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► **To cite this version:**

Manolis Perrot, Florian Lemarié. Energetically consistent Eddy-Diffusivity Mass-Flux schemes for Atmospheric and Oceanic Convection. 2024. hal-04439113v1

**HAL Id: hal-04439113**

**<https://hal.science/hal-04439113v1>**

Preprint submitted on 5 Feb 2024 (v1), last revised 2 Aug 2024 (v3)

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# Energetically consistent Eddy-Diffusivity Mass-Flux schemes for Atmospheric and Oceanic Convection

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## Key Points:

- An Eddy-Diffusivity Mass-Flux parameterization is carefully derived from first principles, making the underlying assumptions explicit
- Closed energy budgets between resolved and subgrid energy reservoirs are outlined, including a new formulation of vertical TKE transport
- Comparisons with Large Eddy Simulations show that the new scheme successfully reproduces TKE and its vertical transport

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**Abstract**

This study aims to introduce a new convective vertical mixing scheme rooted in the Eddy-Diffusivity Mass-Flux (EDMF) approach, itself derived from first principles. The integration of the mass-flux (MF) concept with the Eddy-Diffusivity (ED) approach has long been studied and applied in global and regional atmospheric models for parameterizing convection, both dry and cloudy, and sees a growing interest in ocean models. This type of closure involves separating vertical turbulent fluxes into two components: a diffusion term that addresses local small-scale mixing in a near isotropic environment and a mass-flux transport term that accounts for the non-local transport due to vertically coherent plumes within the environment. Here, we exploit the multi-fluid averaging technique underlying the MF concept to propose an original formulation of a scheme that possesses properties not satisfied by most existing EDMF formulations. Consistent energy budgets between resolved and subgrid scales are derived for different multi-component fluids including seawater and dry atmosphere (in Boussinesq and anelastic cases). This guarantees that all mean kinetic, potential, and internal energy sinks and sources as long as turbulent kinetic energy (TKE) transport associated with EDMF terms are exactly added or subtracted to the TKE budget, effectively rectifying energy biases existing in prior EDMF schemes. Notably, this analysis facilitates a clear separation of convective and turbulent small-scale energy reservoirs. In addition to bulk energy transfers, we provide guidelines to avoid spurious energy fluxes at the fluid's boundary when using EDMF. We illustrate the performance of the proposed *energetically consistent EDMF scheme* in the context of oceanic convection. When compared with Large Eddy Simulations (LES) of oceanic convection, our scheme can reproduce mean fields as well as higher-order moments such as TKE, vertical fluxes, and turbulent transport of TKE. The energetic consistency is key to obtaining realistic TKE and turbulent transport of TKE profiles. To further illustrate that the MF concept is a credible alternative to the traditional approaches used in the oceanic context (using an enhanced vertical diffusion or a counter gradient term *à la* KPP) the proposed scheme is validated in a single-column configuration against observational data of oceanic convection from the LION buoy. Last but not least, during the theoretical development of the scheme, we maintain transparency regarding underlying assumptions and systematically assess their validity in the light of LES data.

**Plain Language Summary**

In Earth system models, various important processes occur on scales that are too fine to be resolved with usual grid resolutions. Parameterizations have to be used to approximate the average effect of such processes on the scales resolved by a numerical model. The general objective of the proposed work is to approach the parameterization problem for boundary-layer turbulence and convective plumes in a “consistent” manner. Here the notion of consistency integrates various aspects: global energetic consistency, consistency with a particular averaging technique for the scale-separation, and the rigorous reduction of a physical system to a scale-aware parametric representation based on well-identified and justifiable approximations and hypotheses. An originality is to jointly consider energy budgets including a subgrid energy reservoir on top of the resolved energies allowing the proper coupling between the parameterization and the resolved fluid dynamics. This research is fundamental to obtain an apt representation of mean fields and higher-order turbulent moments and to pave the way toward an alternative methodology to parameterize oceanic convection across scales. Numerical simulations demonstrate the adequacy of the proposed parameterization.

## 1 Introduction

### 1.1 Convection in the ocean and atmosphere and its parameterization in numerical models

Boundary layer convection occurs in the atmosphere and the ocean due to buoyancy fluxes at the surface, which trigger gravitational instabilities. Buoyant plumes then tend to overturn and mix the fluid. When looking at the mean properties of the fluid, it leads to the formation of a well-mixed layer. The accurate representation of such boundary layers is of paramount importance for short-term forecasts as well as for climate projections in the atmosphere (Bony et al., 2015; Schneider et al., 2017) and the ocean (Martin et al., 2013; Piron et al., 2016; Moore et al., 2015; Fox-Kemper et al., 2019). Regarding current computational capacities, plumes are still unresolved in regional and global numerical models, and thus their effects require parameterization. Moreover in ocean modeling, beyond the requirement in terms of grid resolution, hydrostatic equations used in the overwhelming majority of regional and global studies are not suitable for resolving convective phenomena explicitly (Marshall et al., 1997).

For any quantity  $X$ , standard turbulent mixing models are based on the closure of vertical turbulent fluxes  $\overline{w'X'}$  proportional to the local mean gradient in the form  $-K_X \partial_z \overline{X}$  (which corresponds to the so-called Eddy-Diffusivity (ED) closure). Such a closure leads to a diffusion of  $\overline{X}$ , which is often justified by considering that turbulent fluctuations resemble Brownian motion (Vallis, 2017; Resseguier et al., 2017). Although the ED closure has been widely used in many industrial and geophysical applications, it is known to potentially predict incorrectly higher order moments and even mean fields for complex flows (e.g. Schmitt, 2007). For instance, the inadequacy of ED closures for atmospheric convection has long been highlighted (Deardorff, 1966). Indeed fluctuations are carried by non-local structures, the buoyant plumes, that can be coherent over the whole mixed layer. In particular, in such a layer, mean gradients are close to zero ( $\partial_z \overline{X} \simeq 0$ ) while transport is ensured at leading order by non-zero vertical fluxes  $\overline{w'X'}$  which may even be up-gradient. Indeed, using the assumption of a mixed-layer  $\partial_z \overline{X} \simeq 0$  into a turbulent transport equation of the type  $\partial_t \overline{X} + \partial_z \overline{w'X'} = 0$  implies that  $\overline{w'X'}$  varies linearly with  $z$ . Such linear variation of fluxes in the mixed layer is well-supported by observations and numerical experiments (Garratt, 1994b; Denbo & Skyllingstad, 1996).

To circumvent ED hypothesis, Deardorff (1966) proposed to introduce a constant non-local term  $\gamma_X$  in the form  $\overline{w'X'} = -K_X(\partial_z \overline{X} - \gamma_X)$ . Later on, such a formulation has been refined, where both  $K_X$  and  $\gamma_X$  were prescribed by a self-similar profile function depending on external characteristics of the boundary layer such as surface forcing, stratification at the atmospheric top (or oceanic base) of the mixed layer and implicitly defined mixed layer height (see Troen and Mahrt (1986); Holtslag and Moeng (1991) for atmospheric models, Large et al. (1994) for oceanic models). This approach is still in use in some present-day ocean models (e.g. via the CVMIX library, Van Roekel et al., 2018). Furthermore, in the context of ocean models, two other types of convective parameterization are sometimes used: (i) a buoyancy sorting scheme (a.k.a. adjustment scheme or non-penetrative scheme), in which static instabilities are eliminated in one time-step by mixing downward neighboring vertical levels until a neutral buoyancy profile is attained (e.g. Madec et al., 1991) (ii) an enhanced eddy-viscosity scheme in which the vertical diffusivity coefficient is artificially increased to a high value as soon as static instabilities are found on the density profiles. These two approaches are not grounded on a physical derivation.

The present work builds on the combined Eddy-Diffusivity and Mass-Flux (EDMF) parameterization schemes (Hourdin et al., 2002; Soares et al., 2004). The ED component aims to represent turbulent transport in a nearly isotropic environment, in which convective plumes -modeled by MF terms- support a non-local advective transport. The MF concept was originally introduced in the atmospheric context to represent deep con-

vective clouds (Arakawa & Schubert, 1974), then it has been adapted to represent shallow and dry boundary layer convection in combination with ED schemes. It is intrinsically based on a multi-fluid averaging (Yano, 2014; Thuburn et al., 2018) of the fluid equations. In ocean models the EDMF concept has been first introduced by Giordani et al. (2020), and has been gaining increasing attention (e.g. Garanaik et al. (2024), or a recent implementation in Oceananigans, Ramadhan et al. (2020)).

## 1.2 Parameterization development and physics dynamics coupling

The general objective of the proposed work is to approach the parameterization problem in a “consistent” manner. Here the notion of consistency integrates various aspects: consistency with the laws of physics, energetic consistency at both continuous (e.g. Eden, 2016; Jansen et al., 2019; Eden & Olbers, 2014) and discrete (e.g. Burchard, 2002) levels, consistency with a particular choice of scale-separation operator (Higgins et al., 2013; Lauritzen et al., 2022), and the rigorous reduction of a physical system to a scale-aware parametric representation based on well-identified approximations and hypotheses (Honnert et al., 2016; Tan et al., 2018).

Regarding boundary layer parameterizations, eddy-diffusivity intensity often scales with the turbulent kinetic energy (TKE) which is computed via a parameterized prognostic equation. TKE represents a subgrid kinetic energy that exchanges energy with the resolved reservoirs. The use of mass-flux terms leads to energy transfers and redistributions that must be taken into account in the TKE equation to ensure energetic consistency between resolved and subgrid scales. In addition, the boundary conditions of the mass-flux equations must be consistent between ED and MF to avoid double-counting and artificial energy fluxes at the fluid boundary. Apart from a brief discussion in Tan et al. (2018) for unsteady plume models, the energetically consistent coupling of TKE and standard EDMF schemes has not been, to our knowledge, discussed in the literature. Some modifications of the TKE equation when using a mass-flux model have been proposed for the buoyancy production term (Witek et al., 2011b) and the vertical turbulent transport of TKE (Witek et al., 2011a; Han & Bretherton, 2019). However, these studies are not motivated by considerations of energetic consistency.

## 1.3 Goals and organisation of the paper

The aim of this paper is two-fold. First, we intend to provide an introductory, self-contained, and pedagogical derivation of EDMF schemes starting from first principles, to guide consistency considerations. Second, we derive theoretical energy budgets and provide guidelines to obtain energetically consistent EDMF models. Consequently, this paper is intended to both the oceanographic community as a pedagogical introduction to EDMF, and the atmospheric community seeking to reduce energy biases in EDMF models. The paper is organized as follows. In section 2, we expose the derivation of an EDMF scheme from first principle, systematically discuss the successive assumptions at stake, provide closures according to state-of-the-art practice, and discuss consistent boundary conditions. In section 3, we recall the theoretical resolved and subgrid energy budgets of a horizontally averaged Boussinesq fluid without closures. In section 4, we expose the necessary modification of the parameterized turbulent kinetic energy (TKE) equation to obtain closed energy budgets when using EDMF. Furthermore, we derive vertically averaged energy budgets to reveal the role of boundary conditions on the energy fluxes. In section 5, we analyze the assumptions used in the derivation of the scheme in light of data from Large Eddy Simulation (LES) of idealized oceanic deep convection. Then we evaluate the energetically consistent EDMF scheme against such data, and against realistic data of oceanic deep convection events in the Mediterranean Sea. In appendices, we provide discretization details for interested model developers and energy budgets in the anelastic setting which are more commonly used by the atmospheric community.

## 2 Derivation of EDMF scheme

### 2.1 Formal derivation

We start from the unaveraged Navier-Stokes equations under the Boussinesq assumption in a cubic domain  $L_x \times L_y \times H$ :

$$\nabla \cdot \mathbf{u} = 0 \quad (1)$$

$$\partial_t \mathbf{u} = -\nabla \cdot (\mathbf{u} \otimes \mathbf{u}) - \frac{1}{\rho_0} \nabla p^\dagger + b \mathbf{e}_z + \nu \nabla^2 \mathbf{u} \quad (2)$$

$$\partial_t \phi = -\nabla \cdot (\phi \mathbf{u}) + S_\phi \quad (3)$$

$$b = b_{\text{eos}}(\phi) \quad (4)$$

where  $\mathbf{u} = (u, v, w)$  denotes the velocity field in a local Cartesian frame of reference  $(\mathbf{e}_x, \mathbf{e}_y, \mathbf{e}_z)$ ,  $z$  ranges from 0 to  $H$  in the atmosphere and  $-H$  to 0 in the ocean,  $\rho_0$  is a constant reference density, the pressure has been decomposed as  $p = p_{\text{ref}}(z) + p^\dagger(x, y, z, t)$  with  $\partial_z p_{\text{ref}} = -\rho_0 g$ ,  $b$  is the buoyancy acceleration,  $\phi$  is any entropic variable describing each component of the fluid,  $S_\phi$  is an additional source term (typically molecular diffusion). For instance, in the context of a dry atmosphere modeled as an ideal gas, a simple choice<sup>1</sup> would be  $\phi = \theta$ , where  $\theta$  is the potential temperature, and  $b_{\text{eos}}(\theta) = g(\theta - \theta_0)/\theta_0$ . In the context of ocean dynamics, one would choose conservative temperature and salinity ( $\phi = \theta, S$ ) and a linear equation of state,  $b_{\text{eos}}(\theta, S) = g\alpha(\theta - \theta_0) - g\beta(S - S_0)$  where  $\alpha$  and  $\beta$  are thermal expansion and haline contraction coefficients, respectively, and  $\theta_0$  and  $S_0$  are reference temperature and salinity. Details on source terms  $S_\phi$  are given in section 3. For the sake of simplicity, we do not include the Coriolis term in the present study. Since the Coriolis force is energetically-neutral it does not interfere with the derivations made throughout this paper. Next, we explicit the framework in which vertical mixing parameterizations are usually developed. We adopt a semi-discrete approach, where the *horizontal* fluid domain is divided into a  $N_x \times N_y$  mesh. Each horizontal grid cell has length  $\Delta x_i$  and width  $\Delta y_j$ , and we denote  $(x_i, y_j)$  its center. Note that the time and vertical coordinates  $z$  are kept *continuous*. The spatial domain can be thought of  $N_x \times N_y$  vertical columns stacked together. In a numerical model discretized on such a mesh, the computed variables would be interpreted in a finite volume approach (LeVeque, 2002). For any field  $X = \mathbf{u}, \phi \dots$  one can define the following horizontal average and fluctuation

$$\overline{X}(x_i, y_j, z, t) := \frac{1}{\Delta x_i \Delta y_j} \int_{\Delta x_i \times \Delta y_j} X(x, y, z, t) dx dy, \quad X' = X - \overline{X}$$

If we recast (1)–(3) in the generic form  $\partial_t X + \nabla \cdot (\mathbf{u} X) = S_X$ , and then apply such a horizontal average, we obtain

$$\partial_t \overline{X} + \partial_z (\overline{wX} + \overline{w'X'}) + \frac{1}{\Delta x_i \Delta y_j} \oint_{\partial(\Delta x_i \times \Delta y_j)} X \mathbf{u}_h \cdot d\mathbf{n} = \overline{S_X} \quad (5)$$

where  $\mathbf{u}_h = (u, v, 0)$  denotes the horizontal velocity vector and  $d\mathbf{n}$  is an outward pointing line integral element, i.e.  $\mathbf{u}_h \cdot d\mathbf{n} = u dy - v dx$ . The boundary integral in (5) is the total (resolved and subgrid) horizontal flux of  $X$ . In a numerical model,  $\overline{X}$  would be interpreted as the resolved variable,  $X'$  would be an unresolved fluctuation, the precise form of the horizontal flux would depend on the numerical scheme (and possibly on parameterizations), and the vertical subgrid flux  $\overline{w'X'}$  has to be closed by a parameterization. When focusing on the parameterization of vertical mixing processes, it is common to conceptually isolate one vertical column of fluid to work with a one-dimensional Single-Column

