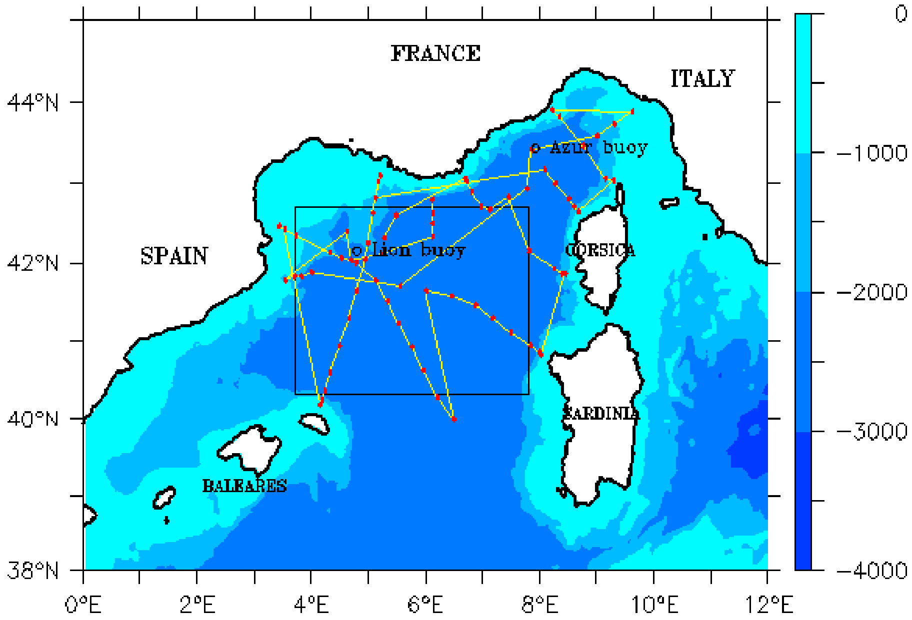

Figure 1. *Bathymetry (m) of the north-western Mediterranean. The black box corresponds to the test area. The 89 CTDs of the MOOSE 2012 hydrological survey (from 2012/07/24 to 2012/08/08) are represented by red dots, the ship trajectory by yellow lines and the position of the anchored AZUR and LION buoys by black circles.*

The method was applied during one seasonal cycle from 2012/08/01 to 2013/07/31, by using most of the data collected in the test area during six hydrological surveys: MOOSE 2012 and MOOSE 2013 (respectively from 2012/07/24 to 2012/08/08 with 89 CTD casts and from 2013/06/13 to 2013/07/09 with 77 CTD casts), DeWEX-1 (from 2012/08/22 to 2012/09/06 with 54 CTD casts) and DeWEX-2 (from 2013/04/05 to 2013/04/24 with 73 CTD casts), as well as the HyMeX-SOP1 in autumn 2012 [*Ducrocq et al.*, 2014] and HyMeX-SOP2 in winter 2013 [*Estournel et al.*, 2016a]. We also used various in-situ data (gliders, ARGO floats, surface drifters, moored buoys) and satellite platforms, either for initialization of the SCM (see below), or for calculating the cost function (subsection 2.5). As mentioned in the introduction, the more numerous the data, stronger is the constraint on the realism of the numerical simulations and finally on the adjusted fluxes.

During the same period, operational and research oceanic models were run and some of their outputs were used. For estimating large scale geostrophic advections of temperature and salinity as well as horizontal Ekman advection of salinity, we used outputs of the operational MERCATOR PSY2V4R4 model [*Drillet et al.*, 2014] (see subsections 2.4.2 and 2.4.3). Moreover, for evaluating the heat budget closure presented in subsection 4.3, the MEDRYS reanalysis [*Hamon et al.*, 2016] and some outputs of the mesoscale research SYMPHONY [*Marsaleix et al.*, 2009, 2012] and MARS3D [*Garreau et al.*, 2011] models were also used. The MEDRYS reanalysis, based on the MERCATOR assimilation system, assimilated numerous in-situ data collected between 2007 and 2013 in the NWM. Unlike MERCATOR and MEDRYS, the SYMPHONY and MARS3D models do not assimilate altimetry nor in-situ data. They were initialized either form MERCATOR fields (MARS3D) or from a mixed of in-situ data and MERCATOR outputs (SYMPHONY) [*Estournel et al.*, 2016b] and forced with fluxes derived from NWPM fields.

The SCM was initialized with 35 CTDs (over 89) collected in the test area during the MOOSE 2012 campaign (Figure 1). The mean temperature and salinity profiles were linearly interpolated on a 5 m regular vertical grid before spatial averaging (Figure 2). The profiles were used as initial state at the central time of the survey (i.e., 2012/08/01). The mean potential temperature profile (Figure 2a) is homogeneous from 2800 m to 100 m due to the presence of WMDW, and covered by well stratified surface waters above 100 m. The mean salinity values (Figure 2b) range between 38.3 and 38.6 from the bottom to about 200 m and exhibit a maximum value of 38.6 near 400 m. Above, salinity drops sharply near the surface to 37.8. Both mean temperature and salinity profiles display substantial spatial variability near the surface, which rapidly decreases with depth (Figure 2).

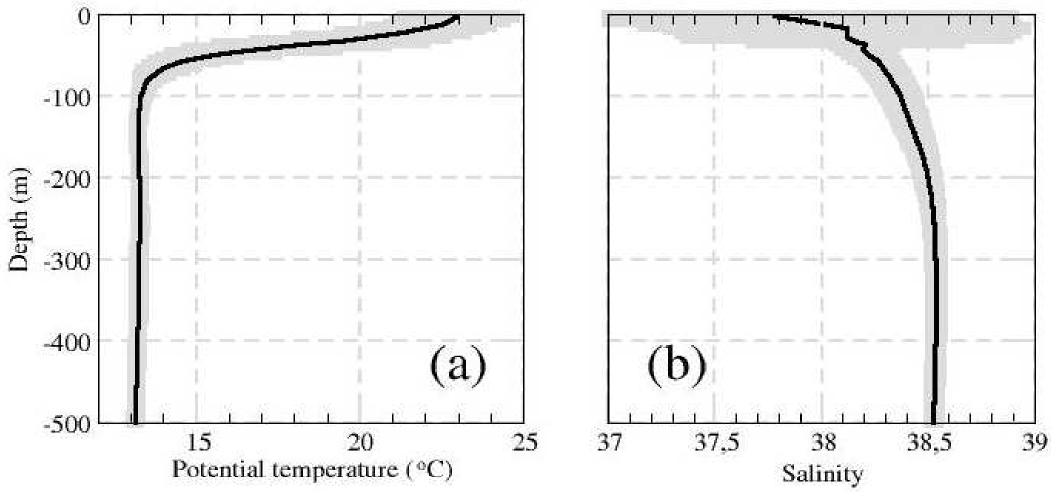

Figure 2. *(a) Area mean temperature (in °C) and (b) salinity profiles from the CTDs collected within the test area (see Figure 1) during the MOOSE 2012 hydrological network with standard deviations in grey.*

2.4. Forcings

2.4.1. Surface Flux Guess

To force the SCM, the flux guess was computed after collecting several surface meteorological and oceanic variables. One of the objectives being to take into account oceanic mesoscales in the surface fluxes, we chose SST fields produced operationally since 2010 by the Centre de Météorologie Spatiale (Météo-France, Lannion), at a daily frequency and analyzed and positioned on a ultra-high resolution 0.02° longitude x 0.02° latitude grid. This production is issued from the MEDSPIRATION project (http://cersat.ifremer.fr/thematic-portals/projects/medspiration) funded by the European Space Agency (ESA). The atmospheric variables (air temperature, humidity, sea level pressure and surface winds) come from the operational Météo-France AROME model [*Bouttier*, 2007]. Its outputs were available every hour on a 0.025° longitude x 0.025° latitude grid and were interpolated on the finer SST grid. Rather than using precipitation from the AROME-France model, we preferred to download TRMM precipitation fields [*Huffman et al.*, 2007], because precipitating clouds or cells are better positioned than in models [*Béranger et al.*, 2006; *Pfeifroth et al.*, 2013], even if the calibration of satellite precipitation over oceans and seas can still be improved [*Serreze et al.*, 2005;]. As

TRMM data were available every three hours on a 0.125° longitude x 0.125° latitude grid, the fields were linearly interpolated every hour at the resolution of the SST grid. The daily SST fields were also interpolated every hour. Finally, the COARE3.0 bulk algorithm [*Fairall et al.*, 2003] was used to produce hourly turbulent fluxes (latent and sensible heat fluxes and wind-stress) on the 0.02° longitude x 0.02° latitude SST grid.