<sup>1</sup> In both oceanic and atmospheric context, we use simple thermodynamic descriptions allowing convection. Although these descriptions are inaccurate for real-world applications, they are sufficient to expose how to build energetically consistent EDMF parameterizations. Energy budgets for the anelastic approximation can be found in Appendix E

197 Model (SCM) (e.g. Zhang et al., 2016). Any quantity is assumed statistically invariant  
 198 along the horizontal direction, meaning that in practice the horizontal fluxes and pres-  
 199 sure gradients are neglected. We further simplify the problem with two additional as-  
 200 sumptions: First, the bottom of the column is considered flat. Along with a non-penetration  
 201 condition, this leads to  $\bar{w}(z = 0) = 0$ . Now the averaged volume conservation under  
 202 the horizontal homogeneity  $\partial_z \bar{w} = 0$  implies that  $\bar{w}(z) = 0$  at any level  $z$ . Second, in  
 203 the vertical momentum budget, the momentum flux divergence  $\partial_z \overline{w'w'}$  is neglected, lead-  
 204 ing to the hydrostatic approximation  $\partial_z \bar{p}^\dagger = b$ . The SCM equations are then

$$\partial_t \bar{\mathbf{u}}_h = -\partial_z \overline{w' \mathbf{u}'_h} \quad (6)$$

$$\partial_t \bar{\phi} = -\partial_z \overline{w' \phi'} + \bar{S}_\phi \quad (7)$$

205 where the molecular viscosity can be safely neglected in the mean momentum budget.  
 206 The remainder of this article will use these SCM assumptions, and indices  $i, j$  will be dropped.  
 207 For readers interested in the inclusion of horizontal fluxes, we refer them to Yano (2014)  
 208 and Tan et al. (2018). As an alternative to the semi-discrete description presented above,  
 209 a fully continuous description can be carried out by replacing the horizontal average by  
 210 smoothing kernels on the scale of the grid size (see for example Thuburn et al. (2018)  
 211 in the context of mass-flux schemes).

212 We now *assume* a formal decomposition of the horizontal column area  $\Delta x \times \Delta y$   
 213 into two horizontal subdomains of areas  $\mathcal{A}_e(z, t)$  and  $\mathcal{A}_p(z, t)$  which also depend on depth  
 214 and time. Such decomposition is meant to isolate the coherent convective structures usu-  
 215 ally referred to as *plumes* (occupying the subdomain of area  $\mathcal{A}_p(z, t)$ ) from the rest of  
 216 the flow, referred to as the *environment* (occupying the subdomain of area  $\mathcal{A}_e(z, t)$ ). We  
 217 introduce the following notations to characterize the subdomain averaged field and *frac-*  
 218 *tional* area (for  $i = e, p$ ):

$$X_i = \frac{1}{\mathcal{A}_i(z, t)} \int_{\mathcal{A}_i(z, t)} X(x, y, z, t) dx dy$$

$$a_i = \mathcal{A}_i(z, t) / (\Delta x \times \Delta y)$$

219 Any mean field can then be decomposed as

$$\bar{X} = a_e X_e + a_p X_p$$

220 In particular, when  $X \equiv 1$  we get the constraint  $a_e = 1 - a_p$ . After some algebra, any  
 221 turbulent flux can be recast as

$$\overline{w'X'} = a_e \overline{w'_e X'_e} + a_p \overline{w'_p X'_p} + a_e (w_e - \bar{w})(X_e - \bar{X}) + a_p (w_p - \bar{w})(X_p - \bar{X}) \quad (8)$$

222 where

$$\overline{w'_i X'_i} = \frac{1}{\mathcal{A}_i(z, t)} \int_{\mathcal{A}_i(z, t)} (X - X_i)(w - w_i) dx dy$$

223 For each subdomain, the  $a_i(w_i - \bar{w})(X_i - \bar{X})$  terms in (8) account for the "mass-flux"  
 224 (i.e. the contribution of coherent structures to the flux), whereas the  $a_i \overline{w'_i X'_i}$  terms are  
 225 a contribution from internal variability. Applying the subdomain average to any conser-  
 226 vation law of the form  $\partial_t X + \nabla \cdot (\mathbf{u}X) = S_X$  and using Reynolds transport theorem  
 227 leads to (see appendix A of Tan et al. (2018) and Yano (2014) for full derivation)

$$\partial_t (a_i X_i) + \partial_z \left( a_i w_i X_i + a_i \overline{w'_i X'_i} \right) + \frac{1}{\mathcal{A}_i} \oint_{\partial \mathcal{A}_i} X \mathbf{u}_r \cdot d\mathbf{n} = a_i S_{X,i} \quad (9)$$

228 where the relative horizontal boundary velocity is  $\mathbf{u}_r = \mathbf{u}_h - \partial_t \mathbf{r}_b - w \partial_z \mathbf{r}_b$  and  $\mathbf{r}_b =$   
 229  $(x_b(z, t), y_b(z, t))$  is the position vector of boundary elements. The three terms that con-  
 230 stitute  $\mathbf{u}_r$  indicate that boundary fluxes can arise respectively due to horizontal veloc-  
 231 ity across the boundary, to (apparent) horizontal velocity of the boundary, or to verti-  
 232 cal velocity if the boundary of the 3D plume is vertically tilted (i.e.  $\partial_z \mathbf{r}_b \neq 0$ ).



233 **2.2 Standard assumptions**

234 **2.2.1 Plume-Environment decomposition**

235 The first standard assumption we have already made is to consider only two sub-  
 236 domains, the convective plume and the environment. This is justified since in convec-  
 237 tive situations the main contribution to the fluxes comes from the plumes. However, the  
 238 framework is flexible enough to incorporate an arbitrary number of components. In par-  
 239 ticular, several studies of the atmospheric convective boundary layer (CBL) underline  
 240 the importance of returning coherent structures around the plumes, often referred to as  
 241 CBL downdrafts (Schmidt & Schumann, 1989; Couvreux et al., 2007; Brient et al., 2023).

242 **2.2.2 Entrainment/Detrainment and Upstream approximation**

243 Net fluid exchange at the horizontal boundary of the plume domain can be further  
 244 decomposed into fluid *entrained* into the plume from the environment, and fluid *detrained*  
 245 out of the plume into the environment, namely

$$\begin{aligned} \frac{1}{\mathcal{A}_p} \oint_{\partial\mathcal{A}_p} \mathbf{u}_r \cdot d\mathbf{n} &= \frac{1}{\mathcal{A}_p} \oint_{\partial\mathcal{A}_p, \mathbf{u}_r \cdot d\mathbf{n} > 0} \mathbf{u}_r \cdot d\mathbf{n} + \frac{1}{\mathcal{A}_p} \oint_{\partial\mathcal{A}_p, \mathbf{u}_r \cdot d\mathbf{n} < 0} \mathbf{u}_r \cdot d\mathbf{n} \\ &= D - E \end{aligned}$$

246 where  $E(> 0)$  is called *entrainment rate* and  $D(> 0)$  is called *detrainment rate*. We fur-  
 247 ther assume that the value of  $X$  at the boundary is either equal to the mean value in  
 248 the environment when entrainment is occurring, or the mean value in the plume when  
 249 detrainment is occurring. This is the so-called *upstream approximation*, formulated as<sup>2</sup>

$$\frac{1}{\mathcal{A}_p} \oint_{\partial\mathcal{A}_p} X \mathbf{u}_r \cdot d\mathbf{n} = X_e E - X_p D \quad (10)$$

250 As a result of this approximation, the plume equation reads

$$\partial_t(a_p X_p) + \partial_z(a_p w_p X_p) = -\partial_z(a_p \overline{w'_p X'_p}) + E X_e - D X_p + a_p S_{X,p} \quad (11)$$

251 In particular when  $X \equiv 1$ , we get the plume area conservation equation:

$$\partial_t a_p + \partial_z(a_p w_p) = E - D \quad (12)$$

252 **2.2.3 Steady plume hypothesis**

253 A common hypothesis is that the plume domain is in a quasi-steady regime, thus  
 254 neglecting the temporal tendency compared to vertical advection. The relevance of this  
 255 hypothesis is numerically tested using idealized cases in section 5.3. An *a priori* scal-  
 256 ing estimation can also be performed. Introducing  $\tau$ ,  $h$ , and  $W$  the characteristic time,  
 257 depth, and vertical velocity scales of the plume, the order of magnitude of the ratio be-  
 258 tween the temporal tendency and vertical advection can be estimated as follows

$$O\left(\frac{\partial_t(a_p X_p)}{\partial_z(a_p w_p X_p)}\right) = \frac{h/\tau}{W} \simeq \frac{w_{\text{ent}}}{W} \quad (13)$$

259 where  $w_{\text{ent}} = \frac{d}{dt}h$  is the boundary layer vertical entrainment velocity. In the limit of  
 260 free convection triggered by a surface buoyancy loss  $B_0 < 0$  into a fluid of constant strat-  
 261 ification  $N_0^2$ , the classical convective scalings  $h \propto \sqrt{-B_0/N_0^2 t}$  and  $W = (-B_0 h)^{1/3}$   
 262 (Turner, 1979; Deardorff, 1970) lead to

$$\frac{w_{\text{ent}}}{W} \propto \frac{1}{(N_0 t)^{2/3}} \quad (14)$$

---

<sup>2</sup> In the context of 3D models, the plume boundary  $\partial\mathcal{A}_p$  can cross the horizontal boundary of the grid cell. The corresponding contribution to the integral can be interpreted as a resolved flux divergence across the grid cell, namely  $\nabla_h \cdot (a_p \mathbf{u}_{h,p} X_p + a_p \overline{\mathbf{u}'_{h,p} X'_p})$  (see section 5.1 of Yano (2014)).



263 In a different context, that of the development of a shear-driven mixed layer forced by  
 264 surface wind stress  $\rho_0 u_*^2$ , Kato and Phillips (1969) showed that  $w_{\text{ent}}/u_* \propto u_*^2/N_0^2 h$ . In  
 265 such a layer  $W \simeq u_*$ , leading to a scaling similar to (14). These scalings suggest that  
 266 as long as the surface forcings (represented here by  $u_*$  and  $B_0$ ) are evolving slowly com-  
 267 pared to  $1/N_0$ , the steady plume hypothesis remains valid. Under such a hypothesis, the  
 268 plume equation for any field  $X$  now reads

$$\partial_z(a_p w_p X_p) = -\partial_z(a_p \overline{w'_p X'_p}) + E X_e - D X_p + a_p S_{X,p} \quad (15)$$

269 As a summary, we rewrite the coupled resolved/plume system in an advective form us-  
 270 ing area conservation and  $\overline{X} = (1 - a_p)X_e + a_p X_p$ :

$$\partial_t \overline{X} = -\partial_z \overline{w' X'} + \overline{S}_X \quad (16)$$

$$\overline{w' X'} = \frac{1}{1 - a_p} a_p w_p (X_p - \overline{X}) + (1 - a_p) \overline{w'_e X'_e} + a_p \overline{w'_p X'_p} \quad (17)$$

$$a_p w_p \partial_z X_p = -\frac{1}{1 - a_p} E (X_p - \overline{X}) - \partial_z(a_p \overline{w'_p X'_p}) + a_p S_{X,p} \quad (18)$$

271 Several authors have recently proposed to relax the steady plume hypothesis (Tan et al.,  
 272 2018; Thuburn et al., 2018). However, the overwhelming majority of mass flux schemes  
 273 implemented in realistic models considers a plume domain in a quasi-steady regime.

#### 274 2.2.4 Small area limit

275 A last standard hypothesis is that the fractional area of the plume is *small* com-  
 276 pared to that of the environment (see section 5.3 for a direct evaluation against LES).  
 277 This generally means considering the formal limit  $a_p \rightarrow 0$  and  $a_e \rightarrow 1$  in the previous  
 278 equations while keeping non-zero mass-flux  $a_p w_p$  and source terms. Yano (2014) proposes  
 279 to assume  $a_p w_p = O(w_e)$  and  $a_p S_{X,p} = O(S_{X,e})$  to retain an order one contribution  
 280 of  $a_p w_p (X_p - \overline{X})$  in (17), and to keep an order one contribution of advection and forc-  
 281 ings in (18). In the small area limit, any environmental field  $X_e$  (except  $w_e$ ) can be ap-  
 282 proximated by the mean field, the vertical turbulent flux (17) becomes

$$\overline{w' X'} = a_p w_p (X_p - \overline{X}) + \overline{w'_e X'_e} \quad (19)$$

283 and the plume equation (18) now reads

$$a_p w_p \partial_z X_p = -E (X_p - \overline{X}) + a_p S_{X,p} \quad (20)$$

284 In the remainder of this study, we will adopt such a small area limit. Noteworthy is the  
 285 effort by some authors to relax this hypothesis to explore the "grey zone" of atmospheric  
 286 turbulence or to devise scale-aware parameterization schemes when the grid is refined  
 287 to the point where  $a_p$  is no longer small (Honnert et al., 2016; Tan et al., 2018). For the  
 288 sake of completeness, we include in Appendix A the system of plume equations obtained  
 289 when relaxing the small area limit while still neglecting subplume fluxes  $\overline{w'_p X'_p}$  (in line  
 290 with Tan et al. (2018)). This system only deviates by factors  $1/(1 - a_p)$  from the "small-  
 291 area" system, making it simple to implement in practice.

292 *Remark:* To our knowledge, the interplay between the small area limit and the steady  
 293 plume hypothesis has been only discussed in Yano (2014) where the author argues that  
 294 the formal limit  $a_p \rightarrow 0$  implies  $\partial_t(a_e X_e) \rightarrow \partial_t \overline{X}$ , and thus recovers the steady-plume  
 295 hypothesis  $\partial_t(a_p X_p) \rightarrow 0$  using (8). Using such formal limit and  $a_p w_p = O(w_e)$  im-  
 296 plies that  $w_p \rightarrow \infty$ . Since plume properties are advected by  $w_p$ , such infinite velocity  
 297 assumption is interpreted as an instantaneous adjustment to any surface perturbation,  
 298 consistently with the steady-plume hypothesis. Using Yano's scaling, an estimate of the  
 299 ratio between temporal tendency and vertical advection is now

$$O\left(\frac{\partial_t(a_p X_p)}{\partial_z(a_p w_p X_p)}\right) = \frac{O(a_p)/\tau}{w_e/h} \rightarrow 0 \text{ if } a_p \rightarrow 0$$

which shows that such scaling indeed implies stationarity. However, the alternative scaling we proposed in (13) decouples the small area limit from the stationarity assumption and is found to be validated in numerical simulations (see 5.3). Moreover, our scaling analysis seems more general since it merely takes into account scales for each field, without further assumptions, and thus justifies the potential use of stationary equations while relaxing the small area assumption.

### 2.3 Standard Closures

Thanks to the assumptions made so far, we have arrived at equations of the general form (20) for the plume, and (19) for vertical turbulent fluxes. At this stage, additional closure assumptions are required to express the entrainment and detrainment rates, the flux  $\overline{w'_e X'_e}$ , and the pressure gradients appearing in the  $S_{w,p}$  and  $S_{u_h,p}$  terms.