The radiative fluxes (incoming longwave and shortwave radiations) were downloaded from the Centre de Météorologie Spatiale (Météo-France, Lannion), where they are produced operationally at a time frequency of one hour on a regular grid of 0.05° longitude x 0.05° latitude [*Brisson et al.*, 1999, 2001]. These data are compared operationally with moored buoys [*Le Borgne et al.*, 2007] and sometimes with ship data during dedicated experiments at sea [e.g., *Eymard et al.*, 1999; *Caniaux et al.*, 2005a]. They provide interesting comparisons with biases less than 2 W m^{-2} and root mean squares ranging from 10 to 20 W m^{-2} (except in some specific cases of Saharan dust aerosols). Their good performance against in-situ data imply that they don’t need to be corrected by the optimization procedure of the inverse method. Like the other flux-relative variables, the radiative fluxes were interpolated on the SST grid. The net longwave radiation F_{LW} was computed from the incoming longwave radiation F_{DLR} and SSTs with the classical expression:

$$F_{LW} = (1-\alpha)F_{DLW} - \varepsilon\sigma(SST + 273.16)^4 \quad (4)$$

with a longwave reflectance α = 0.045 [*Bignami et al.*, 1995], an emissivity ε = 0.97 and a Stefan-Boltzmann constant $\sigma = 5.67 \times 10^{-8}$ W m^{-2} K^{-4}. For the net shortwave radiation an albedo of 0.055 was adopted.

The mean annual surface net heat flux and wind-stress are shown in Figure 3a. The area mean net heat flux is negative (-14.3 W m^{-2}), meaning cooling for the sea. Actually, the area is straddling the zero flux line located on the eastern part of the domain (thick black line in Figure 3a). The area with the lowest heat fluxes corresponds to the area of maximum wind-stress associated with the dominant north-northwesterly continental winds (i.e., the northerly Mistral and north-westerly Tramontane blowing down the Rhône and Garonne river valleys). Figure 3b represents the mean annual E-P budget during the same period. The area mean value is 711 mm yr^{-1}. A belt of higher values is present to the west of the domain, where the strongest winds generate higher evaporation rate, and farther south with values up to 1000 mm yr^{-1} on the warm waters of the Balearic front. The north-eastern portion of our study region has a much lower E-P budget (~100 mm yr^{-1}) attributable to intense precipitation, which mainly affects the Gulf of Genoa during the winter period (associated with the famous Genoa low).

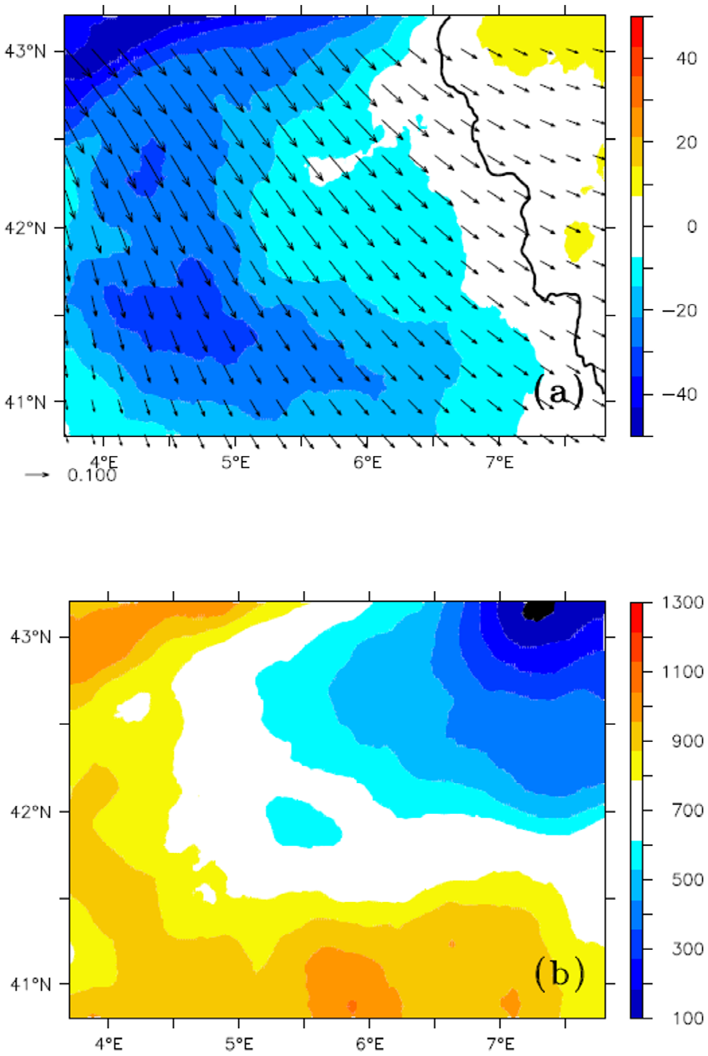

Figure 3. *Map of the year mean (from 2012/08/01 to 2013/07/31) guess for : (a) the surface net heat fluxes (shades, units W m^{-2}) with zero isoline in black and wind-stress every 10 grid point (arrows, units N m^{-2} and scale in the lower left corner); (b) evaporation minus precipitation (mm yr^{-1}).*

2.4.2. Horizontal Ekman Advection

We assumed that the horizontal Ekman advection of temperature could be calculated from satellite SSTs and wind-stress fields. This hypothesis is reasonable because the depth of the Ekman layer is relatively low during most time of the year in the area and less than the mixed layer depth, so that over this depth, the temperature profiles were assumed homogeneous to be taken as SST. The horizontal advection term in equation (3) was thus computed every hour and at the same spatial scale as the surface fluxes, from the following classical expression:

$$-\vec{u}_e.\vec{\nabla}_h T = -\frac{1}{\rho_0 f}\left(\vec{k}\times\vec{\tau}\right)\vec{\nabla}_h SST \quad (5)$$

where $\vec{k}$ is the unit vertical vector, $\vec{\tau}$ the wind-stress and f the Coriolis parameter. According to *Cushman-Roisin* [1987], the Ekman layer depth could be computed from the turbulent velocity as:

$$h = 0.4\frac{u_*}{f} \quad (6)$$

with $u_* = \sqrt{\frac{|\vec{\tau}|}{\rho_0}}$. A similar formulation was used for the horizontal Ekman advection of salinity, in which the SSS values were taken from the MERCATOR PSY2V4R4 model and linearly interpolated every hours on the same spatial grid as SSTs. In the SCM, horizontal Ekman advection was added as an external forcing term on the thickness of the Ekman layer *h*.

Figure 4 represents the annual mean horizontal Ekman advection of temperature, superimposed with the Ekman transport and Ekman layer depth. Over the whole area, the Ekman transport is southwestward, perpendicular to the dominant surface wind-stress. The mean annual transport of temperature is quite noisy, with predominantly positive values in the north and negative values in the south. This configuration, far from reflecting the mean transport of the time mean SST field by the time mean current, reflects the predominant role of the eddy field. The mean annual depth of the Ekman layer, with values ranging from 35 to 50 m, is deeper in the north-western part of the domain due to the influence of the dominant winds.

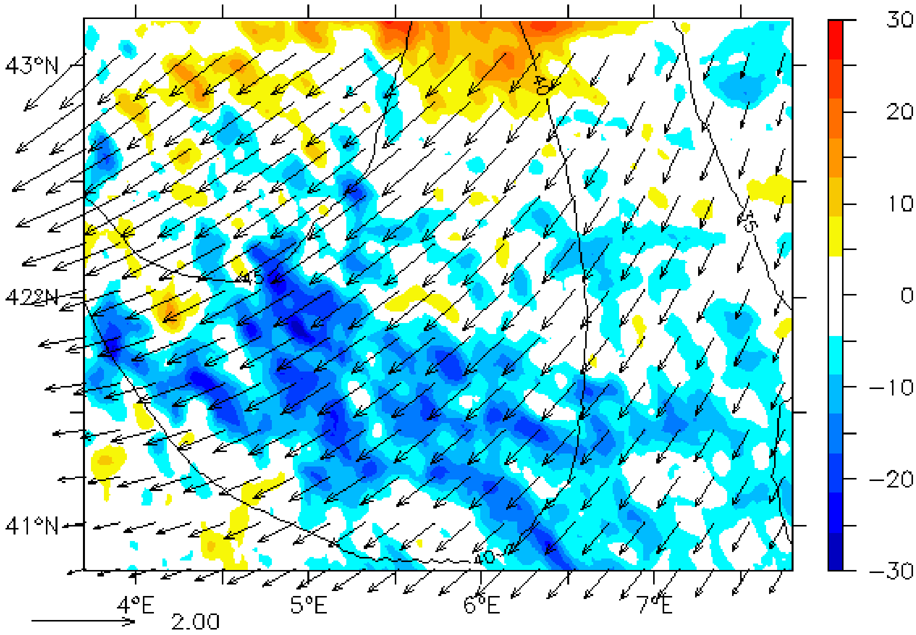

Figure 4. *Same as Figure 3 for the horizontal Ekman advection of temperature (shades, units 10^{-8} °C s^{-1}), Ekman transport (arrows, units m^2 s^{-1} and scale in the lower left corner) every 10 grid point and Ekman depth (contours, units m).*

2.4.3. Horizontal Non-Ekman Advection

For the horizontal non-Ekman advection, we used geostrophic advections derived from the MERCATOR PSY2V4R4 model. This model assimilates altimetry, suggesting that the large-scale circulation in the NWM is better constraints than in models without assimilation. Moreover, many comparisons were done with MARS3D and SYMPHONIE models and with MEDRYS reanalysis during winter 2012-2013 in the NWM (not shown). These comparisons led us to conclude that the MERCATOR model responds quite well to our needs for reconstructing geostrophic advections over the whole water column.