#### 2.3.1 Plume vertical pressure gradient

Plume vertical pressure gradients are usually parameterized as the combination of a virtual mass term (e.g. Bretherton et al., 2004) – representing the reduction of plume buoyancy due to pushing and pulling on the environment –, a reduced entrainment term and a quadratic drag term. Several formulations have been proposed (see Roode et al. (2012) for an intercomparison in the context of shallow cumulus convection). In line with usual practices in the atmospheric context (e.g. Pergaud et al., 2009; Rio et al., 2010) we consider

$$a_p \left( \frac{1}{\rho_0} \partial_z p^\dagger \right)_p = (a-1)a_p B_p + (b-1)(-E w_p) + b' a_p w_p^2 \quad (21)$$

leading to the plume vertical momentum budget

$$a_p w_p \partial_z w_p = a a_p B_p - b E w_p - \sigma_o^a b' a_p w_p^2 \quad (22)$$

where  $a$ ,  $b$  and  $b'$  are positive parameters,  $\sigma_o^a = +1$  in the atmosphere and  $-1$  in the ocean, and  $B_p = b_p - \bar{b}$ . Note that in the case of dry atmosphere or seawater with a linearized equation of state, we have  $b_p - \bar{b} = b_{\text{eos}}(\phi_p) - b_{\text{eos}}(\bar{\phi})$ .

#### 2.3.2 Horizontal momentum budget

Based on the work of Rotunno and Klemp (1982) and Wu and Yanai (1994), Gregory et al. (1997) proposed a parameterization of the plume horizontal pressure gradient as an advective correction of the form

$$a_p \left( \frac{1}{\rho_0} \nabla_h p^\dagger \right)_p = a_p w_p C_u \partial_z \bar{u}_h \quad (23)$$

where  $C_u$  is a parameter. We show in Section 4.5 that energy constraints impose  $0 \leq C_u < 1$ .

#### 2.3.3 Eddy-Diffusivity closure

The environment is thought of as a subdomain where only small-scale turbulence occurs, thus supporting the hypothesis of a closure of the vertical flux with an eddy-diffusivity,  $\overline{w'_e X'_e} = -K_X \partial_z X_e \underset{a_p \ll 1}{\simeq} -K_X \partial_z \bar{X}$ . This leads to the eddy-diffusivity mass-flux closure of subgrid fluxes

$$\overline{w' X'} = \underbrace{-K_X \partial_z \bar{X}}_{\text{ED}} + \underbrace{a_p w_p (X_p - \bar{X})}_{\text{MF}} \quad (24)$$

In the present study, the eddy viscosity  $K_u$  and diffusivity  $K_\phi$  in turbulent vertical fluxes are computed from a turbulence closure model based on a prognostic equation for the

336 turbulent kinetic energy (TKE)  $k = \overline{\mathbf{u}' \cdot \mathbf{u}'}/2$  and a diagnostic computation of appropriate  
 337 length scales (a.k.a. 1.5-order turbulence closure). For the numerical tests in the  
 338 oceanic context presented in Sec. 5, we use a formulation close to that of the Nucleus  
 339 for European Modelling of the Ocean model (NEMO, Madec et al., 2019). The eddy-  
 340 viscosity and diffusivity are classically assumed to be related to TKE by

$$\begin{aligned} K_u &= c_m l_m \sqrt{k} \\ K_\phi &= K_u (\text{Pr}_t)^{-1} \end{aligned}$$

341 with  $l_m$  a mixing length scale,  $\text{Pr}_t$  the non-dimensional turbulent Prandtl number, and  
 342  $c_m$  is a constant (further details on the computations of these quantities are given in Ap-  
 343 pendix B). Details of the prognostic equation for  $k$ , in connection with energetic con-  
 344 sistency requirements, are given in Sec. 3. We acknowledge that since ED represents tur-  
 345 bulance in the environment, one should use the environmental TKE  $1/2\overline{\mathbf{u}'_e \cdot \mathbf{u}'_e}$  instead  
 346 as it is done in Tan et al. (2018). Although no significant effect could be seen in prelim-  
 347 inary idealized numerical tests, this point should be further explored.

### 348 **2.3.4 Entrainment and detrainment closures**

349 Entrainment and detrainment closures are still a topic of extensive research in the  
 350 atmospheric modeling community. One difficulty is that a given closure can only be spe-  
 351 cific to a certain type of convection (de Rooy et al., 2013). To close entrainment and de-  
 352 trainment rates<sup>3</sup>, we adapt the formulation proposed by Rio et al. (2010), namely

$$E = a_p \beta_1 \max(0, \partial_z w_p) \quad (25)$$

$$D = -a_p \beta_2 \min(0, \partial_z w_p) + \sigma_o^a a_p w_p \delta_0 \quad (26)$$

353 where the two parameters  $\beta_1$  and  $\beta_2$  are positive,  $\delta_0$  is a positive minimum detrainment.  
 354 In order to guarantee  $0 \leq a_p \leq 1$ , it is sufficient to impose  $0 \leq \beta_1 \leq 1$  and  $1 \leq \beta_2 <$   
 355  $2$  (see Appendix F).

356 To summarize the formal derivation made so far, the closure of fluxes and associ-  
 357 ated plume equations of the resulting EDMF scheme are provided in Tab. 1.

## 358 **2.4 Consistent boundary conditions for mean and plume equations**

### 359 **2.4.1 General concepts**

360 Under the aforementioned assumptions, the budget equations governing plume quan-  
 361 tities simplify into a system of non-linear first-order ordinary differential equations with  
 362 respect to the variable  $z$ . Accordingly, a single boundary condition at  $z = 0$  (i.e., the  
 363 top of the water column or the bottom of the air column depending on the fluid under  
 364 consideration) is sufficient for the computation of plume variables. At the boundary  $z =$   
 365  $0$ , consistent boundary conditions for the plume variable  $X_p$  and the mean variable  $\overline{X}$   
 366 must comply with the EDMF flux decomposition (24)

$$\overline{w'X'}(0) = -K_X \partial_z \overline{X}(0) + a_p(0)w_p(0)(X_p(0) - \overline{X}(0)) \quad (27)$$

367 Such a constraint should guide modeling choices concerning boundary conditions. In-  
 368 deed, it systematically guarantees the correct partition of surface fluxes, and thus avoids  
 369 double-counting biases linked to non-physical energy sources/sinks at the boundary (see  
 370 Sec. 4.5). For instance, suppose the values of  $\overline{w'X'}(0)$ ,  $a_p(0)$ ,  $w_p(0)$  and  $X_p(0)$  are jointly

---

<sup>3</sup>In the literature, closures are usually provided for *fractional* entrainment and detrainment rates, re-  
 spectively  $\epsilon = E/(\sigma_o^a a_p w_p)$  and  $\delta = D/(\sigma_o^a a_p w_p)$ , where  $-a_p w_p$  is the oceanic mass-flux and  $+a_p w_p$  is the  
 atmospheric mass-flux.

$\frac{\overline{w'\phi'}}{\overline{w'\mathbf{u}'_h}} = a_p w_p (\phi_p - \bar{\phi}) - K_\phi \partial_z \bar{\phi}$	Vertical turbulent flux for component $\phi$
$\frac{\overline{w'\mathbf{u}'_h}}{\overline{w'\mathbf{u}'_h}} = a_p w_p (\mathbf{u}_{h,p} - \bar{\mathbf{u}}_h) - K_u \partial_z \bar{\mathbf{u}}_h$	Vertical turbulent momentum flux
$\partial_z(a_p w_p) = E - D$	Plume area conservation equation
$a_p w_p \partial_z \phi_p = E(\bar{\phi} - \phi_p)$	Plume equation for component $\phi$
$a_p w_p \partial_z \mathbf{u}_{h,p} = E(\bar{\mathbf{u}}_h - \mathbf{u}_{h,p}) + a_p w_p C_u \partial_z \bar{\mathbf{u}}_h$	Plume horizontal momentum equation
$a_p w_p \partial_z w_p = -bE w_p + a_p \{aB_p - \sigma_o^a b'(w_p)^2\}$	Plume vertical velocity equation
$B_p = b_{\text{eos}}(\phi_p) - b_{\text{eos}}(\bar{\phi})$	Buoyancy forcing term
$K_u = c_m l_m \sqrt{k}$	Eddy-viscosity
$K_\phi = K_u (\text{Pr}_t)^{-1}$	Eddy-diffusivity

Table 1: Summary of the vertical turbulent flux formulation and plume equations in the small area limit under the steady plume hypothesis detailed in sections 2.1, 2.2 and 2.3. The mean terms quantities  $\bar{\mathbf{u}}_h$  and  $\bar{\phi}$  are the prognostic variables of the model and the equation for  $k$  is given in Sec. 4 and in Tab. 2.

371 specified. Then (27) would turn into a Robin (a.k.a type 3) boundary condition for the  
 372  $\bar{X}$  equation which arises naturally in advection-diffusion equations (e.g. Hahn and Özişik  
 373 (2012), chapter 1-5). At the boundary  $z = \sigma_o^a H$ , a no-flux condition is imposed for the  
 374 mean equation. For the specific case of oceanic convection reaching the ocean bottom,  
 375 a possibility is to add a penalization term to ensure the condition  $w_p(z = -H) = 0$ .

#### 376 2.4.2 Oceanic context

377 For oceanographic applications, we consider that a surface flux  $\overline{w'X'}(0)$  is prescribed.  
 378 The mass flux component becomes non-zero close to the surface as soon as the entrain-  
 379 ment rate (25) is itself non-zero. In this case the conservation of volume reads

$$\partial_z(a_p w_p) = a_p w_p \left( \beta_1 \frac{1}{w_p} \partial_z w_p + \delta_0 \right)$$

380 which can be easily integrated vertically to obtain

$$a_p(z)w_p(z) = (a_p(0)w_p(0)) \left( e^{\delta_0 z} \left( \frac{w_p(z)}{w_p(0)} \right)^{\beta_1} \right)$$

381 As  $\beta_1 < 1$ , non-trivial solutions are obtained if and only if non-zero boundary values  
 382 for  $a_p$  and  $w_p$  are chosen. In the remainder, we adopt the following simple choice,

$$X_p(0) = \bar{X}(0), \quad a_p(0) = a_p^0, \quad w_p(0) = w_p^0$$

383 where  $a_p^0$  and  $w_p^0$  are parameters. According to (27), it implies that all the surface flux  
 384 is allocated in the ED component, as advocated by Tan et al. (2018). This particular choice  
 385 of boundary condition is also motivated by the fact that it implies at the discrete level  
 386 that convection is triggered as soon as the surface Brünt-Väisälä frequency  $\partial_z b(0)$  is neg-  
 387 ative (see Appendix F for further details). As a result, (27) turns into the Neumann bound-  
 388 ary condition  $-K_X \partial_z X(0) = \overline{w'X'}(0)$ , which is standard practice for ED-only closures.

389 Alternatively, Soares et al. (2004) proposed that close to the surface, the plume/mean  
 390 buoyancy difference  $B_p$  should depend on the surface buoyancy flux, leading to

$$b_p(z) = \bar{b}(z) + \beta \frac{\overline{w'b'}(0)}{\sqrt{k}(z)} \quad (28)$$

391 where  $\beta$  is a constant. We show in Appendix C that our formulation is in fact equiva-  
 392 lent to (28) for if  $\beta = z/(c_b l_b(0))$  and  $k(z) \simeq k(0)$ . However, when using this type of  
 393 boundary condition exactly at the surface (as in Pergaud et al., 2009), special attention  
 394 must be paid when providing the ED flux, since the EDMF decomposition (27) imposes

$$-K_b(0)\partial_z \bar{b}(0) = \left(1 - \frac{a_p(0)w_p(0)\beta}{\sqrt{k(0)}}\right) \overline{w'b'(0)}$$

395 which is different from the standard Neumann condition used for ED-only closures.

### 396 **2.4.3 Atmospheric context: consistency with Monin-Obukhov theory**

397 For atmospheric applications, boundary conditions for the mean variables are com-  
 398 monly imposed using Monin-Obukhov similarity theory (MOST), which assumes that  
 399 in a surface layer located between  $z = 0$  and  $z = z_1$  fluxes are constant, and mean vari-  
 400 ables obey a quasi-logarithmic profile. To properly include a surface layer obeying MOST,  
 401 then the EDMF flux decomposition must be imposed at the new model boundary  $z =$   
 402  $z_1$ , namely

$$\overline{w'X'}(z_1) = -K_X(z_1)\partial_z \bar{X}(z_1) + a_p(z_1)w_p(z_1)(X_p(z_1) - \bar{X}(z_1)) \quad (29)$$

403 At this stage, we can point the following ambiguity. When the MF term is non-zero, it  
 404 is not clear whether the flux arising from MOST – which is an ED flux – should be al-  
 405 located to the ED term  $-K_X(z_1)\partial_z \bar{X}(z_1)$ , or to the total flux  $\overline{w'X'}(z_1)$  using the con-  
 406 stant flux assumption. Although not discussed transparently, it seems that the second  
 407 option is a common practice. However, in such a case, special attention would be required  
 408 to compute the total flux entering in energy budget computations.

409 Although beyond the scope of this article, we would like to point out that MOST is known  
 410 to fail in strongly unstable conditions (Johansson et al., 2001; Li et al., 2018). Recently,  
 411 Li et al. (2021) proposed corrections to formulate departure from MOST in the form of  
 412 an EDMF closure including updraft *and* downdraft contributions. This approach could  
 413 potentially help provide physically consistent boundary conditions to EDMF models.

414 At this stage, we have provided all the elements and underlying assumptions re-  
 415 quired to formulate an EDMF-type scheme (see Appendix F for the discretization as-  
 416 pects). Before studying the energetic impacts of using MF components, we derive the-  
 417oretical horizontally averaged energy budgets.

## 418 **3 Horizontally Averaged Energy budgets**

419 The total specific energy  $E_{\text{tot}}$  of the fluid is the sum of the mean kinetic energy  $E_k =$   
 420  $(\bar{\mathbf{u}}_h \cdot \bar{\mathbf{u}}_h)/2$ , the turbulent kinetic energy  $k = (\overline{\mathbf{u}' \cdot \mathbf{u}'})/2$ , the potential energy  $E_p = gz$   
 421 and the mean internal energy  $E_i$ . In the following sections, we recall the expression of  
 422 these energy reservoirs under the Boussinesq approximation, and we derive budgets for  
 423 each of these reservoirs, regardless of flux parameterization. For completeness, energy bud-  
 424 gets for anelastic models of dry atmosphere are derived in Appendix E.

### 425 **3.1 Kinetic energies**

426 Under the SCM assumptions exposed in Sec. 2.1, we can derive budgets for the re-  
 427 solved kinetic energy  $E_k$  and the turbulent kinetic energy  $k$ :

$$\partial_t E_k + \partial_z T_{E_k} = \overline{w'\mathbf{u}'_h} \cdot \partial_z \bar{\mathbf{u}}_h \quad (30)$$

$$\partial_t k + \partial_z T_k = -\overline{w'\mathbf{u}'_h} \cdot \partial_z \bar{\mathbf{u}}_h + \overline{w'b'} - \bar{\epsilon}_\nu \quad (31)$$

428 where  $\bar{\epsilon}_\nu = \overline{\nu \partial_z \mathbf{u}' \cdot \partial_z \mathbf{u}'}$  is the viscous dissipation of energy, whereas  $T_{E_k} = \overline{w'\mathbf{u}'_h} \cdot \bar{\mathbf{u}}_h$   
 429 and  $T_k = \overline{w' \frac{\mathbf{u}' \cdot \mathbf{u}'}{2}} + \frac{1}{\rho_0} \overline{w'p'}$  redistribute energy on the vertical. Exchanges be-  
 430 tween the resolved and subgrid reservoirs of kinetic energy are done via the mechanical

431 shear term  $\overline{w'\mathbf{u}'_h \cdot \partial_z \bar{\mathbf{u}}_h}$ . To close the budgets, we provide in the following sections a bud-  
 432 get for internal and potential energy.

### 433 3.2 Internal and Potential energies

434 For a generic fluid, the unaveraged specific internal energy can be written as

$$\mathcal{E}_i = \mathcal{h}(p, \phi) - \frac{p}{\rho} \quad (32)$$

435 where  $\mathcal{h}$  is the specific enthalpy and  $\phi$  is any entropic variable describing components  
 436 of the fluid. Under the Boussinesq approximation, internal energy is (Tailleux & Dubos,  
 437 2023)

$$\mathcal{E}_i = \mathcal{h}(p_0, \phi) + (p_{\text{ref}} - p_0) \partial_p \mathcal{h}(p_0, \phi) - \frac{p_{\text{ref}}}{\rho_0} \quad (33)$$

438 where we recall that  $p_{\text{ref}}(z) = -\rho_0 g z + p_0$ , and the specific volume is by definition  $1/\rho :=$   
 439  $\partial_p \mathcal{h}$ . In particular, this implies that under the Boussinesq approximation  $b(\phi) := -g(\rho(p_0, \phi) -$   
 440  $\rho_0)/\rho(p_0, \phi)$  (e.g. sec. 3.4 of Eldred & Gay-Balmaz, 2021). The sum of unaveraged in-  
 441 ternal and potential energies can then be written as

$$\mathcal{E}_i + E_p = z(g - b) + \mathcal{h}(p_0, \phi) - \frac{p_0}{\rho_0} \quad (34)$$

442 which leads to the unaveraged budget (Young, 2010; Tailleux, 2012)

$$\partial_t(\mathcal{E}_i + E_p) + \nabla \cdot ((\mathcal{h}(p_0, \phi) + gz) \mathbf{u}) = \epsilon_\nu - wb \quad (35)$$

443 Upon averaging and using the SCM assumptions, the budget of mean internal energy  
 444  $E_i = \bar{\mathcal{E}}_i$  and potential energy reads

$$\partial_t(E_i + E_p) + \partial_z(\overline{\partial_\phi \mathcal{h}_0} \overline{w' \phi'}) = \bar{\epsilon}_\nu - \partial_z(\overline{\phi} \overline{w' \partial_\phi \mathcal{h}'_0} + \overline{\phi' w' \partial_\phi \mathcal{h}'_0}) - \overline{w' b'} \quad (36)$$

445 where we introduced the notation  $\mathcal{h}_0(\phi) := \mathcal{h}(p_0, \phi)$ . Remark that if  $\mathcal{h}(p_0, \phi)$  is linear  
 446 in  $\phi$ , we have closed relations  $\overline{\mathcal{h}(p_0, \phi)} = \mathcal{h}(p_0, \bar{\phi})$  and  $\overline{b(\phi)} = b(\bar{\phi})$ .

447 As a summary, the budgets of mean kinetic energy, turbulent kinetic energy and  
 448 the sum of mean internal and potential energy are

$$\begin{cases} \partial_t E_k + \partial_z T_{E_k} & = \overline{w' \mathbf{u}'_h \cdot \partial_z \bar{\mathbf{u}}_h} \\ \partial_t k + \partial_z T_k & = -\overline{w' \mathbf{u}'_h \cdot \partial_z \bar{\mathbf{u}}_h} + \overline{w' b'} - \bar{\epsilon}_\nu \\ \partial_t(E_i + E_p) + \partial_z(\overline{\partial_\phi \mathcal{h}_0} \overline{w' \phi'}) & = -\partial_z(\overline{\phi} \overline{w' \partial_\phi \mathcal{h}'_0} + \overline{\phi' w' \partial_\phi \mathcal{h}'_0}) - \overline{w' b'} + \bar{\epsilon}_\nu \end{cases} \quad (37)$$

449 where conversion of  $E_k$  into  $k$  occurs via mean shear, conversion of  $k$  into  $E_i$  occurs via  
 450 viscous dissipation, and conversion of  $k$  into  $E_i + E_p$  occurs via buoyancy fluxes.

451 In the following, we illustrate these budgets for dry atmosphere and seawater.

#### 452 3.2.1 Dry atmosphere

453 The specific enthalpy for a dry atmosphere modeled as an ideal gas  $p = \rho R_d T$  is

$$\mathcal{h}(p, \theta) = c_p \left( \frac{p}{p_0} \right)^{R_d/c_p} \theta \quad (38)$$

454 which is linear in the potential temperature  $\theta = T(p/p_0)^{-R_d/c_p}$ . Using (33) the sum  
 455 of mean internal and potential energy within the Boussinesq approximation is

$$E_i + E_p = \left( c_p - \frac{gz}{\theta_0} \right) \bar{\theta} + 2gz - \frac{p_0}{\rho_0} \quad (39)$$

456 and buoyancy is  $b(\bar{\theta}) = g(\bar{\theta} - \theta_0)/\theta_0$ . The budget of  $E_i + E_p$  is

$$\partial_t(E_i + E_p) = \left(c_p - \frac{gz}{\theta_0}\right) \partial_t \bar{\theta} = \bar{\epsilon}_\nu - \partial_z \left(c_p \frac{\theta_0}{g} \overline{w'b'}\right) - \overline{w'b'} \quad (40)$$

457 where  $\overline{w'b'} = \frac{g}{\theta_0} \overline{w'\theta'}$ . As a summary, the budgets of mean kinetic energy, turbulent ki-  
458 netic energy and the sum of mean internal and potential energy for a *dry atmosphere* within  
459 the Boussinesq approximation are

$$\begin{cases} \partial_t E_k + \partial_z T_{E_k} & = \overline{w'\mathbf{u}'_h} \cdot \partial_z \bar{\mathbf{u}}_h \\ \partial_t k + \partial_z T_k & = -\overline{w'\mathbf{u}'_h} \cdot \partial_z \bar{\mathbf{u}}_h + \frac{g}{\theta_0} \overline{w'\theta'} - \bar{\epsilon}_\nu \\ \left(c_p - \frac{gz}{\theta_0}\right) \partial_t \bar{\theta} + -\partial_z (c_p \overline{w'\theta'}) & = -\frac{g}{\theta_0} \overline{w'\theta'} + \bar{\epsilon}_\nu \end{cases} \quad (41)$$

### 460 3.2.2 Seawater with linearized equation of state

461 For an ocean with a linearized equation of state, Boussinesq buoyancy is

$$b(\theta, S) = g\alpha(\theta - \theta_0) - g\beta(\theta - S_0) \quad (42)$$

462 and specific enthalpy is

$$h(p_0, \theta, S) = c_p \theta - gz(1 + \alpha(\theta - \theta_0) - \beta(\theta - S_0)) \quad (43)$$

463 Using (33), the budget of mean internal and potential energy is

$$\partial_t (c_p \bar{\theta} - z\bar{b}) = \bar{\epsilon}_\nu - \partial_z (c_p \overline{w'\theta'} - z\overline{w'b'}) - \overline{w'b'} \quad (44)$$

464 The budgets of mean kinetic energy, turbulent kinetic energy, and the sum of mean in-  
465 ternal and potential energy for *seawater* with a linearized equation of state are

$$\begin{cases} \partial_t E_k + \partial_z T_{E_k} & = \overline{w'\mathbf{u}'_h} \cdot \partial_z \bar{\mathbf{u}}_h \\ \partial_t k + \partial_z T_k & = -\overline{w'\mathbf{u}'_h} \cdot \partial_z \bar{\mathbf{u}}_h + \overline{w'b'} - \bar{\epsilon}_\nu \\ \partial_t (c_p \bar{\theta} - z\bar{b}) + \partial_z T_{E_i + E_p} & = -\overline{w'b'} + \bar{\epsilon}_\nu \end{cases} \quad (45)$$

466 Using the salt budget  $\partial_t \bar{S} = -\partial_z \overline{w'S'}$ , we can split this last equation as

$$\partial_t \bar{\theta} = \frac{\bar{\epsilon}_\nu}{c_p - \alpha gz} - \partial_z \overline{w'\theta'} \quad (46)$$

$$\partial_t (-z\bar{b}) = -zg\alpha \frac{\bar{\epsilon}_\nu}{c_p - \alpha gz} + \partial_z (z\overline{w'b'}) - \overline{w'b'} \quad (47)$$

467 Since the energy increase due to viscous dissipation is negligible in the ocean,  $-z\bar{b}$  is of-  
468 ten used as a proxy for "potential" energy (e.g. McDougall, 2003; Olbers et al., 2012).  
469 We nevertheless retain this dissipative heating in (46) to work with a properly closed en-  
470 ergy budget in theoretical descriptions.

## 471 4 Consistency of TKE equation with EDMF closures

472 Based on the energy budgets described in the previous section, we provide a new  
473 parameterization of the TKE budget to obtain an energetically consistent model mim-  
474 icking (37). Indeed, the following TKE equation is commonly used in TKE-based nu-  
475 merical models regardless of whether ED or EDMF closure is used,

$$\partial_t k + \partial_z (-K_k \partial_z k) = K_u \partial_z \bar{\mathbf{u}}_h \cdot \partial_z \bar{\mathbf{u}}_h - K_\phi \partial_z \bar{b} - \bar{\epsilon}_\nu \quad (48)$$

476 where  $k$  represents the turbulent kinetic of the whole grid cell, *i.e.*  $1/2 \overline{\mathbf{u}' \cdot \mathbf{u}'}$ . In (48),  
477 turbulent fluxes have been closed using ED. However, we argue that if an EDMF clo-  
478 sure is used in the mean equations (for momentum, temperature, and salinity or humid-  
479 ity), the TKE equation should be modified by MF terms to ensure energetic consistency  
480 as shown below. Note that Tan et al. (2018) made a different choice by considering a bud-  
481 get for the *environmental* TKE,  $k_e = 1/2 \overline{\mathbf{u}'_e \cdot \mathbf{u}'_e}$ .



482

#### 4.1 Shear and Buoyancy terms

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We have seen in (37) that sources of turbulent kinetic energy could arise from the mean kinetic energy via mean shear  $-\overline{w'\mathbf{u}'_h} \cdot \partial_z \bar{\mathbf{u}}_h$ , or from internal and potential energies via buoyancy production  $\overline{w'b'}$ .

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When the EDMF approach is used to close fluxes in the diagnostic equations of  $\bar{\mathbf{u}}_h$  and  $\bar{\phi}$ , then the same closures must be used in turbulent kinetic energy budget to ensure energetic consistency. As a consequence, the shear term must be closed as

$$-\overline{w'\mathbf{u}'_h} \cdot \partial_z \bar{\mathbf{u}}_h \Big|_{\text{EDMF}} = -[K_u \partial_z \bar{\mathbf{u}}_h + a_p w_p (\mathbf{u}_{h,p} - \bar{\mathbf{u}}_h)] \cdot \partial_z \bar{\mathbf{u}}_h \quad (49)$$

489

In the case of *dry atmosphere*, the buoyancy production term is

$$\overline{w'b'} \Big|_{\text{EDMF}} = \frac{g}{\theta_0} [-K_\theta \partial_z \bar{\theta} + a_p w_p (\theta_p - \bar{\theta})] \quad (50)$$

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whereas in the case of *seawater* with linearized equation of state and  $K_\phi = K_\theta = K_S$ ,

$$\begin{aligned} \overline{w'b'} \Big|_{\text{EDMF}} &= g\alpha [-K_\theta \partial_z \bar{\theta} + a_p w_p (\theta_p - \bar{\theta})] - g\beta [-K_S \partial_z \bar{S} + a_p w_p (S_p - \bar{S})] \\ &= -K_\phi \partial_z \bar{b} + a_p w_p (b_p - \bar{b}) \end{aligned}$$

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#### 4.2 Fluxes of TKE

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The redistribution terms of TKE are often little discussed in turbulence parameterization since they do not contribute directly to the vertically integrated energy budgets. However, they are of great importance in convective conditions where non-local transport dominates (Witek et al., 2011a). For instance, in the atmosphere, the TKE produced close to the surface due to destabilizing buoyancy fluxes is then transported by coherent plumes in the mixed layer. Taking into account MF transport of TKE is thus essential to achieve local energetic consistency, and model accurately TKE at any level  $z$ .

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Turbulent fluxes of TKE arise from the contribution of a TKE transport term, a pressure redistribution term and a viscous flux,

$$T_k = \frac{1}{2} \overline{w'\mathbf{u}' \cdot \mathbf{u}'} + \frac{1}{\rho_0} \overline{w'p'} - \nu \partial_z k \quad (51)$$

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For atmospheric and oceanic flow, the viscous flux is negligibly small and will be omitted. We will assume the pressure redistribution term to be small compared to the transport of TKE, as it is usually done in CBL schemes (e.g. Mellor, 1973). In numerical models, TKE transport is usually parameterized via K-diffusion, namely

$$\partial_z \left( \overline{w' \frac{\mathbf{u}' \cdot \mathbf{u}'}{2}} \right) \simeq -\partial_z (K_k \partial_z k) \quad (52)$$

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However, within the framework exposed in section 2.1, we can apply the two-domain decomposition of the horizontal average to get the exact relation

$$\begin{aligned} \overline{w' \frac{\mathbf{u}' \cdot \mathbf{u}'}{2}} &= \sum_{i=e,p} a_i \underbrace{\frac{1}{2} \overline{\mathbf{u}'_i \cdot \mathbf{u}'_i w'_i}}_{\text{I}_i} + \underbrace{a_i (\mathbf{u}_i - \bar{\mathbf{u}}) \cdot \overline{\mathbf{u}'_i w'_i}}_{\text{II}_i} \\ &\quad + \underbrace{a_i (w_i - \bar{w}) \frac{1}{2} \overline{\mathbf{u}'_i \cdot \mathbf{u}'_i}}_{\text{III}_i} + \underbrace{a_i \frac{1}{2} (\mathbf{u}_i - \bar{\mathbf{u}})^2 (w_i - \bar{w})}_{\text{IV}_i} \end{aligned} \quad (53)$$

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where:  $\text{I}_i$  is an intra-subdomain turbulent TKE transport;  $\text{II}_i$  is a transport of Reynolds stress by the coherent velocities;  $\text{III}_i$  is a transport of subdomain TKE by the coherent velocities (*i.e.* transport of TKE by mass-flux);  $\text{IV}_i$  is a transport of convective kinetic

510 energy by coherent velocities. Based on LES simulations (see Sec. 5.3), we found that:  
 511 (i)  $I_p$  can be neglected, consistently with the small area limit; (ii)  $\Pi_e$  and  $\Pi_p$  are almost  
 512 compensating, thus the sum  $\Pi_e + \Pi_p$  can be neglected. Using  $a_p w_p = -a_e w_e$ , we can  
 513 conveniently reformulate the remaining terms:

$$\text{III}_e + \text{III}_p + \text{IV}_e + \text{IV}_p = a_p w_p \frac{1}{1-a_p} \left( k_p + \frac{1}{2} \|\mathbf{u}_p - \bar{\mathbf{u}}\|^2 - k \right) \quad (54)$$