The seasonal evolution of the mean temperature geostrophic advection versus depth is presented in Figure 5. The plot confirms that advections are the strongest in the surface layers down to a depth of about 150 m. From January to March, geostrophic advections were weaker than during the rest of the year because during this period intense cooling significantly reduced horizontal gradients of temperature and salinity across the area, despite the intensification of the rimcurrent. During the rest of the year, alternatively warm and cold subsurface advections reflect the presence of mesoscale features (eddies and filaments) mainly transiting along the Balearic Front around 40°N. At the surface and after one annual cycle, geostrophic advection tends to warm SSTs and freshen SSSs in the test area.

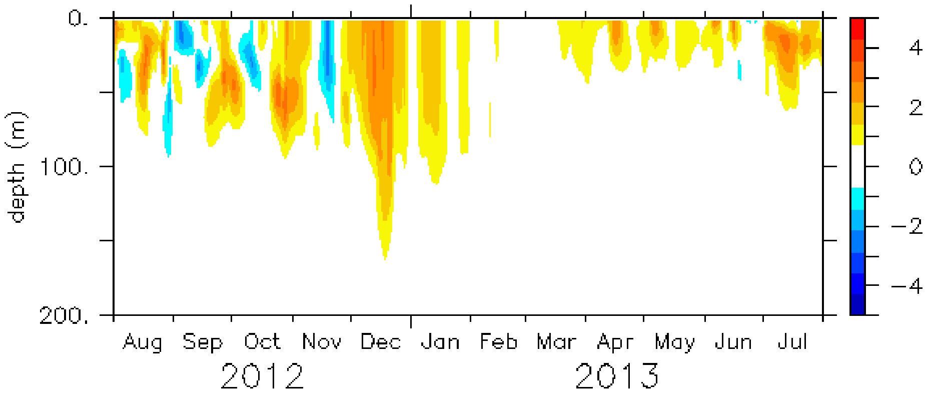

Figure 5. *Temporal evolution of the domain average geostrophic advection of temperature (10^{-7} °C s^{-1}) as a function of depth (m).*

2.4.4. Vertical Ekman Advection

At any point of the test area and at each time step, a vertical Ekman velocity w_e was evaluated from the wind-stress curl and then averaged over the test area. For computing vertical advections of temperature and salinity, we must further impose a vertical profile for $\langle w_e \rangle$. As in *Caniaux et al.* [2005b], we chose zero at the surface, maximum at the Ekman layer depth, and decreasing to zero at the bottom of the water column. In the SCM, vertical Ekman advections were calculated at each level of the SCM from vertical gradients of temperature and salinity and from the vertical profile of $\langle w_e \rangle$ with an upstream numerical scheme compatible with the other schemes of the model.

The mean annual Ekman pumping is displayed in Figure 6. An ascending positive (subsiding negative) pumping zone is present on the right cyclonic (left anticyclonic) side of dominant winds. The two areas of opposite sign are separated by a nearly 110 km wide corridor corresponding to the main pathway of the dominant winds in the area. Note that the patterns of higher and lower pumping values are consistent with the patterns of higher temporal variability (yearly standard deviations > 40 10^{-6} m s^{-1}). The north-eastern area with positive pumping plays an important role for preconditioning water masses, by maintaining the doming of isopycnals inside the gyre interior, as underlined by *Gascard* [1978] and *Madec et al.* [1996] in the Gulf of Lion or by *Pickart et al.* [2003] in the Irminger Sea, where the Greenland tip jets generate elevated heat loss and strong wind-stress curl in the lee of Cape Farewell. As the magnitude of the positive wind-stress curl and its extension are larger than that of the negative pumping zone, a mean annual positive value is expected in the test area.

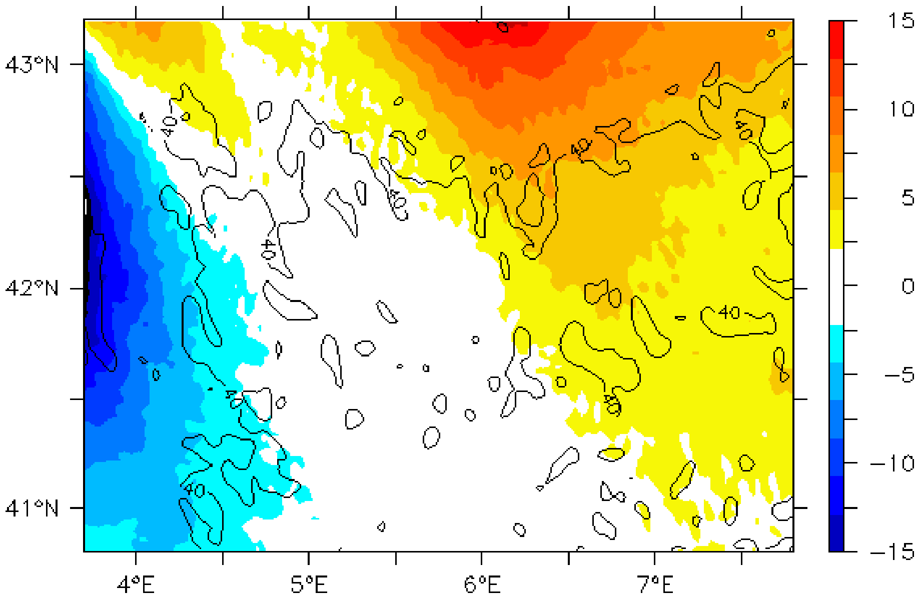

Figure 6. *Same as Figure 3 for the Ekman pumping (shades, units 10^{-6} m s^{-1}) and temporal standard deviation (contours, units 10^{-6} m s^{-1}). Contour intervals are 40×10^{-6} m s^{-1}.*

2.4.5. Subgrid Scale Vertical Mixing

This term, symbolized in equation (3) by $\partial_z \langle K'' \partial_z T'' \rangle$, represents a physical process that increases vertical mixing. As in *Caniaux et al.* [2005b], we suppose that the subgrid scale fluctuations of this process were due to spatial heterogeneities in the wind field throughout the test area. To parameterize this process, we considered that the wind-stress was increased by a factor taking into account the spatial standard deviation σ of the wind magnitude $\langle |\vec{U}| \rangle$, i.e., by multiplying the wind-stress by the factor $\gamma = 1 + \frac{\sigma}{\langle |\vec{U}| \rangle}$. All year long, the time series of γ displays a high frequency variability but with no significant trend (not shown). Consequently, a constant value for this factor was specified to be equal to its mean annual value (γ = 1.34).

2.5. Optimization

The optimization of the model simulations needs first to select some adjustable parameters (i.e., poorly known constants of the model or constants leading to a great sensitivity to the results) and to introduce other parameters to correct the surface fluxes. Among the first, two adjustable constants in the parameterization of the incoming solar penetration were selected because tests proved that SSTs were very sensitive to R and d_2 in *Paulson and Simpson* [1977]'s parameterization:

$$I(z) = R.\exp(-\frac{z}{d_1}) + (1-R).\exp(-\frac{z}{d_2}) \quad (7)$$

where z is the depth; R denotes a partition parameter between the red and blue-green parts of the solar radiation spectrum penetrating down to the extinction depths d_1 and d_2 respectively. As the simulations were quite insensitive to d_1, the value of the standard type III waters in *Jerlov* [1976]'s classification was adopted and set to be 1.4 m.

Among the second adjustable parameters, five coefficients were introduced in the expressions of the area mean surface fluxes. These coefficients a supposed to represent corrections to be brought either to the input parameters or to the exchange coefficients of the bulk formulae:

1. coefficient β_w corresponds to the errors affecting the surface wind. This parameter plays an important role because it affects directly wind-stress, latent and sensible heat fluxes, and horizontal and vertical Ekman advections.

2. Coefficients β_{ws} and β_l represent the uncertainty affecting the exchange coefficients of wind-stress and of latent heat flux (and evaporation) respectively. Both are multiplicative factors.

3. For sensible heat flux, a bias β_s was introduced instead of a multiplicative factor, because sensible heat may frequently change sign in the NWM, air temperatures being frequently close to SSTs.

4. β_p for correcting satellite rainfall.

Finally, the corrected fluxes were written as:

$$\begin{aligned}
\langle \tau \rangle &= \beta_w^2 \beta_{ws} \langle \tau \rangle^* \\
\langle Q_{lat} \rangle &= \beta_l \beta_w \langle Q_{lat} \rangle^* \\
\langle Q_{sens} \rangle &= \beta_w \langle Q_{sens} \rangle^* - \beta_s \\
\langle P \rangle &= \beta_p \langle P \rangle^*
\end{aligned} \qquad (8)$$

in which τ stands for the magnitude of the wind-stress, Q_{lat} the latent heat flux, Q_{sens} the sensible heat flux and P the precipitation, and in which the area mean guess fluxes are affected by a star. The ranges of values of the seven adjustable parameters are given in Table 1. They were determined so as to be large enough to be sure to get the optimum, but in reasonable intervals to discard unphysical solutions.