514 where we have used the following exact decomposition of TKE:

$$k = \frac{1}{2} a_e \|\mathbf{u}_e - \bar{\mathbf{u}}\|^2 + a_e k_e + \frac{1}{2} a_p \|\mathbf{u}_p - \bar{\mathbf{u}}\|^2 + a_p k_p \quad (55)$$

515 and  $k_i := 1/2 \overline{\mathbf{u}'_i \cdot \mathbf{u}'_i}$  ( $i = e, p$ ). In EDMF closures, turbulence is assumed isotropic in  
 516 the environment, thus we close  $\frac{1}{2} \overline{\mathbf{u}'_e \cdot \mathbf{u}'_e w'_e}$  with K-diffusion, similar to the standard prac-  
 517 tice for TKE-only schemes. Then assuming  $\frac{1}{1-a_p} \simeq 1$  (i.e. the small area limit) we have

$$\overline{w' \frac{\mathbf{u}' \cdot \mathbf{u}'}{2}} \simeq \underbrace{-K_k \partial_z k}_{\text{ED}} + \underbrace{a_p w_p \left( k_p - k + \frac{1}{2} \|\mathbf{u}_p - \bar{\mathbf{u}}\|^2 \right)}_{\text{MF}} \quad (56)$$

518 It is interesting to note that we can recover existing formulations from the proposed clo-  
 519 sure (56): if  $a_p w_p = 0$  it boils down to the classical eddy-diffusivity closure; if  $k_p = k$   
 520 and  $\mathbf{u}_{h,p} = \bar{\mathbf{u}}_h$  the term  $1/2 w_p^3$  proposed by Witek et al. (2011a) is recovered; if  $\mathbf{u}_p =$   
 521  $\bar{\mathbf{u}}$  then the formulation proposed by Han and Bretherton (2019) is recovered. However,  
 522 we should mention that the latter authors treat TKE as a tracer to include the term  $a_p w_p (k_p -$   
 523  $k)$ . This justification is incorrect because  $\overline{w' \mathbf{u}' \cdot \mathbf{u}' / 2}$  is not a second-order moment, but  
 524 a third-order moment which requires a proper treatment as seen in (53).

525 Finally, one still needs to provide a value for  $k_p$ . Without any assumption, its prog-  
 526 nostic equation reads (Tan et al., 2018, eq. (11))

$$\begin{aligned} \partial_t(a_p k_p) + \partial_z(a_p w_p k_p) &= -a_p \overline{w'_p \mathbf{u}'_{h,p}} \cdot \partial_z \mathbf{u}_{h,p} + a_p \overline{w'_p b'_p} \\ &+ E \left( k_e + \frac{1}{2} \|\mathbf{u}_e - \mathbf{u}_p\|^2 \right) - D k_p \\ &- \partial_z \left( a_p w'_p \frac{\mathbf{u}'_p \cdot \mathbf{u}'_p}{2} + a_p \mathbf{u}'_p \cdot \frac{1}{\rho_0} (\nabla p^\dagger)'_p \right) \\ &- a_p (\epsilon_\nu)_p \end{aligned}$$

527 As a first attempt, we propose to retain advection, entrainment, detrainment and dis-  
 528 sipation terms, which lead to the simplified form of the previous equation:

$$\partial_z(a_p w_p k_p) = E \left( k_e + \frac{1}{2} \|\mathbf{u}_e - \mathbf{u}_p\|^2 \right) - D k_p - a_p (\epsilon_\nu)_p \quad (57)$$

$$= E \left( \frac{1}{1-a_p} k - \frac{a_p}{1-a_p} k_p + \frac{1}{1-a_p} \frac{1}{2} (\mathbf{u}_p - \bar{\mathbf{u}})^2 \right) - D k_p - a_p (\epsilon_\nu)_p \quad (58)$$

529 where we have used the identity  $(\mathbf{u}_e - \mathbf{u}_p)^2 = \frac{1}{(1-a_p)^2} (\mathbf{u}_p - \bar{\mathbf{u}})^2$  and substituted  $k_e$  us-  
 530 ing (55). Using area conservation, we get the advective form

$$a_p w_p \partial_z k_p = E \frac{1}{1-a_p} \left( k - k_p + \frac{1}{2} (\mathbf{u}_p - \bar{\mathbf{u}})^2 \right) - a_p (\epsilon_\nu)_p \quad (59)$$

531 Finally assuming  $\frac{1}{1-a_p} \simeq 1$  (i.e. the small area limit) we have

$$a_p w_p \partial_z k_p = E \left( k - k_p + \frac{1}{2} (\mathbf{u}_p - \bar{\mathbf{u}})^2 \right) - a_p (\epsilon_\nu)_p \quad (60)$$

532 As a summary, the proposed closure of TKE transport is given by

$$w' \frac{\mathbf{u}' \cdot \mathbf{u}'}{2} = -K_k \partial_z k + a_p w_p \left( k_p - k + \frac{1}{2} \|\mathbf{u}_p - \bar{\mathbf{u}}\|^2 \right) \quad (61)$$

$$a_p w_p \partial_z k_p = E \left( k - k_p + \frac{1}{2} (\mathbf{u}_p - \bar{\mathbf{u}})^2 \right) - a_p (\epsilon_\nu)_p \quad (62)$$

### 533 4.3 Viscous dissipation

534 The total viscous dissipation rate is often parameterized as  $\bar{\epsilon}_\nu = \frac{c_\epsilon}{l_\epsilon} k^{3/2}$  in stan-  
535 dard ED schemes, we do the same for the plume viscous dissipation rate

$$(\epsilon_\nu)_p = \frac{c_\epsilon}{l_\epsilon} k_p^{3/2}$$

536 where  $c_\epsilon = \sqrt{2}/2$  is a numerical constant and the dissipation length is  $l_\epsilon = \sqrt{l_{\text{up}} l_{\text{dwn}}}$   
537 (e.g. Gaspar et al., 1990) with  $l_{\text{up}}$  and  $l_{\text{dwn}}$  defined in Appendix B.

### 538 4.4 Boundary conditions

539 In general, providing physically relevant boundary conditions for the TKE equa-  
540 tion is a complex question that we do not intend to answer in this study. However, once  
541 modelling choices are made, we can provide guidelines to utilize such boundary condi-  
542 tion consistently within an EDMF scheme.

#### 543 4.4.1 Generic constraint

544 According to (61), the boundary condition should verify at  $z = 0$

$$w' \frac{\mathbf{u}' \cdot \mathbf{u}'}{2} = -K_k \partial_z k + a_p w_p \left( k_p - k + \frac{1}{2} \|\mathbf{u}_p - \bar{\mathbf{u}}\|^2 \right) \quad (63)$$

545 In general if plume variables are specified at  $z = 0$ , then (63) is again a Robin bound-  
546 ary condition for the TKE equation.

#### 547 4.4.2 Oceanic context

548 In the ocean, we will assume the following boundary conditions,

$$w' \frac{\mathbf{u}' \cdot \mathbf{u}'}{2} = 0, \quad k_p(0) = k(0)$$

549 along with  $\mathbf{u}_p(0) = (\bar{u}(0), \bar{v}(0), w_p^0)$ . In this case, (63) implies the following Neumann  
550 condition for TKE,

$$K_k \partial_z k(0) = \frac{1}{2} a_p^0 (w_p^0)^3 \quad (64)$$

551 Our formulation could handily include non-zero TKE flux at the surface, as proposed  
552 in the presence of wave-breaking (Craig & Banner, 1994; Mellor & Blumberg, 2004).

#### 553 4.4.3 Atmospheric context

554 In atmospheric models, a value of TKE depending on friction and convective ve-  
555 locities is usually imposed at or near the surface, following field measurements of Wyngaard  
556 and Coté (1971). As long as the plume contribution to the surface TKE flux is imposed  
557 to be zero, the previous approach can be still used. If not, special care would have to be  
558 taken to enforce (63) and avoid spurious energy fluxes.

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#### 4.5 EDMF-parameterized budgets

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Within the Boussinesq approximation, the budget of resolved kinetic energy, sub-grid kinetic energy, and resolved internal+potential energy for a *dry atmosphere* with EDMF closure is

$$\begin{cases} \partial_t E_k + \partial_z T_{E_k} & = -K_u (\partial_z \bar{\mathbf{u}}_h)^2 + a_p w_p (\mathbf{u}_{h,p} - \bar{\mathbf{u}}_h) \cdot \partial_z \bar{\mathbf{u}}_h \\ \partial_t k + \partial_z T_k & = \frac{g}{\theta_0} [-K_\theta \partial_z \bar{\theta} + a_p w_p (\theta_p - \bar{\theta})] + K_u (\partial_z \bar{\mathbf{u}}_h)^2 - a_p w_p (\mathbf{u}_{h,p} - \bar{\mathbf{u}}_h) \cdot \partial_z \bar{\mathbf{u}}_h - \bar{\epsilon}_\nu \\ \partial_t \left[ \left( c_p - \frac{gz}{\theta_0} \right) \bar{\theta} \right] + \partial_z T_{E_i+E_p} & = -\frac{g}{\theta_0} [-K_\theta \partial_z \bar{\theta} + a_p w_p (\theta_p - \bar{\theta})] + \bar{\epsilon}_\nu \end{cases} \quad (65)$$

563

where the flux terms are

$$T_{E_k} = (-K_u \partial_z \bar{\mathbf{u}}_h + a_p w_p (\mathbf{u}_{h,p} - \bar{\mathbf{u}}_h)) \cdot \bar{\mathbf{u}}_h \quad (66)$$

$$T_k = -K_k \partial_z k + a_p w_p \left( k_p - k + \frac{1}{2} \|\mathbf{u}_p - \bar{\mathbf{u}}\|^2 \right) \quad (67)$$

$$T_{E_i+E_p} = -c_p K_\theta \partial_z \bar{\theta} + c_p a_p w_p (\theta_p - \bar{\theta}) \quad (68)$$

564

Equivalently, in the case of *seawater* with linearized equation of state

$$\begin{cases} \partial_t E_k + \partial_z T_{E_k} & = -K_u (\partial_z \bar{\mathbf{u}}_h)^2 + a_p w_p (\mathbf{u}_{h,p} - \bar{\mathbf{u}}_h) \cdot \partial_z \bar{\mathbf{u}}_h \\ \partial_t k + \partial_z T_k & = -K_\phi \partial_z \bar{b} + a_p w_p (b_p - \bar{b}) + K_u (\partial_z \bar{\mathbf{u}}_h)^2 - a_p w_p (\mathbf{u}_{h,p} - \bar{\mathbf{u}}_h) \cdot \partial_z \bar{\mathbf{u}}_h - \bar{\epsilon}_\nu \\ \partial_t (c_p \bar{\theta} - z \bar{b}) + \partial_z T_{E_i+E_p} & = -(-K_\phi \partial_z \bar{b} + a_p w_p (b_p - \bar{b})) + \bar{\epsilon}_\nu \end{cases} \quad (69)$$

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where the flux of internal and potential energy is

$$T_{E_i+E_p} = -\partial_z (c_p (-K_\phi \partial_z \bar{b} + a_p w_p (b_p - \bar{b})) - z (-K_\phi \partial_z \bar{b} + a_p w_p (b_p - \bar{b}))) \quad (70)$$

566

and the conservative temperature equation is

$$\partial_t \bar{\theta} = \frac{\bar{\epsilon}_\nu}{c_p - \alpha g z} - \partial_z (-K_\phi \partial_z \bar{b} + a_p w_p (b_p - \bar{b}))$$

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A summary of EDMF energy budgets is provided in Fig. 1 and in Tab. 2.

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#### 4.6 Vertically integrated energy budgets

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In this section, we provide global energy budgets to highlight the role of mass-flux terms in bulk energy exchange as well as sinks/sources at boundaries. Let us introduce the vertical average  $\langle X \rangle_z = 1/(\sigma_o^a H) \int_0^{\sigma_o^a H} X dz$ , and the boundary operator  $[X]_0^{\sigma_o^a H} = 1/(\sigma_o^a H)(X(z = \sigma_o^a H) - X(z = 0))$ . Then for any advected field  $X$  with source term  $S_X$ , we have (see Appendix D for a detailed derivation):

$$\begin{aligned} \frac{1}{2} \partial_t \langle \bar{X}^2 \rangle_z &= \overbrace{-\langle K_X (\partial_z \bar{X})^2 \rangle_z}^{<0} - \overbrace{\left\langle \frac{E+D}{2} (X_p - \bar{X})^2 \right\rangle_z}^{<0} \\ &+ \langle \bar{X} \bar{S}_X \rangle_z + \langle a_p (S_X)_p (X_p - \bar{X}) \rangle_z \\ &- \left[ \bar{X} w' \bar{X}' + a_p w_p \frac{(X_p - \bar{X})^2}{2} \right]_0^{\sigma_o^a H} \end{aligned}$$

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Consequently, the entrainment and detrainment processes contribute on average to decreasing the mean variance, similar to eddy-diffusivity terms. Although not sufficient in the context of nonlinear equations, monotonically decreasing variance is usually a necessary property to ensure analytical well-posedness of transport partial differential equations (e.g. Evans, 2010). Interestingly, the last term of the budget implies that a non-zero MF flux at the boundary leads to an additional sink of resolved variance (which is exactly compensated by an equal and opposite boundary source for  $\bar{X}'^2$ ).

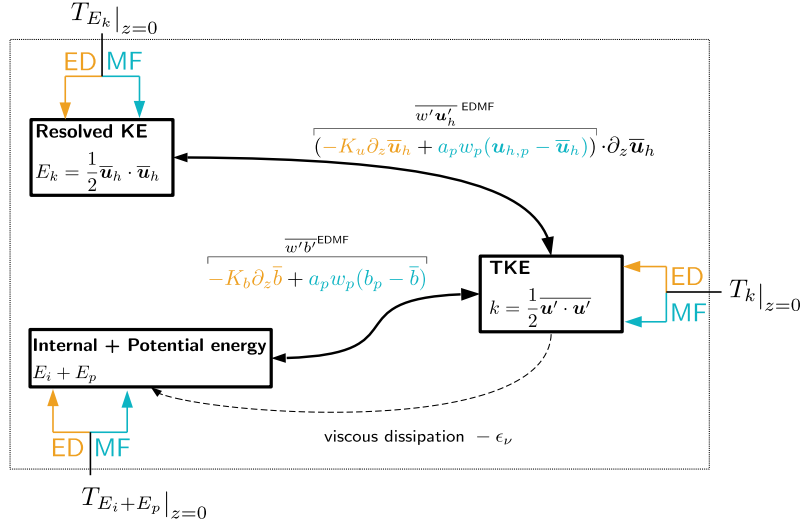


Figure 1: Schematic representation of bulk and boundary energy fluxes within EDMF closure (KE: kinetic energy, TKE: turbulent kinetic energy).