Parameter (unit)	Range of values	Optimum
R	0.3 – 0.7	0.463
d_2 (m)	5 – 25	20.000
β_w	0.8 – 1.2	1.066
β_{ws}	0.5 – 1.0	0.750
β_l	0.7 – 1.1	0.900
β_s (W m^{-2})	-10 – +10	+4.526

β_p	0.6 – 1.2	1.138

Table 1. *List of adjustable parameters, with their range of values and the optimum obtained with the genetic algorithm.*

The optimization of the SCM simulations was carried out using a genetic algorithm [*Carroll*, 1996]. This tool is derived from genetics and population evolution. It is used for seeking the extreme of particularly complex functions, sometimes with discontinuities, like in numerical models. The genetic algorithm searches in a N-dimensional space the N parameters that minimize a cost function *CF* evaluated for each run of the model. In the algorithm, the set of N parameters to be optimized are coded in a binary form called chromosome. The algorithm starts with a randomly chosen population of chromosomes, after which it evaluates the fitness value of each chromosome by computing a cost function, using the corresponding set of parameters to run the model. Then, the three genetic processes of selection, crossover and mutation are performed upon the chromosomes in sequence. During the selection, chromosomes are copied in proportion to their fitness values based on a probability of selection. Crossover acts on the selected chromosomes, using a crossover probability: this operator selects a crossover site within paired strings and exchanges between the two chromosomes the parts located to the right of the crossover site. Lastly, mutation is applied to the chromosomes in order to maintain diversity. After these processes, the new chromosomes are compared to those of the previous generation, and accepted or rejected based on an update probability. The procedure is repeated until convergence or stopped by fixing a maximum number of generations. The output of the algorithm is a set of N optimal parameters obtained after running a generally high number of model simulations (here 50.000). In the present study N = 7 for R, d_2, β_w, β_{ws}, β_l, β_s and β_p.

The cost function (*CF*) is defined as follows:

$$
\begin{aligned}
CF = {} & \alpha_{SST} \sum_i \frac{1}{\sigma_{SST}^2} \left(\langle SST_{\mathrm{mod}} \rangle - \langle SST_{obs} \rangle \right)^2 \\
& + \alpha_{SSS} \sum_j \frac{1}{\sigma_{SSS}^2} \left(\langle SSS_{\mathrm{mod}} \rangle - \langle SSS_{obs} \rangle \right)^2 \\
& + \alpha_T \sum_3 \sum_z \frac{1}{\sigma_T^2} \left(\langle T_{\mathrm{mod}}(z) \rangle - \langle T_{obs}(z) \rangle \right)^2 \\
& + \alpha_S \sum_3 \sum_z \frac{1}{\sigma_S^2} \left(\langle S_{\mathrm{mod}}(z) \rangle - \langle S_{obs}(z) \rangle \right)^2 \\
& + \alpha_{RB} \sum_j \frac{1}{\sigma_{RB}^2} \left(\langle RB_{\mathrm{mod}} \rangle - \langle RB_{obs} \rangle \right)^2
\end{aligned}
\tag{9}
$$

In this expression, each term is normalized by the variance σ_k^2 of the series (k refers to the area mean *SST*s, *SSS*s, temperature (*T*) and salinity (*S*) profiles and residual buoyancy *RB*). $\langle SST_{obs} \rangle$ represents the area mean daily satellite SST series (the same as those of the guess fluxes) during the period of simulation (i = 365 days). $\langle SSS_{obs} \rangle$ is the area mean surface salinities obtained from daily objective analyses performed by one of the co-authors [*Giordani et al.*, 2014] during the winter period (i.e., j = 119 days) from all the data collected in the NWM (gliders, floats, CTDs, drifters and satellite). For the analyses, temperature and salinity data were first carefully checked to detect any erroneous values. They were then interpolated onto 800 vertical levels (with a 5 m vertical resolution from the surface to the bottom) and objectively analyzed onto a 1/12° horizontal grid following the procedure used by *Giordani et al.* [2005]. The first guess of the analyses was derived from the operational MERCATOR PSY2V4R4 model. At each grid point, the PSY2V4R4 analysis was corrected with the observations which lie within one influence time/space radius around the grid point, following the procedure of *De Mey and Ménard* [1989]. A space correlation radius of 10 km, consistent with the mesoscale structures of the NWM, and a decay e-folding time of one day were chosen.

In equation (9), $\langle T_{obs}(z) \rangle$ and $\langle S_{obs}(z) \rangle$ are the area mean temperature and salinity profiles deduced from CTDs collected during the DeWEX-1, DeWEX-2 and MOOSE 2013 hydrological networks, respectively centered on 2013/02/01, 2013/04/14 and 2013/06/30. Residual buoyancy $\langle RB_{obs} \rangle$ (units in $m^2\ s^{-2}$), an integral measure of the stratification of the water column, was computed from the objectively analyzed temperature and salinity fields during the 119 days period, as:

$$RB = \int_{-H}^{0} zN^2(z)dz \qquad (10)$$

where $N^2(z)$ is the Brunt-Vaïsala frequency computed from *McDougall* [1987] and H the depth of the ocean (2250 m). Finally in equation (9), α_k (k = 1,5) are weighting coefficients chosen inversely proportional to the number of data in the series and function of the confidence we have in the quality of the data. They were taken as 1, 0.8, 0.1, 0.1 and 0.1 respectively.

3. Results

3.1. Adjusted Parameters

The optimization with the genetic algorithm was performed after running 50.000 simulations of the SCM during one annual cycle. For each simulation, the adjustable parameters were chosen by the genetic algorithm in their preselected range of values (Table 1) and the cost function computed. In Figure 7, the fitness function (10000 times the inverse of the function cost) is plotted against the value of each adjustable coefficient. Each black point corresponds to the fitness value evaluated for each simulation and the red circle is the maximum fitness function. The latter provides the optimal adjustable set of coefficients, which also figure in Table 1.

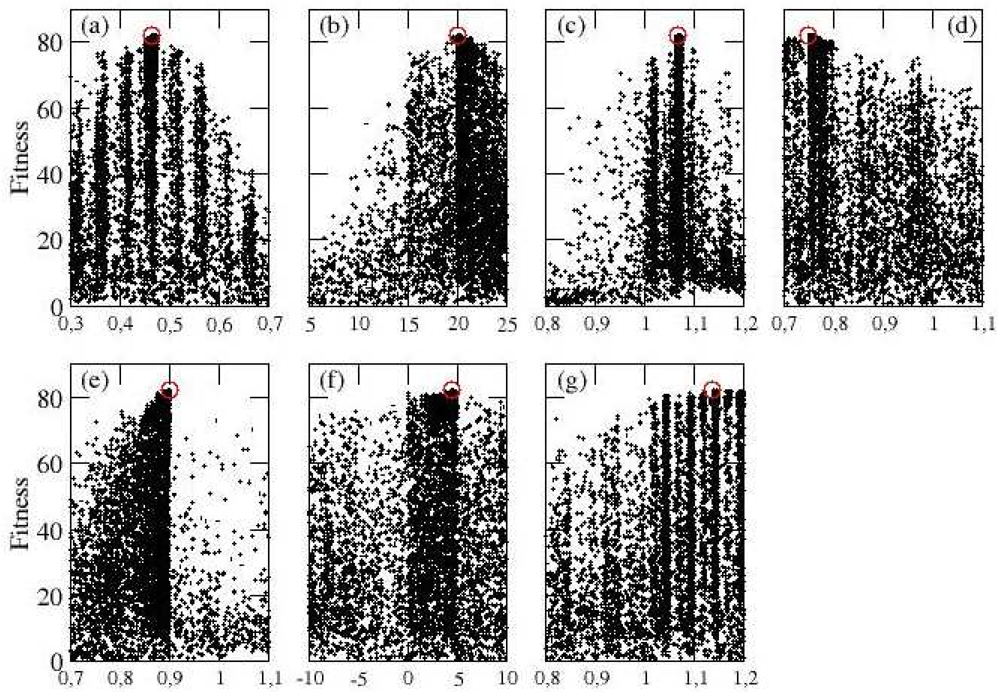

Figure 7. *Fitness function for each adjustable parameter: (a) R, (b) d_2, (c) β_w, (d) β_{ws}, (e) β_l, (f) β_s, (g) β_p. The maximum fitness values are circled.*

The optima for R and d_2 (Table 1 and Figure 7a-b) are close to the values in *Jerlov* [1976]'s classification, although R appears slightly underevaluated compared to type III waters. However, the adjusted values represent a mean annual value for different water types, which may change during the year and through the area. In Figure 7, sharp peaks of the fitness function correspond to well identified optimum values. This is the case for the wind coefficient β_w (Figure 7c) and the latent heat flux coefficient β_l (Figure 7e). Conversely, the sensitivity of the simulations to the adjustable coefficient is lower for the sensible heat flux coefficient β_s (Figure 7f) and for the precipitation coefficient β_p (Figure 7g) for which the values of the fitness function form almost a plateau.

In Table 1, the optimum of β_w means that the wind needed to be slightly increased by a factor of 1.066, for optimizing both the wind-stress, the latent (as well as evaporation) and sensible heat fluxes, the horizontal and vertical Ekman advections. On the other side, the optimum of β_{ws} (supposed to correct the exchange coefficient of the wind-stress) being 0.75 means that the guess wind-stress was largely overestimated and according to equation (8) had to be reduced by a final factor of 0.75*1.066² = 0.85. Similarly, the exchange coefficient of the latent heat flux had to be multiplied by a factor of 0.9 and the guess flux by a factor of 0.9*1.066 = 0.96. Note that the TRMM precipitation fields were underestimated by an factor of 1.138 for adjusting the model near surface salinity. Accordingly, when the flux correction is applied to each grid point of the test area with equation (8), and during one annual cycle the mean latent and sensible heat fluxes were reduced by 4.7 and 3.5 W m^{-2} respectively (Table 2); this led to an increase of the net heat flux by 8.2 W m^{-2}. Similarly, the adjusted E-P balance is reduced by 163 mm yr^{-1}, due to an overestimation of evaporation (60 mm yr^{-1}) and an underestimation of precipitation (103 mm yr^{-1}) of the guess. The average value of the adjusted wind-stress is lowered by about 0.02 N m^{-2}.