581 We use (71) to get the vertically integrated mean kinetic energy budget,

$$\begin{aligned} \partial_t \langle E_k \rangle_z &= - \langle K_u (\partial_z \bar{\mathbf{u}}_h)^2 \rangle_z - \left\langle \frac{E + D}{2(1 - C_u)} (\mathbf{u}_{h,p} - \bar{\mathbf{u}}_h)^2 \right\rangle_z \\ &\quad - [\bar{\mathbf{u}}_h \cdot \overline{w' \mathbf{u}'_h}]_0^{\sigma_a^H} - \left[ \frac{a_p w_p}{2(1 - C_u)} (\mathbf{u}_{h,p} - \bar{\mathbf{u}}_h)^2 \right]_0^{\sigma_a^H} \end{aligned}$$

582 and the vertically integrated TKE budget

$$\begin{aligned} \partial_t \langle k \rangle_z &= - \langle K_\phi \partial_z \bar{b} \rangle_z + \langle a_p w_p (b_p - \bar{b}) \rangle_z \\ &\quad + \langle K_u (\partial_z \bar{\mathbf{u}}_h)^2 \rangle_z + \left\langle \frac{E + D}{2(1 - C_u)} (\mathbf{u}_{h,p} - \bar{\mathbf{u}}_h)^2 \right\rangle_z \\ &\quad - \langle \bar{\epsilon}_\nu \rangle_z - [T_k]_0^{\sigma_a^H} + \left[ \frac{a_p w_p}{2(1 - C_u)} (\mathbf{u}_{h,p} - \bar{\mathbf{u}}_h)^2 \right]_0^{\sigma_a^H} \end{aligned}$$

583 It is interesting to note that the parameterization of the plume horizontal pressure gra-  
584 dient introduced in 2.3.2 and characterized by the parameter  $C_u$  induces a hyperbolic  
585 enhancement of the transfer from  $E_k$  to  $k$  due to entrainment/detrainment processes.  
586 Additionally, the vertically integrated potential energy and resolved internal energy bud-  
587 get reads

$$\partial_t \langle E_i + E_p \rangle_z = \langle K_\phi \partial_z \bar{b} \rangle_z - \langle a_p w_p (b_p - \bar{b}) \rangle_z + \langle \bar{\epsilon}_\nu \rangle_z - [T_{E_i+E_p}]_0^{\sigma_a^H} \quad (71)$$

588 To illustrate potential biases, let us examine the atmospheric surface flux at  $z = 0$

$$T_{E_i+E_p}(0) = -c_p K_\theta \partial_z \bar{\theta}(0) + c_p a_p(0) w_p(0) (\theta_p(0) - \bar{\theta}(0))$$

589 and assume that the boundary condition is  $-K_\theta \partial_z \bar{\theta}(0) = \overline{w' \theta'}$  (for instance using  
590 MOST), along with a plume initialization of the form (28). Then we would have

$$T_{E_i+E_p}(0) = c_p \overline{w' \theta'}(0) + c_p \overline{w' \theta'}(0) \frac{a_p(0) w_p(0) \beta}{\sqrt{k(0)}}$$

$\partial_t E_k + \partial_z T_{E_k}$	$= -K_u(\partial_z \bar{\mathbf{u}}_h)^2 + a_p w_p (\mathbf{u}_{h,p} - \bar{\mathbf{u}}_h) \cdot \partial_z \bar{\mathbf{u}}_h$	Resolved kinetic energy budget
$\partial_t (E_i + E_p) + \partial_z T_{E_i + E_p}$	$= -(-K_\phi \partial_z \bar{b} + a_p w_p (b_p - \bar{b})) + \bar{\epsilon}_\nu$	Internal and potential energy budget
$\partial_t k - \partial_z (K_k \partial_z k)$	$= K_u(\partial_z \bar{\mathbf{u}}_h)^2 - K_\phi \partial_z \bar{b}$	ED related TKE production terms
	$-a_p w_p (\mathbf{u}_{h,p} - \bar{\mathbf{u}}_h) \cdot \partial_z \bar{\mathbf{u}}_h + a_p w_p (b_p - \bar{b})$	MF related TKE production terms
	$-\partial_z \left( a_p w_p \left[ k_p - k + \frac{1}{2} \ \mathbf{u}_p - \mathbf{u}\ ^2 \right] \right)$	MF related TKE transport term
	$-\bar{\epsilon}_\nu$	TKE dissipation
$a_p w_p \partial_z k_p$	$= E \left( k - k_p + \frac{1}{2} \ \mathbf{u}_p - \mathbf{u}\ ^2 \right) - a_p (\epsilon_\nu)_p$	Plume related TKE
$K_k$	$= c_k l_m \sqrt{k}$	TKE eddy-diffusivity

Table 2: Complementary equations to those presented in Tab. 1, derived from energy consistency constraints in Sec. 4.

591 where the second term leads to an unphysical source of energy for  $a_p(0)w_p(0) \neq 0$ . This  
 592 bias is due to an inconsistent partitioning of the physical boundary flux  $c_p w' \theta'(0)$  into ED  
 593 and MF fluxes.

## 594 5 Evaluation of the EDMF-Energy scheme using a single column model

595 In this section, we numerically evaluate the proposed EDMF formulation on three  
 596 cases of oceanic deep convection. The first two cases are performed in an idealized set-  
 597 ting and compared to Large Eddy Simulation (LES) data, whereas the last case is ini-  
 598 tialized and forced with realistic data and compared to *in situ* measurements at the LION  
 599 buoy in the Mediterranean Sea.

### 600 5.1 Description of idealized cases

601 The two idealized cases considered are reminiscent of typical deep convective condi-  
 602 tions in the ocean (e.g. Marshall & Schott, 1999), where convection into a initially rest-  
 603 ing ocean of constant stratification  $\Delta\theta = 1 \text{ K}/1000 \text{ m}$  (corresponding  $N_0^2 = 1.962 \times$   
 604  $10^{-6} \text{ s}^{-2}$ ) is triggered by a surface cooling of  $Q_0 = -500 \text{ W m}^{-2}$  (corresponding to a  
 605 surface buoyancy loss of  $B_0 = -2.456 \times 10^{-7} \text{ m}^2 \text{ s}^{-3}$ ). In both cases, salinity is kept  
 606 uniform at  $S = 32.6 \text{ psu}$ . The first case (FC500) consists of free convection, where no  
 607 wind stress is applied. In the second idealized case (W005\_C500) a uniform wind stress  
 608 along the meridional direction, of magnitude  $(u_*^a)^2 = 0.05 \text{ m}^2 \text{ s}^{-2}$ , is applied. A sum-  
 609 mary of the parameters for each case can be found in table 3. To characterize wind-shear  
 610 effects, we introduce the Froude number (Haghshenas & Mellado, 2019)

$$Fr_* = \frac{u_*^2}{N_0 L_0} \quad (72)$$

611 where the length scale  $L_0 = (B_0/N_0^3)^{1/2}$  can be interpreted as an Ozmidov scale  $(\bar{\epsilon}_\nu/N^3)^{1/2}$   
 612 (Garcia & Mellado, 2014) which is a measure of the smallest eddy size affected by a back-  
 613 ground stratification  $N_0^2$  in a turbulent field characterized by a viscous dissipation rate  
 614  $\epsilon_\nu$ . After  $t_f = 72 \text{ h}$  of simulation leading to a mixed layer depth  $h$  (defined as the depth  
 615 at which the buoyancy flux is minimum) of several hundred meters, various non-dimensional  
 616 numbers can be used to characterize the flow. Their values can be found in Tab. 4. The  
 617 ratio of the mixed layer depth to the Obukhov length (Obukhov (1971) and Zheng et

Table 3: Idealized cases parameters

Case	$Q_0$ ( $\text{W m}^{-2}$ )	$(u_*^a)^2$ ( $\text{m}^2 \text{s}^{-2}$ )	$N_0^2$ ( $\text{s}^{-2}$ )	$t_f$ (h)	$Fr_*$
FC500	-500	0	$1.962 \times 10^{-6}$	72	0
W005_C500	-500	0.05	$1.962 \times 10^{-6}$	72	0.56

Table 4: Idealized cases non-dimensional parameters after 72 h of simulation

Case	$h/L_{Ob}$	$Ri_h$	$Ri_*$
FC500	$\infty$	$\infty$	97
W05_C500	5.7	310	97

618 al. (2021) in the oceanic context)  $h/L_{Ob}$ , where

$$L_{Ob} = \frac{(u_*^o)^3}{-B_0}$$

619 is an estimate of the depth at which the production of TKE by turbulent shear is of the  
 620 same order of magnitude as the production of TKE by buoyancy fluxes. Noting  $w_* =$   
 621  $(-B_0 h)^{1/3}$  the convective velocity scale (Deardorff, 1970), we get

$$\frac{h}{L_{Ob}} = \left(\frac{w_*}{u_*}\right)^3 \quad (73)$$

622 We also recall that the oceanic friction velocity  $u_*^o$  satisfies  $\rho_o(u_*^o)^2 = \rho_a(u_*^a)^2$ . The Richard-  
 623 son number at the mixed layer base,

$$Ri_h = \frac{N_0^2}{\left(\frac{u_*^o}{h}\right)^2}$$

624 measures the destabilization by surface shear stresses of a stably stratified water column.  
 625 At  $t_f = 72$  h, the case W005\_C500 can be described by  $h/L_{Ob} \simeq 5.7$  and  $Ri_h \simeq 310$ ,  
 626 which corresponds to a regime of strong deepening of the MLD according to Legay et  
 627 al. (2023). Finally, for free convection cases (no wind) a convective Richardson number  
 628 can be built as

$$Ri_* = \frac{N_0^2}{(w_*/h)^2} = \frac{N_0^2 h^{4/3}}{(-B_0)^{2/3}} = Ri_h \left(\frac{L_{Ob}}{h}\right)^{2/3}$$

629 It can be interpreted as follows. The time evolution of the mixed layer depth can be ac-  
 630 curately described by the scaling (Turner, 1979; Van Roekel et al., 2018)

$$h \propto h_{\text{enc}} \quad (74)$$

631 where the *encroachment* depth is  $h_{\text{enc}}(t) := \sqrt{2 \frac{(-B_0)}{N_0^2} t}$ . Then the ratio of the entrain-  
 632 ment velocity  $w_e = \frac{d}{dt} h$  to the convective velocity  $w_* = (-B_0 h)^{1/3}$  reads

$$\frac{w_e}{w_*} \propto Ri_*^{-1} \quad (75)$$

## 633 5.2 LES model description and conditional sampling

634 The LES data have been generated by the Ocean-LES version of the non-hydrostatic  
 635 model Méso-NH (Lac et al., 2018). It is solving an anelastic Lipps-Hemler system adapted



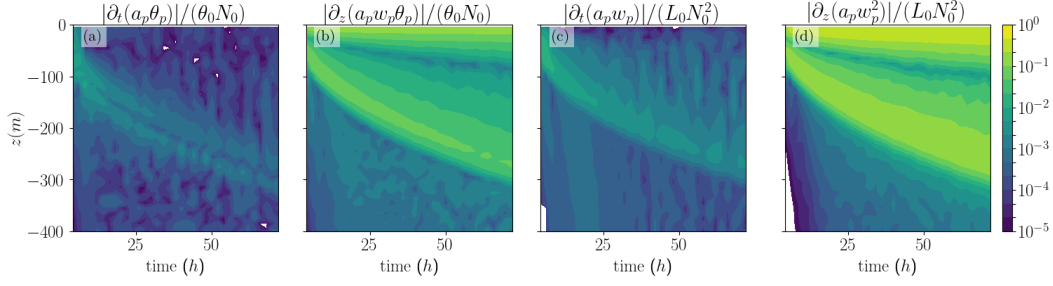


Figure 2: Temporal evolution of the normalized plume tendency  $\partial_t(a_p X_p)$  and plume advection  $\partial_z(a_p w_p X_p)$  terms, for the case FC500.

636 to the ocean, along with a linearized equation of state. The model uses a second-order  
 637 Runge-Kutta time stepping and spatial discretization of advection operators is performed  
 638 with a fourth-order centered scheme. Explicit subgrid scale closures are computed via  
 639 a 3-D turbulence scheme based on a prognostic equation of the subgrid turbulent kinetic  
 640 energy using a mixing-length scale, computed from the volume of a grid cell (Cuxart et  
 641 al., 2000). The domain size is 1000 m on the vertical and  $7.5 \text{ km} \times 7.5 \text{ km}$  on the horizon-  
 642 tal, where doubly periodic conditions are applied. A resolution of 10 m on the vertical  
 643 and 15 m on the horizontal is used. Each configuration is run for 72 h with a time-step  
 644 of 10 s. To assess the quality of the simulations, we checked that the subgrid TKE was  
 645 never exceeding 20% of the TKE explicitly resolved by the LES (Pope, 2004). Via anal-  
 646 ysis of the total TKE budget, we checked that a quasi-steady regime is reached after a  
 647 few hours of simulation (e.g. Garcia & Mellado, 2014). Moreover, at the end of the sim-  
 648 ulations, the typical size of coherent structures, which can be quantified by the horizon-  
 649 tal integral length scale in the bulk of the mixed layer, is of the order  $O(500 \text{ m}) \ll 7.5 \text{ km}$ .  
 650 This suggests that the horizontal domain is large enough to provide a satisfactory sam-  
 651 pling of turbulent structures.

652 To identify plumes, we use a velocity-based conditional sampling adapted from Pergaud  
 653 et al. (2009), namely the plume area is defined as

$$A_p(z, t) = \left\{ (x, y, z, t) \text{ such that } \bar{w}(z, t) - w(x, y, z, t) > m \times \max(\sqrt{w'^2}(z, t), \sigma_{\min}(z, t)) \right\} \quad (76)$$

654 where the minimum standard deviation is chosen as  $\sigma_{\min}(z, t) = 0.05 / (-z) \int_z^0 \sqrt{w'^2}(z', t) dz'$ .  
 655 We checked that the qualitative results were not sensitive to  $m$ , and used  $m = 1$  for  
 656 the remainder. We do not use the tracer-based sampling of Couvreux et al. (2010) since  
 657 it is valid only for small variations of the mixed layer depth. We neither utilize the "strong  
 658 updraft" sampling of (Siebesma et al., 2007) since it assumes that  $a_p$  is a given constant.  
 659 However, we checked that similar conclusions could be drawn from such samplings (not  
 660 shown).