Flux	Guess	Adjusted	Difference guess-adjusted
Sensible heat flux	-16.4	-12.9	-3.5
Latent heat flux	-113.8	-109.1	-4.7
Net heat flux	-14.3	-6.1	-8.2
Wind-stress	0.156	0.133	0.023
E	1460.8	1400.9	59.9
P	749.3	852.3	-103.0
E-P	711.5	548.6	162.9

Table 2. *Comparison of guess and adjusted mean annual fluxes. Domain considered: 3.71°E-7.79°E – 40.31°N-42.69°N; period considered: 2012/08/01 to 2013/07/31. Heat fluxes are in W m^{-2}, wind-stress in N m^{-2} and water fluxes in mm yr^{-1}.*

3.2. The Optimized Simulation

We now compare the evolution of the area mean satellite SST, reanalyzed SSS and residual buoyancy evolutions (considered as our reference) with the model simulations after introducing successively first the three advection terms (geostrophic advection, horizontal Ekman advection, vertical Ekman advection), then the surface fluxes and finally the adjusted surface fluxes. Figure 8 displays the contribution and order of magnitude of each process during one annual cycle and how the simulations of SST, SSS and residual buoyancy are improved with the adjusted fluxes. Satellite SSTs present a significant seasonal cycle with a peak to peak amplitude of 15°C (black curve in Figure 8a). The annual cycle is flattened in winter because SSTs never fall below 12.8°C when the mixed layer is deep. Some marked cooling events punctuated the seasonal cycle in autumn (e.g., in early December) and some warming events in spring (e.g., mid-April and mid-June) in response to intense surface fluxes. After introducing geostrophic advection alone (dark green curve in Figure 8a), the SST series is marked by a regular warming with a final yearly gain of 2.6°C. When adding horizontal Ekman advection (green curve in Figure 8a), the SST trend drops to about 1°C, while with vertical Ekman advection (cyan curve) the yearly trend is reduced to zero. Obviously, the surface flux is the main process, which allows to reconstruct the annual cycle and the intraseasonal warming and cooling short events (orange curve in Figure 8a). Remarkably, the modeled SST series obtained with the adjusted fluxes (red curve) is quite close to the daily satellite SST series, with a bias of 0.011°C (0.06 %) and a mean standard deviation of the differences between the two series of 0.017°C.

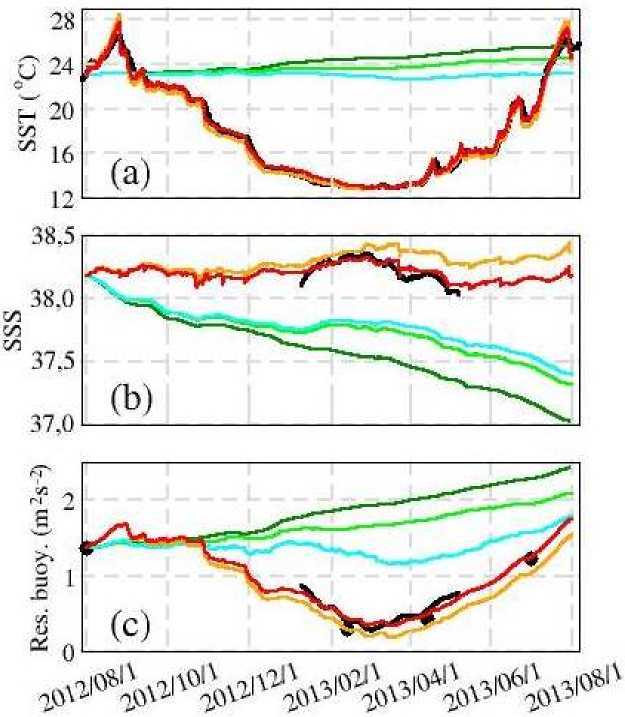

Figure 8. *Temporal evolution of (a) SST (°C), (b) SSS and (c) residual buoyancy (m² s^{-2}) simulated by the model, when activating only geostrophic advection (dark green curve), then successively adding horizontal Ekman advection (green), vertical Ekman advection (cyan), surface fluxes (orange), and when using the adjusted surface fluxes (red curve). The black curves correspond to the reference (a) mean satellite SSTs, (b) analyzed SSSs from in-situ data during the period 2013/01/09 to 2013/05/07 and (c) residual buoyancy (computed from the 3D analyses during the same period). The black points correspond to the residual buoyancy calculated from the CTDs collected in the test area during MOOSE 2012 (median date 2012/08/01), DeWEX-1 (2013/02/13), DeWEX-2 (2013/04/14) and MOOSE 2013 (2013/06/30).*

For SSSs, our reference is the analyzed wintertime series (see subsection 2.5). SSS values range from 38.04 to 38.36 with a maximum reached in late February 2013 (black curve in Figure 8b). By introducing geostrophic advection, SSS undergoes a strong but quite steady decrease of 1.2 unit after one year (dark green curve in Figure 8b). Horizontal Ekman advection reduces the yearly trend and introduces seasonal variability in autumn and winter (green curve). Vertical Ekman advection generates higher salinity values associated with an import of salinity from depth and helps to further reduce the negative trend (cyan curve in Figure 8b). With the guess fluxes, the annual range of SSS drops significantly (orange curve in Figure 8b). Finally, with the adjusted fluxes (red curve in Figure 8b), the daily wintertime difference with the analyses falls to 0.011 (0.03%) and the standard deviation of the differences between the series to 0.004. Some brief events, that cause sudden SSS drop (e.g., late March, late April), were associated with substantial rainfall. These events are not very well reconstructed by the analyses; the source of this discrepancy must lie in the smoothing effect inherent to the optimal interpolation technique. Note that during the simulation period, SSSs exhibit an overall insignificant negative trend due to the quasi-balance between the surface fluxes and the advection terms, despite a positive input of salinity in January associated with a positive horizontal Ekman advection.

The residual buoyancy was evaluated from the wintertime daily temperature and salinity analyses (see subsection 2.5), as well as from CTDs of the four hydrological networks (black curve and black dots in Figure 8c). The residual buoyancy rapidly decreases from mid January 2013 and reaches a minimum at the end of February, when the surface area occupied by low stratified waters presents its maximum extension in the test area, after which the residual buoyancy increases during the spring restratification. Geostrophic advection (dark green curve in Figure 8c) produces a marked residual buoyancy increase up to 1 $m^2 s^{-2}$ after one year. The effect of horizontal Ekman advection is to reduce the trend (green curve). Added to horizontal advection, vertical Ekman advection results in the destratification of the water column in winter and restratification in spring (cyan curve). If the Ekman pumping effect was reduced on the SSTs and SSSs series (see Figure 8a-b), its effect on residual buoyancy, thus on the seasonal cycle of the upper top 300 m, is obvious. After introducing the surface fluxes, the peak to peak annual cycle is enhanced (orange curve in Figure 8c). Finally, the effect of the adjusted fluxes is striking: the bias between the model and analyzed series falls to –0.029 $m^2 s^{-2}$ and the standard deviation of the difference to 0.005 $m^2 s^{-2}$. This has the effect of producing a fairly good agreement with the values of the reanalyzed MOOSE 2013 network (red curve) after almost one seasonal cycle.

4. Evaluations

4.1. Comparison With Fluxes at the LION and AZUR Buoys

The adjusted fluxes were calculated over a larger area than the test area (0°E-12°E, 38°N-44.5°N; see Figure 1), i.e., the simulation domain of the operational Météo-France AROME model over the Mediterranean Sea. However, the spatial resolution was reduced to a grid of 0.04° longitude x 0.04° latitude to avoid spatial interpolations near the coast. The calculation was performed by applying equation (8) at each grid point of the large domain area, every hour and during one year (2012/08/01 – 2013/07/31). In this section, we evaluated the adjusted fluxes locally, through their comparison with the in-situ data collected at the LION and AZUR buoys (see locations in Figure 1). The buoy datasets include radiative fluxes (incoming longwave and shortwave radiations) and all the near-surface meteorological observables needed to estimate the turbulent fluxes, except precipitation. Previously, the variables downloaded from the HyMeX website were scrupulously checked. Out-of-range values were cleaned and sequence values deemed to be unreliable or displaying periods of constant values were rejected. The data were then placed on a regular, hourly temporal grid, and isolated missing data or short sequences of missing data were linearly interpolated from adjacent ones. Compatibility between relative humidity and dew-point measurements was checked and corrected if necessary (for example, dew-point values could excess air temperatures, under high humidity or saturated conditions). Finally, because of missing sequences and rejected data, only 1818 and 514 hourly fluxes (over 8760) were available at the LION and AZUR buoys respectively for the comparison.

Moreover, for comparing the adjusted and the buoy net heat fluxes, we preferred to use several bulk algorithms instead of selecting only one, due to errors affecting bulk formulae. For that, we selected seven bulk formulae, established over various oceanic basins of the world ocean, i.e., *Anderson* [1993], *Brut et al.* [2005], *Fairall et al.* [2003], *Dupuis et al.* [2003], *Persson et al.* [2005], *Caniaux et al.* [2005a] as well as *Smith* [1980], whose wind-stress parameterization was associated with *De Cosmo et al.* [1986] for the latent and sensible heat fluxes. Figure 9 represents the scatter plots at the two buoys of the adjusted net heat flux series versus the median of the seven net heat flux estimates, as well as their inter-quartile range (IQR hereafter).

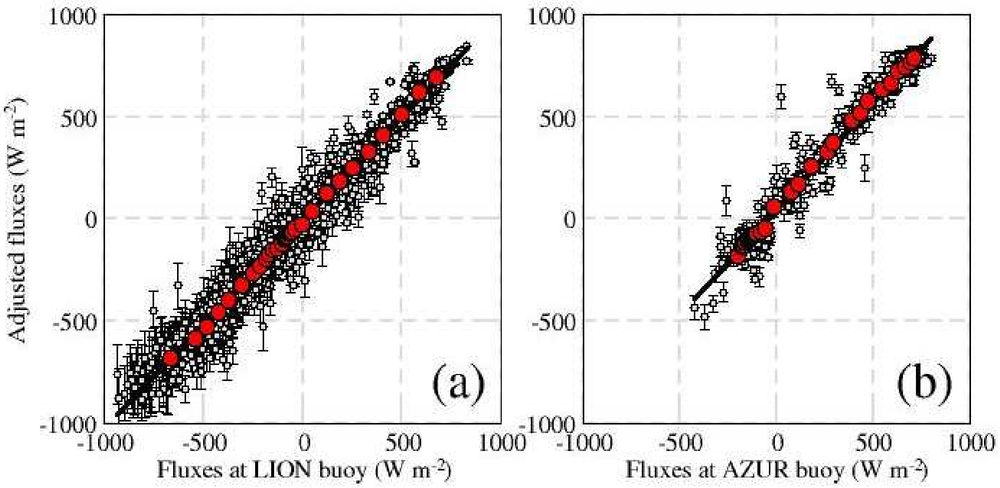

Figure 9. *Scatter (grey points) and Q-Q (red points for the 30-quantiles) plots comparing the adjusted fluxes with the surface net heat fluxes estimated from in-situ measurements: (a) at the LION (N = 1818; r^2 = 0.96) and (b) AZUR buoys (N = 514; r^2 = 0.96). The turbulent fluxes were evaluated with 7 bulk formulae and the medians of each of the 7 estimates are plotted with their inter-quartile range represented by bars. The comparison covers the period 2012/08/01 to 2013/07/31.*

The net heat flux at the buoys is predominantly governed by turbulent heat flux and solar radiation and its sign depends on the seasonal balance between net solar radiation and latent heat flux. At the LION buoy (Figure 9a), the range of the net heat flux is much larger (~1700 W m^{-2}) than at the AZUR buoy (~1200 W m^{-2}) (Figure 9b), a consequence of limited sampling at AZUR buoy, and in part because the LION buoy is located on the passage of the prevailing stronger winds with frequent intrusions of cold and dry air from the north. The adjusted and the median of the in-situ fluxes are in fair agreement (r^2 = 0.96 at the two buoys), with only a weak spread of the data around the first diagonal of the diagram. Note that the IQR of the medians at the two buoys are much more important at low (negative) than at high (positive) flux values, due to greater uncertainties in the turbulent heat flux exchange coefficients at high wind, and large contrast of temperature and humidity between the air and the oceanic surface. The agreement of the series remains good over the whole range of values with no skew, even for low or high fluxes, as indicated by the 30-th quantiles of the Q-Q plot (red dots in Figure 9).

4.2. Evaluation of NWPM Fluxes

In this section, we compare the adjusted fluxes, considered as a reference, with fluxes of four operational NWPM: the French ARPEGE [*Courtier et al.*, 1991] and AROME [*Bouttier*, 2007] models, the NCEP and ECMWF models and one reanalysis, ERA-INTERIM [*Dee and al.*, 2011]. The fluxes of the five products were linearly interpolated on the same horizontal grid (0.02° x 0.02°) as the adjusted fluxes and compared over the test area. Table 3 provides mean annual values of the individual flux components of the net heat and water fluxes as well as the wind-stress, along with the standard deviations.

	ARPEGE	AROME	NCEP	ECMWF	ERA-INTERIM	Adjusted
Sensible heat flux	-23.2 (56.3)	-27.0 (64.3)	-21.4 (55.3)	-17.7 (38.6)	-16.2 (37.2)	-12.9 (34.9)
Latent heat flux	-124.7 (152.8)	-109.0 (127.5)	-118.6 (143.8)	-109.5 (117.8)	-98.9 (105.9)	-109.1 (114.5)
Net longwave	-76.9 (23.8)	-79.6 (22.8)	-77.4 (23.0)	-80.5 (20.5)	-79.0 (21.1)	-66.3 (17.2)
Net shortwave	+172.7 (216.4)	+190.7 (223.2)	+192.7 (228.9)	+184.5 (221.0)	+179.8 (219.1)	+182.2 (266.7)
Net heat flux	-52.1 (317.2)	-24.9 (311.1)	-24.7 (327.0)	-23.2 (284.0)	-14.4 (274.3)	-6.1 (319.4)
Wind-stress	0.143 (0.189)	0.149 (0.202)	0.105 (0.145)	0.145 (0.188)	0.117 (0.148)	0.133 (0.167)
E	1599.8 (1962.1)	1398.7 (1632.5)	1456.4 (1772.4)	1380.9 (1485.5)	1247.5 (1335.4)	1400.9 (1468.5)
P	727.9 (1988.0)	688.1 (2317.4)	731.0 (2098.0)	685.6 (1861.9)	654.6 (1833.0)	852.3 (2851.4)
E-P	871.9 (2625.8)	710.6 (2770.0)	725.4 (2550.5)	695.3 (2280.3)	592.9 (2237.8)	548.6 (3133.5)

Table 3. *Comparison of the operational NWPM: ARPEGE, AROME, NCEP, ECMWF and of the ERA-INTERIM reanalysis with the adjusted fluxes; standard deviation values in parenthesis.*

Domain considered: 3.71°E-7.79°E – 40.31°N-42.69°N; period considered: 2012/08/01 to 2013/07/31. Heat fluxes are in W m^{-2}, wind-stress in N m^{-2} and water fluxes in mm yr^{-1}.

All model products display a net heat loss by the sea, but they all underestimate the adjusted fluxes, sometimes dramatically like ARPEGE (the difference reaches 40 W m^{-2}), others weaker like ERA-INTERIM (8 W m^{-2}). Note the substantial dispersion between the various NWPM products with a more than twofold intervariation (the range, 38 W m^{-2}, is of the same order of magnitude as the median, -25 W m^{-2}). The model products differ from the adjusted fluxes for different reasons; the differences are primarily the result of differences in either the sensible heat flux for AROME and APREGE (the heat loss difference exceeds 10 W m^{-2}), in the latent heat flux for ARPEGE (< -15 W m^{-2}) and ERA-INTERIM (> +10 W m^{-2}), in the net longwave radiation for the ECMWF and AROME (< -13 W m^{-2}), or in the net shortwave radiation for the NCEP (> +10 W m^{-2}). On average, the NCEP and ERA-INTERIM underestimate the adjusted wind-stress by 0.028 N m^{-2} and 0.016 N m^{-2} respectively, while the other products overestimate the adjusted wind-stress over 0.01 N m^{-2}.

The model E-P budgets display a high dispersion (Table 3). Moreover, all NWPM overestimate the adjusted water budget, sometimes radically, with ARPEGE exhibiting the greatest difference with the adjusted fluxes (323 mm yr^{-1}). Again, ERA-INTERIM is the model that most agrees with the adjusted fluxes (44 mm yr^{-1}), certainly a consequence of a greater amount of data assimilated in the reanalysis. This behavior results from differences in evaporation and from systematic and substantial underestimate of precipitation by the NWPM (the difference with the model mean is -155 mm yr^{-1}). All model products underestimate the uncorrected TRMM precipitation as well (not shown). A similar conclusion was reached by *Alhammoud et al.* [2014] who noted that rainfall and specially convective rainfall in ERA-INTERIM over the Mediterranean Sea were systematically underestimated compared to microwave satellite retrievals. The large dispersion between NWPM, both for heat and water fluxes, suggest the importance of errors and drift affecting model runs, when ocean models are forced with atmospheric NWPM flux fields without any corrections [e.g., *Sanchez-Gomez et al.*, 2011; *Valdivieso et al.*, 2015]. Surprisingly, all the model products appreciably underestimate the variability of the satellite shortwave radiation (Table 3) as well as the variability of satellite precipitation compared with adjusted (Table 3) and even with uncorrected TRMM fields (not shown). Consequently, the variability of the E-P budget is also underestimated by all the model products.