### 661 5.3 Validity of the steady plume hypothesis and small area limit

662 In this section, we directly evaluate the validity of the assumptions made in Sec.  
 663 2.2 during the derivation of the proposed EDMF scheme against LES data. Fig. 2 shows  
 664 that the plume temporal tendency terms are  $O(10^{-2})$  smaller than plume advective terms  
 665 which is consistent with the scaling in  $1/(N_0 t)$  derived in 2.2.3. This justifies the use of  
 666 the steady plume hypothesis. Fig. 3 shows vertical profiles of temperature, vertical ve-  
 667 locity, plume fractional area, and temperature flux for the FC500 case. The small area  
 668 assumption is roughly validated, with values of  $a_p(z)$  between 10% and 20% of the total  
 669 area, as exposed in previous studies (e.g. Couvreux et al., 2010). This justifies ques-

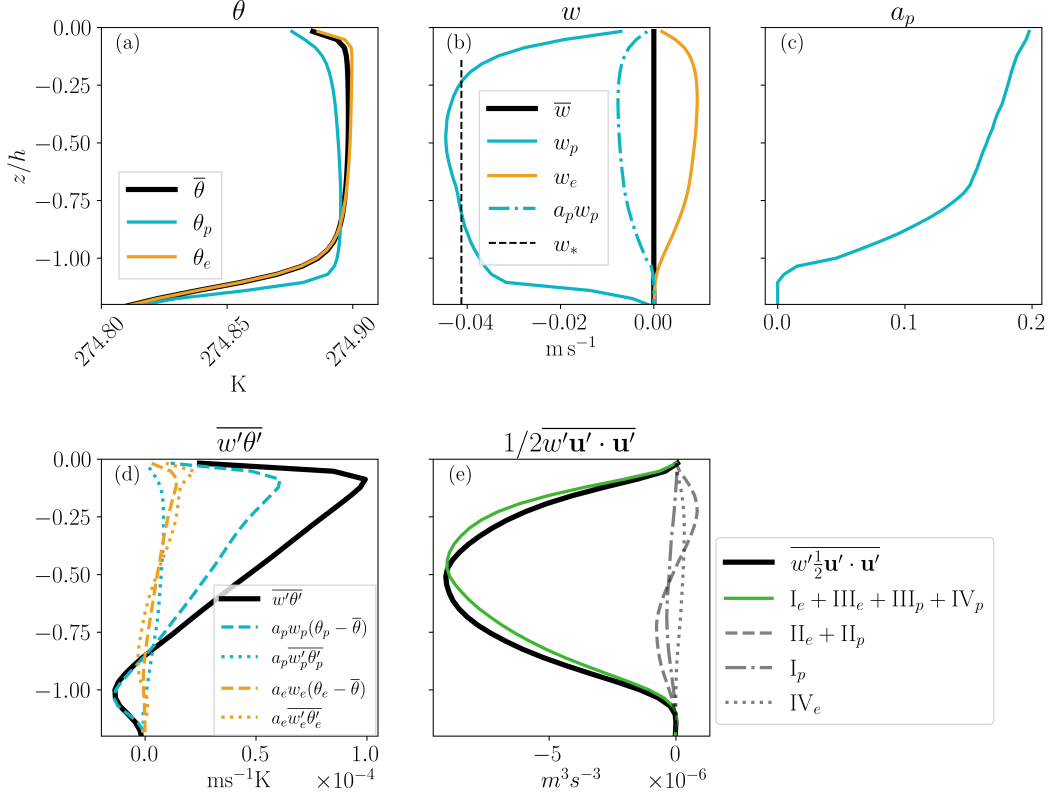


Figure 3: LES vertical profiles of (a) temperature, (b) vertical velocities, (c) plume fractional area, (d) temperature flux and (e) TKE flux for the FC500 case after 72 h of simulation. For each field, the black lines represent an horizontal average over the whole grid cell, the blue lines represent an average over the plume area and the orange lines represent an average over the environment area. In panel (b) the blue dotted line represents  $a_p w_p$ , and the gray dashed line represents the value of the free convective velocity scale  $w_*$ . In panel (d), total flux is in black, plume fluxes in blue (MF is dashed and subplume is dotted), and environment fluxes in orange (same linestyles). In panel (e) are represented the total flux (black) and the contributions from the combined terms  $I_e + III_e + III_p + IV_p$  (blue),  $II_e + II_p$  (dashed gray),  $I_p$  (dash-dotted gray) and  $III_p$  (dotted gray) (see 4.2 for details).

670 tioning the relevance of this assumption and considering the system described in Appendix  
 671 A. The convective velocity  $w_*$  is found to be a good estimate of the plume vertical  
 672 velocity  $w_p$ . The contribution of the mass-flux term  $a_p w_p (\theta_p - \bar{\theta})$  to the total tempera-  
 673 ture flux is increasing with depth, until reaching a quasi-perfect match in the entrain-  
 674 ment layer. The rough validity of assumption  $a_p w_p (\theta_p - \bar{\theta}) \gg a_p \overline{w'_p \theta'_p}, a_e w_e (\theta_e - \bar{\theta})$  is  
 675 consistent with the rough validity of  $a_p \ll 1$ . The plume/environment decomposition  
 676 of the vertical transport of TKE  $1/2 \overline{w' \mathbf{u}' \cdot \mathbf{u}'}$  is presented in Fig. 3(e). The dominant  
 677 terms exposed in (54) explain well the total flux.

678 All the previous findings are also verified for the W005\_C500 case (not shown).

#### 679 5.4 SCM evaluation

680 In this section, we evaluate three different configurations of the SCM against LES  
 681 data. First, a setup where only an eddy-diffusivity closure is used (referred as "ED"), and

682 where the TKE equation (48) does not contain MF terms, which is equivalent to setting  
 683  $a_p w_p = 0$ . Second, an EDMF scheme in which an ED closure of the TKE equation (48)  
 684 is used (referred as "EDMF"). This configuration is not energetically consistent as ex-  
 685 plained in Sec. 4. It would be the result of a naive independent coupling of TKE and  
 686 MF schemes. Finally, the third configuration consists of the previously detailed EDMF  
 687 scheme in which the TKE equation is modified as in (69) to include the contribution of  
 688 MF terms to energy transfers (referred to as "EDMF-Energy"). Since the small area hy-  
 689 pothesis is approximately valid in LES, we also tested the relaxed version of table 1. How-  
 690 ever, we could not identify significant impacts on such an idealized setup (not shown).  
 691 For the three configurations, the constants  $c_m, c_e, c_k$  used in the ED terms are the same  
 692 as the constants used in the TKE equation of the LES model. The parameters used for  
 693 the plume equations closures have been chosen as  $\beta_1 = 0.99, \beta_2 = 1.99, a = 1.0, b =$   
 694  $1.25, b' = 0.003 \text{ m}^{-1}, C_u = 0.5, a_p^0 = 0.2, \delta_0 = 0.005 \text{ m}^{-1}$ . A careful tuning and uncer-  
 695 tainty quantification of the parameters, using for instance statistical method (e.g. Souza  
 696 et al., 2020; Couvreur et al., 2021), is left for future studies.

697 The examination of mean temperature and flux of temperature profiles shows that  
 698 ED fails to reproduce the so-called vertical entrainment zone (e.g. Garcia & Mellado,  
 699 2014), in which penetrative convection generates negative temperature flux and sharp-  
 700 ens the temperature gradients at the base of the mixed layer. The lack of penetrative  
 701 convection is known to reduce the deepening rate (e.g. chap. 6, Garratt, 1994a), thus  
 702 producing an important bias of a hundred meters regarding the mixed layer depth com-  
 703 pared to LES. On the other hand, EDMF and EDMF-energy equally perform in repre-  
 704 senting these profiles. The absence of a noticeable effect of the energetic consistency on  
 705 the temperature mean and flux profiles is a consequence of the small value of the ED fluxes  
 706 (dashed lines) in the mixed layer. When considering the TKE profile, ED can model the  
 707 correct order of magnitude, however, the TKE does not penetrate enough. EDMF fails  
 708 to reproduce TKE due to energetic inconsistency. Indeed, looking at temperature and  
 709 velocity fluxes allows us to infer that the losses of resolved energy due to buoyancy and  
 710 shear are dominated by the MF contributions. However, such contributions are not in-  
 711 cluded as sources of TKE for the EDMF scheme, leading to the very low levels of TKE  
 712 observed in the simulation. EDMF-energy can reproduce accurate profiles of TKE. The  
 713 main discrepancies arise close to the surface and at the base of the mixed layer. Neither  
 714 ED nor EDMF can reproduce the vertical transport of TKE, whereas EDMF-energy re-  
 715 produces well the profile. Similar conclusions are drawn from the WC005\_C500 case (see  
 716 Fig. 5).

717 In Fig. 6, we represent the vertically integrated energy budget of the SCM for the  
 718 case W005\_C500 (FC500 is similar), namely the quantity

$$\int_{-H}^0 \partial_t (E_k + k + E_i + E_p) dz + [T_{E_k} + T_k + T_{E_i+E_p}]_{-H}^0 \quad (77)$$

719 As expected, EDMF-energy conserves energy, whereas EDMF does not. The energy loss  
 720 due to inconsistent energetics is equal to

$$\int_{-H}^0 (-a_p w_p (b_p - \bar{b}) + a_p w_p (\mathbf{u}_{h,p} - \bar{\mathbf{u}}_h) \cdot \partial_z \bar{\mathbf{u}}_h) dz \quad (78)$$

721 and scales with  $B_0 h$ .

## 722 5.5 Realistic case: Hymex/ASICS-MED campaign

723 We now move to more realistic situations corresponding to a sequence of strong con-  
 724 vective events which were documented in the Northwestern Mediterranean during the  
 725 winter 2013 of the HyMeX/ASICS-MED experiment at the LION buoy. This experiment  
 726 was also carried out by Giordani et al. (2020) and we use a similar setup here (similar  
 727 vertical grid as well as similar initial and surface boundary conditions). The experiments

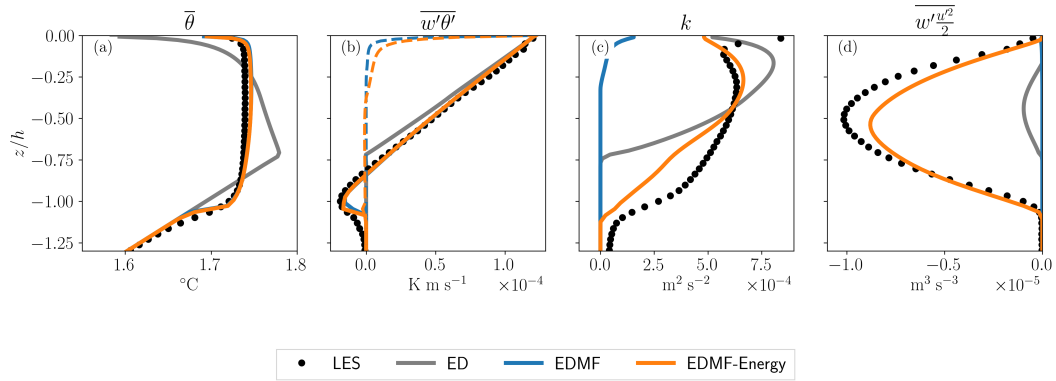


Figure 4: Vertical profiles of (a) temperature, (b) temperature flux, (c) turbulent kinetic energy and (d) turbulent transport of TKE for the FC500 case after 72h of simulation. LES data (black dots), ED-only scheme (grey line), standard EDMF scheme (blue line) and energetically consistent EDMF (orange line) are represented, along with the ED contribution to the temperature fluxes (dashed lines).

728 are performed with a SCM similar to (6) and (7) but including additional Coriolis and  
 729 solar penetration (using a standard Jerlov law) terms. We consider conservative tem-  
 730 perature and salinity as entropic variables which are related to buoyancy via a nonlin-  
 731 ear equation of state. We also include penalization terms in the SCM to account for  
 732 the effect of the bottom (which is at a depth of 2400 m at the LION buoy). Thanks to the  
 733 penalization term a no-slip boundary condition is imposed at the bottom and a no-gradient  
 734 condition is imposed for tracers. The vertical grid resolution ranges from 1 m near the  
 735 surface to 150 m near the bottom located at  $z = -2400$  m. Parameters of the TKE  
 736 scheme are set to the standard NEMO values,  $\mathbf{c} = (c_m, c_e, c_k) = (0.1, \frac{\sqrt{2}}{2}, 0.1)$ .

737 A series of 30-days numerical simulations were carried out starting from January  
 738 15, 2013. The surface boundary conditions are shown in Fig. 7. In particular, very strong  
 739 cooling events occurred during the period of interest. Two simulations were made sys-  
 740 tematically with an eddy-diffusivity term activated. A first simulation was done with En-  
 741 hanced Vertical Diffusion (referred to as ED+EVD) which is the standard practice for  
 742 climate simulations using NEMO, a second one using a mass flux scheme on tracers, dy-  
 743 namics, and with the additional terms for energetic consistency in the TKE equation (re-  
 744 ferred to as EDMF-energy). To get a more concrete idea of the improvements brought  
 745 about by the mass flux scheme over the usual practice for NEMO applications (ED+EVD),  
 746 we show in Fig. 7 (bottom panel) the temporal evolution of the mixed layer depth  $h_{\text{mixl}}$   
 747 computed from mooring data and single-column numerical simulations.  $h_{\text{mixl}}$  is defined  
 748 as the depth where the following criterion is met

$$\int_{h_{\text{mixl}}}^{z_{\text{ref}}} \partial_z b_{\text{eos}}(\theta, S = 38.5 \text{ psu}) dz = \frac{g}{\rho_0} \rho_c$$

749 with  $z_{\text{ref}} = 300$  m and  $\rho_c = 0.01 \text{ kg m}^{-3}$ . We had to consider a constant salinity in  
 750 the buoyancy calculation because the salinity data from the LION buoy are noisy in the  
 751 vertical and did not allow for a robust diagnostics. The bottom panel in Fig. 7 illustrates  
 752 the fact that the penetration depth of convective plumes is significantly better represented  
 753 by the EDMF-Energy scheme than by the ED+EVD approach. Moreover, a direct compar-  
 754 ison with temperature and salinity from mooring data is shown in Fig. 8 at differ-  
 755 ent times. In particular several phases can be identified during the experiment (e.g. Cop-  
 756 pola et al., 2017; Waldman et al., 2017): (i) in the period 15-25 January 2013 winter  
 757 convection starts to deepen the mixed layer down to around  $-800$  m to the point of erod-

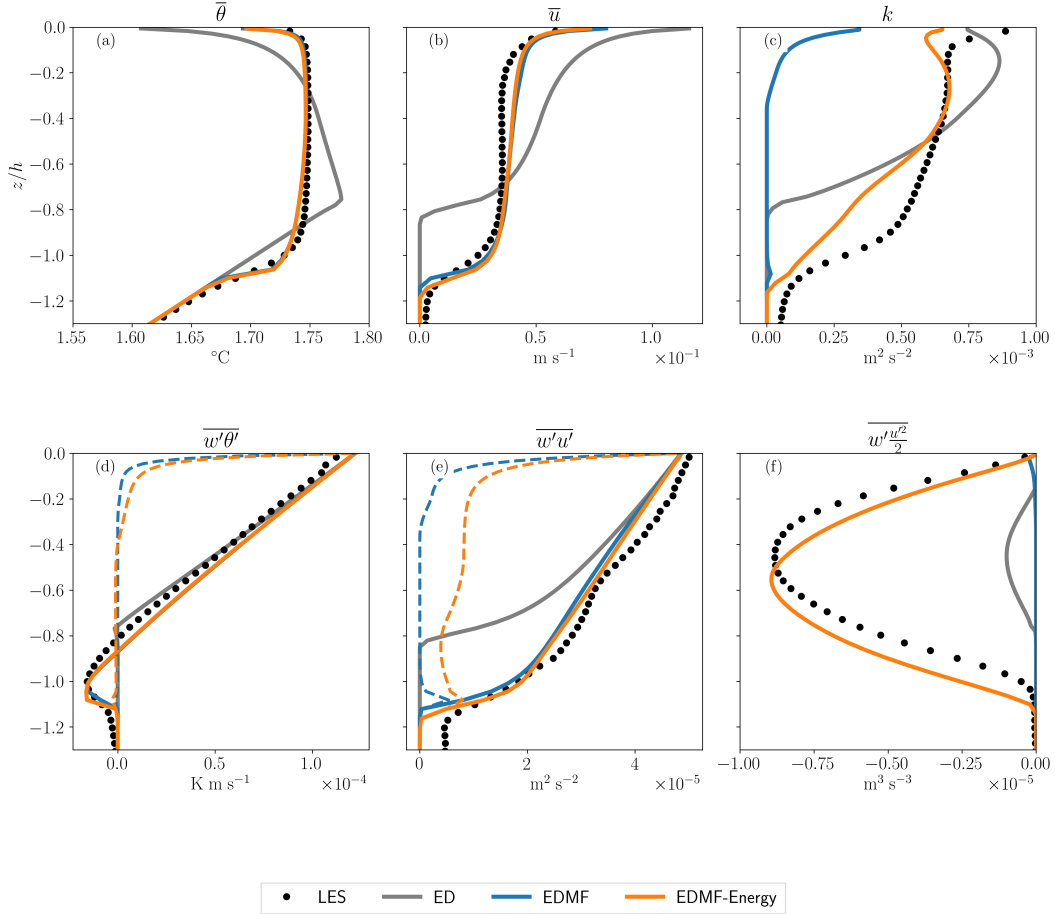


Figure 5: Vertical profiles of (a) mean temperature, (b) mean zonal current, (c) turbulent kinetic energy, (d) temperature flux, (e) zonal momentum flux, (d) turbulent transport of TKE for the FC500 case after 72h of simulation. LES data (black dots), ED-only scheme (grey line), standard EDMF scheme (blue line) and energetically-consistent EDMF (orange line) are represented, along with the ED contribution to the temperature and momentum fluxes (dashed lines).