Figures 10 and 11 compare the mean annual adjusted flux fields over the larger domain with ARPEGE and ERA-INTERIM fields, respectively the farthest and closest models in comparison with the adjusted fluxes. The spatial patterns of the annual net heat flux (Figure 10) are similar, with heat loss between the Gulf of Lion and Sardinia, reflecting the dominant wind pattern, in the Gulf of Genoa and east of Sardinia. The maximum heat loss (~ -60 W m^{-2}) is located in the Gulf of Lion, along the continental margin (Figure 10a). A belt of positive values (heat gain for the ocean of about 10 to 20 W m^{-2}) extends between the southern Pyrenees, the Balearic islands and along the Sardinia and Corsica islands. In both models, the amplitudes differ considerably with the adjusted fluxes with differences reaching locally up to 60 W m^{-2}. In ARPEGE, the zero flux line is hardly present in the vicinity of the Balearic islands (Figure 10b), while in ERA-INTERIM (Figure 10c) the zero flux line delimits a much larger surface area than in the adjusted fluxes.

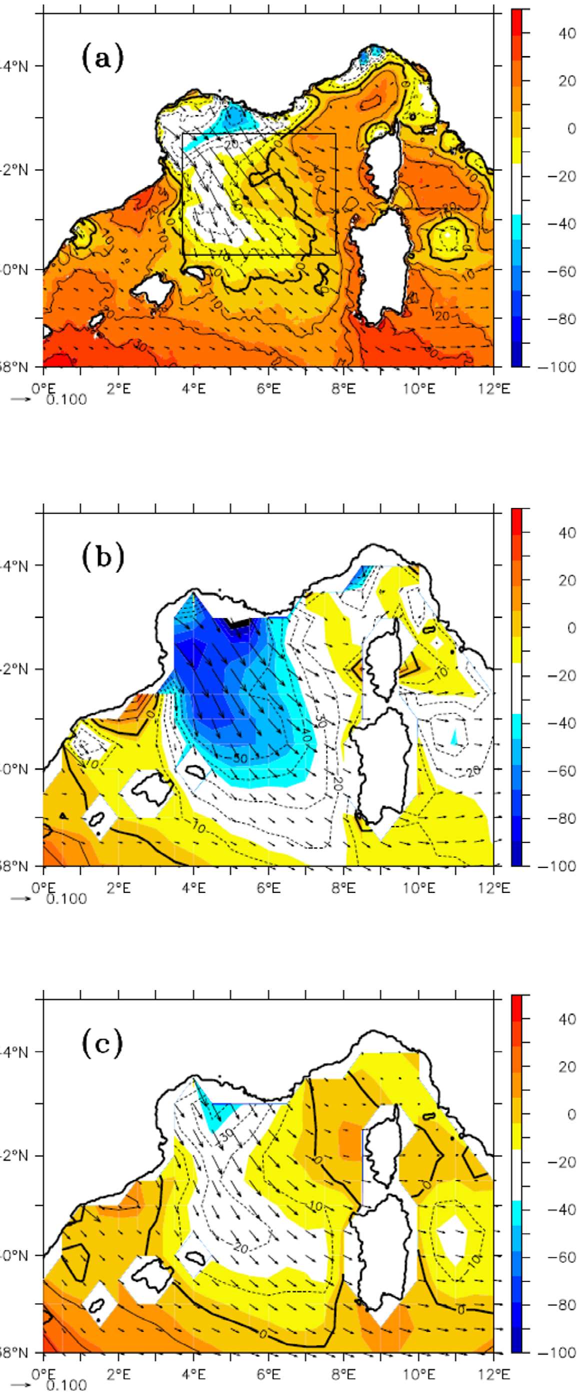

Figure 10. *Maps of the annual net heat flux (shades, W m-2) and wind-stress (arrows, N m-2 and scale in the lower left corner) for (a) the adjusted flux dataset, (b) the ARPEGE model, and (c) ERA-INTERIM. Period considered: 2012/08/01 to 2013/07/31. Contour intervals are 10 W m-2. In (a) the wind-stress is represented every 10 grid point.*

For the water fluxes (Figure 11), the spatial pattern of the adjusted fluxes displays higher values in the Gulf of Lion and from the Balearic to Sardinia islands (750 to 1000 mm yr^{-1}) and much lower values in the Gulf of Genoa, with an excess of precipitation over evaporation rates (Figure 11a). The flux fields of the two models present the same longitudinal gradient pattern but with less mesoscale features than the adjusted fluxes (Figure 11b-c), like in the net heat flux fields. The absence of mesoscale features in the NWPM mean annual heat and water flux fields results from the coarser spatial resolution of SST fields used in NWPM. Actually, most of them use the 6 km resolution OSTIA analysis [*Donlon et al*., 2012] which is derived form coarser resolution (mostly satellite) products, which alter the SST and thus the flux mesoscales, compared to the ~4 km resolution of our flux retrievals based on the ~2 km resolution SST product. The ARPEGE model presents an obvious excess of evaporation and stronger wind-stress from the Gulf of Lion to southern Sardinia, while the region of rainfall excess in the Gulf of Genoa is unrealistically underestimated (Figure 11b).

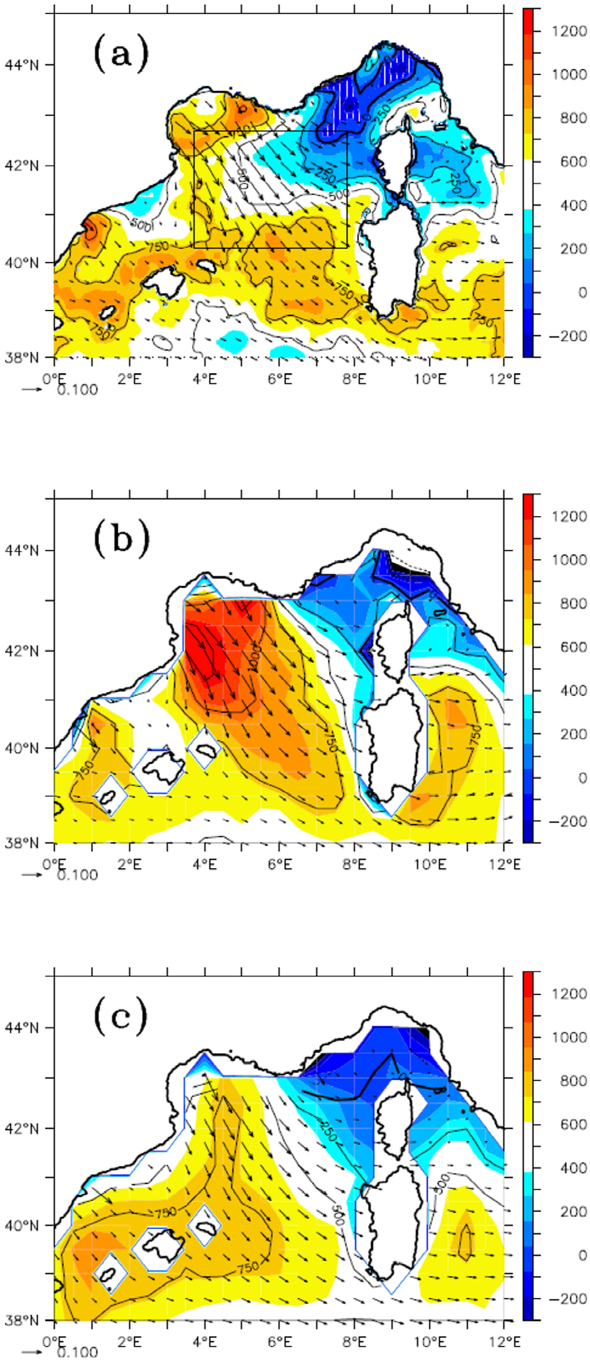

Figure 11. *Same as Figure 10 for the net water flux in mm yr*$^{-1}$*. Contour intervals are 250 mm yr*$^{-1}$*.*

4.3. Evaluation of the Heat and Water Budget Closure

The objective of this section is to show how the fluxes deduced from the inverse method allows to close the heat and water budgets. A heat budget throughout the water column was performed on the test area between MOOSE 2012 and MOOSE 2013 surveys separated by 333 days. The tendency, surface flux, geostrophic and Ekman advections and a residual were calculated independently, either from in-situ data, or from objective analyses of the CTD networks, or from the ocean models, which were run between the two MOOSE networks. The ocean models include the MERCATOR PSY2V4R4 model, the MEDRYS reanalysis, and the mesoscale models SYMPHONY and MARS3D, as well as the SCM forced with the adjusted fluxes.

Each term of the heat and water budgets were computed as box and whisker plots to highlight their contribution and spread (Figure 12). The tendency term was calculated from seven different way: from the mean CTDs collected in the test area during MOOSE 2012 and MOOSE 2013, as well as from objectively analyzed fields deduced from the two hydrological surveys These analyzed fields were produced exactly like the wintertime temperature and salinity analyses (see subsection 2.5), except that they only include the survey CTDs [*Giordani et al.*, 2014]. Other tendency term estimates were provided by the ocean 3D models, the MEDRYS reanalysis and the SCM. The seven estimates of the tendency term are reported in the first column of Figure 12a. The median is negative, meaning cooling of the water column (-16 W m^{-2} with an IQR of 6 W m^{-2}). For getting more than one estimate of the adjusted fluxes, four optimization experiments were performed, wherein only the geostrophic advection was changed (i.e., the MERCATOR geostrophic advection was replaced by the MEDRYS, MARS3D and SYMPHONY ones), because this term is estimated to be the main sensitive term and source of errors in our flux retrieval. For these four estimates (second column of Figure 12a), the median is –21 W m^{-2} (IQR = 12 W m^{-2}), which again corresponds to cooling for the ocean.

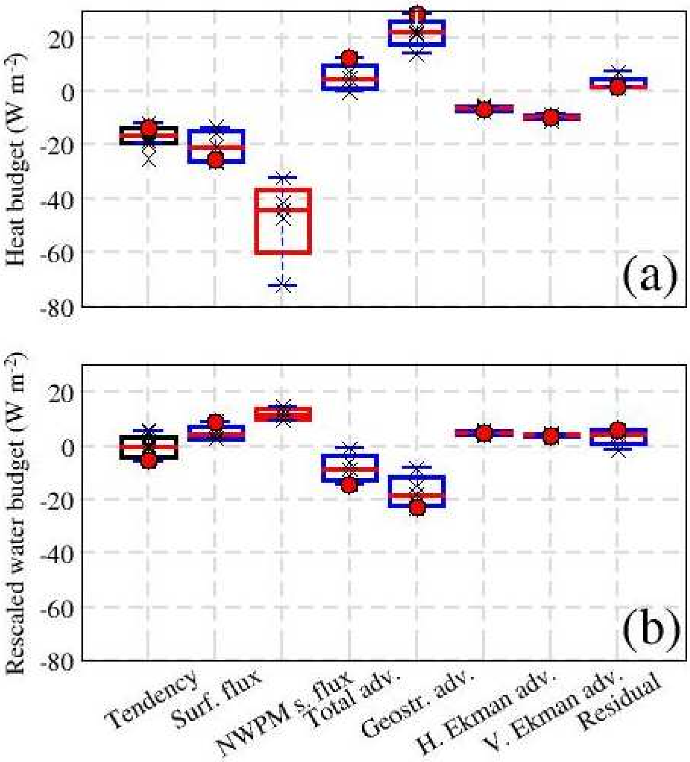

Figure 12. *Box and whisker plot of the (a) heat and (b) rescaled water budgets (in W m^{-2}) in the test area for the period 2012/08/01 to 2013/06/30 (333 days). From left to right: the black box represents the lower and upper quartiles of the tendency term (7 estimates); the blue box the lower and higher quartile of the four flux retrievals obtained after replacing the MERCATOR geostrophic advection by the SYMPHONY, MARS3D and MEDRYS geostrophic advections; the red box corresponds to the five NWPM surface fluxes (ARPEGE, AROME, NCEP, ECMWF and ERA-INTERIM); the last five blues boxes are the lower and higher quartiles of total advection, geostrophic advection, horizontal Ekman advection, vertical Ekman advection and the residual (four estimates each). Each individual estimates are represented by an X; medians are represented by red horizontal lines, and the maximum and minimum values after discarding outliers are represented by blue lines joined by blue vertical dotted lines.*

In the third column of Figure 12a, the surface fluxes of the five NWPM presented and evaluated in previous subsection are reported. The negative median (-44 W m^{-2}), almost three times the median of the adjusted fluxes (-16 W m^{-2}) and the large spread between model fluxes (IQR = 23 W m^{-2}, twice the IQR of the adjusted fluxes) are in agreement with the conclusions of the previous section. The total advection terms (column 4 of Figure 12a), i.e., the sum of horizontal geostrophic advections, horizontal and vertical Ekman advections (represented respectively in columns 5, 6, 7), were estimated with the geostrophic advections of the ocean models and the horizontal and vertical Ekman advections derived from the flux guess corrected with the adjusted coefficients of equation (8). The positive median value of total advection (22 W m^{-2}) is the result of the positive contribution of geostrophic advection, balanced by the weaker negative contribution of horizontal and vertical Ekman advections. Note the weak spread of both the latter (IQR $<$ 2 W m^{-2}). Finally, the individual residuals were obtained as the difference between the tendency estimated from the mean CTDs, minus the adjusted net heat fluxes and total advection from the various models. The residuals (last column of Figure 12a) are weak and poorly spread (median $=$ 1 W m^{-2}, IQR $=$ 3 W m^{-2}).

This means that the heat budget, estimated from various datasets and model outputs, can be considered almost closed with the adjusted fluxes. This is not the case with the NWPM fluxes, for which the heat budget is far from closure. The median of the residuals obtained with the NWPM fluxes (calculated with the tendency deduced from CTDs and with the MERCATOR geostrophic advection) was estimated to +18 W m^{-2}, i.e., nearly the same order of magnitude as the geostrophic advection term. Actually, NWPM provide surface fluxes computed without any oceanic constraint, apart from the SSTs used in bulk parameterization. On the contrary, the inverse method applied in the present study, is highly constrained by the realistic simulation of the underlying whole water column and in particular by the observed heat and water budgets through the minimization of the cost function.

Note that in our best flux estimates (represented by the red dots in Figure 12a), the negative tendency term results from the balance between the dominant negative surface flux term and the positive geostrophic advection term, plus the both slightly negative horizontal and vertical Ekman advection terms. This result means that during the period considered, advection, mostly its geostrophic component, was actively bringing heat from the surroundings toward the convective area in compensation of the surface heat loss. In addition, Figure 12a shows that errors on the adjusted fluxes can be mainly attributed to errors on geostrophic advection of temperature, an important term in the first top 150 meters (see Figure 6).

The same budget was estimated for salinity (Figure 12b). The different terms (multiplied by $\rho_0 C_p$ times the saline contraction coefficient and divided by the thermal expansion coefficient) were rescaled into W m^{-2} to be compared with the heat budget. The median of the tendency term is closed to zero, meaning that between MOOSE 2012 and MOOSE 2013, the various estimates led to a quasi-balance between positive surface fluxes and negative advection. Positive surface fluxes correspond to an excess of evaporation over precipitation rates over the test area. Figure 12b also allows to conclude that the water budget is more difficult to close than for heat (the median of the residual is +5 W m^{-2} compared with +1 W m^{-2} for heat). This is mainly due to the spread of geostrophic advection (IQR = 11 W m^{-2}), larger than the spread of geostrophic advection for heat (IQR = 8 W m^{-2}). This illustrates the importance of salt injection into the area. As mentioned in the previous subsection, all the NWPM water fluxes overestimate the adjusted E-P fluxes, and all the residuals of the water budgets estimated with the NWPM are higher (median = +7 W m^{-2}) than the ones obtained with the adjusted fluxes.

5. Conclusions

Two sets of surface fluxes were produced, the first one on an area of 300 km x 300 km in the north-western Mediterranean (NWM), the second on a wider area (1000 km x 700 km). The first dataset, the guess, was obtained from the best available products collected from several platforms (satellites and model outputs) to calculate each component of the surface heat and water fluxes on a 0.02° longitude x 0.02° latitude grid. These fluxes, spatially averaged, were used to force a single-column model (SCM) and to simulate the evolution of mean potential temperature and salinity profiles for this region. Through the specific form of its equations, the model was also able to represent the evolution of subgrid scales. The SCM was forced by advection terms: horizontal and vertical Ekman advections deduced from the guess fields, and geostrophic advection deduced from a 3D model, which, by assimilating altimetry, represented realistically the large-scale oceanic circulation of the NWM.

After running some 50,000 SCM simulations, chosen by a genetic algorithm in varying 7 adjustable parameters –two model parameters and five coefficients correcting the surface fluxes—, a best simulation was obtained. Using the optimized set of adjustable parameters, the hourly surface flux guess was corrected at each point of the grid on which they were initially calculated (as well as on a larger domain): this is the second surface flux dataset, or adjusted fluxes. This dataset was thus directly derived from the closure of the heat and water budgets which were observed in the region. Indeed, with the optimization by the genetic algorithm, the model trajectory was forced to be close to the observations used in the cost function. This means that in the inverse method, the fluxes were highly constrained by the underlying ocean layers, and not only by SSTs, as was the case with the flux guess. More generally, in NWPM, in satellite retrievals and in fluxes merged from model outputs and from satellite retrievals, SSTs are the only weak oceanic constraints acting on the surface fluxes. Accordingly, the examples provided in section 4, which compare the ARPEGE, AROME, NCEP, ECMWF and ERA-INTERIM models, not only display a large spread but also a poor capacity to close the heat and water budgets of the NWM.

The ultimate goal of surface fluxes is to force three-dimensional ocean models and to simulate realistically the surface layers without any flux correction or relaxation, to obtain a correct description of surface, mid-depth and deep water masses, and to produce an oceanic circulation in agreement with the water masses produced. The same inverse method has already been applied successfully in a low-energetic region of the northeast Atlantic [*Caniaux et al.*, 2005b]. Here, we showed that the same inverse method could be applied with only minor adaptation in a distinct, more energetic area, also characterized by intermittent wintertime deep convection. The flux dataset produced, which takes into account the oceanic mesoscale, is thought to improve simulations in this area of the Mediterranean Sea, more precisely the intensity and timing of oceanic deep convective events, and to help reduce errors on surface fluxes, the major problem of numerical simulations in this basin [e.g., *Tsimplis et al.*, 2006; *Béranger et al.*, 2010; *Jordà et al.*, 2016].

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