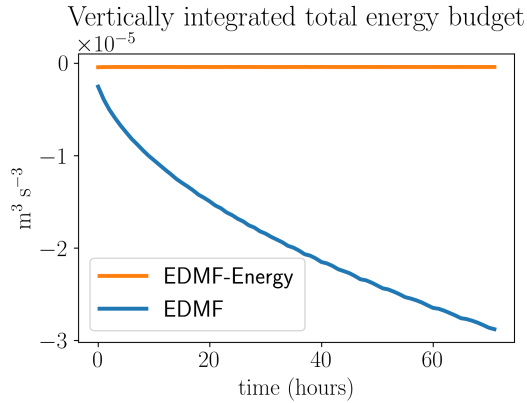


Figure 6: Time series of the vertically integrated energy budget (77) for the case W005\_C500 (see text for details).

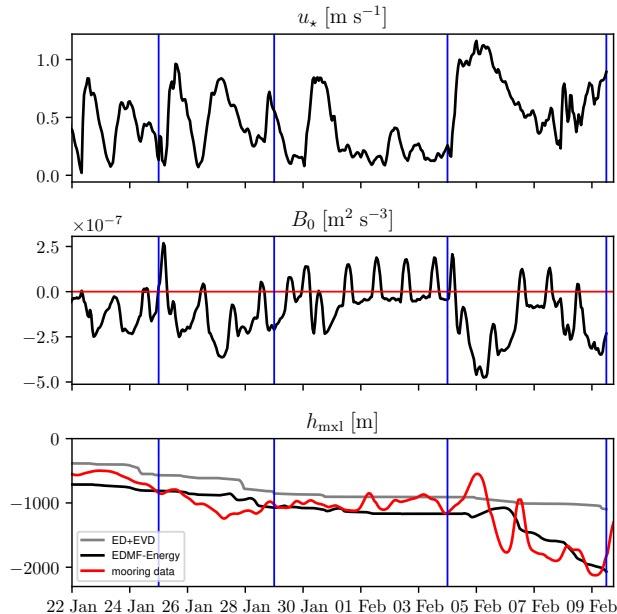


Figure 7: Time series of the friction velocity  $u_*$  ( $\text{m s}^{-1}$ , top panel) and surface buoyancy flux  $B_0$  ( $\text{m}^2 \text{s}^{-3}$ , middle panel) computed from atmospheric forcings. Time series of mixed layer depth  $h_{\text{mixl}}$  (m, bottom panel) obtained from observations at the LION buoy (red line) and from single column numerical experiments using ED+EVD (solid gray line) and EDMF-Energy (solid black line). The vertical blue lines correspond to the dates at which the vertical temperature and salinity profiles derived from observations and numerical simulations are compared in Fig. 8.

758 ing the Levantine intermediate waters. (ii) in the period 26–29 January 2013 the mixed  
 759 layer keeps thickening to the depth of the western Mediterranean deep water ( $\approx -1250$  m)  
 760 (iii) in the period 4–9 February 2013 a new intense convective event associated with a  
 761 strong Mistral event contributes to deepen the mixed layer down to the bottom (reached  
 762 in 9 February). This is followed by a restratification phase involving horizontal processes  
 763 that cannot be represented in our SCM formalism which explains why we do not ana-  
 764 lyze solutions beyond February 9.

## 765 6 Discussion and conclusion

766 In this work, we have presented the theoretical derivation of an EDMF scheme with  
 767 special attention paid to energetic aspects in a simple thermodynamic setting, for both  
 768 dry atmosphere and seawater with linearized equation of state. During the derivation,  
 769 we systematically reviewed the approximations used and provided both *a priori* scaling  
 770 estimations, and direct evaluations of their validity on two idealized LES of oceanic con-  
 771 vection. Closed energetics at the SCM level is a necessary step to obtain energetically  
 772 consistent 3D models and thus reduce spurious energy biases. Theoretical horizontally  
 773 averaged energy budgets are guiding the derivation of consistent energy budgets for SCM  
 774 with EDMF closure. In particular, we have exposed the necessary modification of the  
 775 standard TKE equation that incorporates EDMF terms to obtain closed energy budgets.  
 776 Besides taking into account MF terms in shear and buoyancy terms, we propose an MF  
 777 parameterization of TKE transport based on LES diagnostics. It generalizes previous  
 778 formulations and implies the consideration of a subplume TKE (Han & Bretherton, 2019).

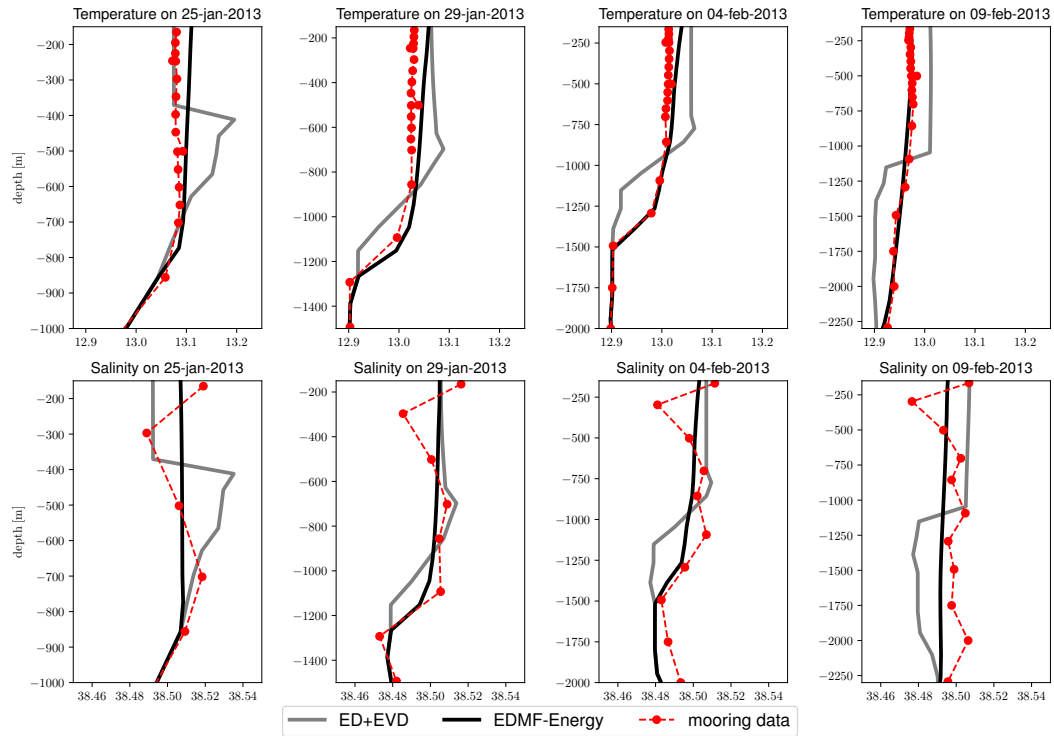


Figure 8: Temperature ( $^{\circ}\text{C}$ , top panels) and salinity (psu, bottom panels) profiles obtained from single column experiments at the location of the LION buoy using an eddy-diffusivity closure with enhanced vertical diffusion (ED-EVD, solid gray lines) and energetically-consistent EDMF (EDMF-Energy, solid black lines). Results from numerical experiments are compared to observations from the LION buoy (dashed red lines) for 4 dates represented on the Fig. 7 by vertical blue lines.



779 We also show that boundary conditions on both mean and plume variables should be  
 780 consistent with the EDMF decomposition to avoid spurious energy fluxes at the bound-  
 781 ary and subsequent inconsistent energetics. We evaluate the performance of the proposed  
 782 energetically consistent EDMF scheme in the context of idealized oceanic convection. When  
 783 compared with LES of idealized oceanic convection, our scheme can reproduce mean fields  
 784 and vertical fluxes of temperature and momentum as well as a non-energetically closed  
 785 EDMF scheme. However energetic consistency is key to obtaining realistic TKE and tur-  
 786 bulent transport of TKE profiles. To further illustrate that the MF concept is a cred-  
 787 ible alternative to the traditional approaches used in the oceanic context (using an en-  
 788 hanced vertical diffusion or a counter gradient term *à la* KPP (Large et al., 1994)) the  
 789 proposed scheme is validated in a single-column configuration against observational data  
 790 of oceanic convection from the LION buoy.

791 Even if the proposed derivation may seem tedious, the energetically consistent param-  
 792 eterization obtained is rather simple to implement, whether in a code with an ex-  
 793 isting "non-energetically consistent" EDMF scheme or, more generally, in any code re-  
 794 lying on a prognostic TKE equation. The MF terms are obtained by solving a straight-  
 795 forward system of ODEs and take the form of vertical advection terms in the mean equa-  
 796 tions (see Appendix F for practical details). The proposed approach can also be applied  
 797 in the case where the ED closure does not use TKE. In this case, it would require to add  
 798 a prognostic or diagnostic TKE equation (even if it does not interact with the ED term)  
 799 to enforce energetic consistency.

800 This paper was intentionally oriented toward the theoretical description of ener-  
 801 getically consistent EDMF schemes. The first idealized test cases were not conclusive on  
 802 several new aspects which should be further assessed using more realistic SCM/LES in-  
 803 tercomparisons in future studies. Among these aspects, we can mention: the impact of  
 804 choosing the total TKE  $k$  instead of the environmental TKE  $k_e$  to compute eddy-diffusivities  
 805 (sec. 2.3.3); the impact of relaxing the small-area assumption presented in Appendix A;  
 806 the impact of energetic consistency on the accuracy of the mean fields.

807 The development of energetically consistent EDMF schemes can be continued in  
 808 several ways. First, for real-world applications, the present work has to be extended to  
 809 more complex thermodynamics models (i.e. moist atmosphere, Pauluis (2008), and sea-  
 810 water with a non-linear equation of state, Tailleux and Dubos (2023)). As a starting point,  
 811 we provided in Appendix E a derivation of EDMF energy budgets in the anelastic set-  
 812 ting from a dry atmosphere. The proposed framework is flexible enough to be readily  
 813 extended to other coherent structures of the boundary layer contributing to transport,  
 814 such as atmospheric downdraft (Han & Bretherton, 2019; Brient et al., 2023). For at-  
 815 mospheric models, the ED-based Monin-Obukhov similarity theory should be reconciled  
 816 with the EDMF representation of fluxes (Li et al., 2021) to provide unambiguous and  
 817 consistent boundary conditions and thus avoid potential spurious boundary energy fluxes.

818 To implement and then assess the impact of this energetically consistent param-  
 819 eterization on realistic 3D oceanic simulations a calibration of the remaining "free" pa-  
 820 rameters must be achieved (Hourdin et al., 2017; Couvreux et al., 2021). It should be  
 821 performed on parameters whose universality can sometimes be statistically assessed (Souza  
 822 et al., 2020), and should be mathematically and physically constrained as much as pos-  
 823 sible (see e.g. section 4.6). We believe that designing energetically consistent parame-  
 824 terization is a way to achieve more realistic models before their tuning.

## 825 **Appendix A Relaxing the small area limit**

826 The small-area assumption can be relaxed with no additional complexity if the sub-  
 827 plume fluxes  $\overline{w'_p \phi'_p}$  are still neglected. A summary of the EDMF-Energy parameteriza-  
 828 tion in such a regime is presented in Tab. A1.

$\tilde{\alpha} = \frac{1}{1 - a_p}$	Rescaling coefficient
$\frac{w'\phi'}{w'\mathbf{u}'_h} = \tilde{\alpha}a_pw_p(\phi_p - \bar{\phi}) - K_\phi\partial_z\bar{\phi}$	Vertical turbulent flux for component $\phi$
$\frac{w'\mathbf{u}'_h}{w'\mathbf{u}'_h} = \tilde{\alpha}a_pw_p(\mathbf{u}_{h,p} - \bar{\mathbf{u}}_h) - K_m\partial_z\bar{\mathbf{u}}_h$	Vertical turbulent momentum flux
$\partial_z(a_pw_p) = E - D$	Plume area conservation equation
$a_pw_p\partial_z\phi_p = \tilde{\alpha}E(\bar{\phi} - \phi_p)$	Plume equation for component $\phi$
$a_pw_p\partial_z\mathbf{u}_{h,p} = \tilde{\alpha}E(\bar{\mathbf{u}}_h - \mathbf{u}_{h,p}) + a_pw_pC_u\partial_z\bar{\mathbf{u}}_h$	Plume horizontal momentum equation
$a_pw_p\partial_zw_p = -(\tilde{\alpha}b)Ew_p + a_p\{aB_p - \sigma_o^a(\tilde{\alpha}b')w_p^2\}$	Plume vertical velocity equation
$B_p = b_{\text{eos}}(\phi_p) - b_{\text{eos}}(\bar{\phi})$	Buoyancy forcing term
$\partial_t k - \partial_z(K_k\partial_z k) = K_m(\partial_z\bar{\mathbf{u}}_h)^2 - K_\phi\partial_z\bar{b}$	ED related TKE production terms
$\quad - \tilde{\alpha}a_pw_p((\mathbf{u}_{h,p} - \bar{\mathbf{u}}_h) \cdot \partial_z\bar{\mathbf{u}}_h - (b_p - \bar{b}))$	MF related TKE production terms
$\quad - \partial_z\left(\tilde{\alpha}a_pw_p\left[k_p - k + \frac{1}{2}\ \mathbf{u}_p - \mathbf{u}\ ^2\right]\right)$	MF related TKE transport term
$\quad - \bar{\epsilon}_\nu$	TKE dissipation
$a_pw_p\partial_zk_p = \tilde{\alpha}E\left((k - k_p) + \frac{1}{2}\ \mathbf{u}_p - \mathbf{u}\ ^2\right) - a_p(\epsilon_\nu)_p$	Plume related TKE

Table A1: Same as table 1, but with a relaxation of the small area limit. Note that under the small area limit we would have  $\tilde{\alpha} \equiv 1$ .

## Appendix B Mixing length computations

For the oceanic applications detailed in this article, we have chosen a formulation of eddy-diffusivity and viscosity close to that used in the NEMO ocean model (Madec et al., 2019). The eddy-viscosity and diffusivity are classically assumed to be related to TKE by

$$\begin{aligned} K_u &= c_m l_m \sqrt{k} \\ K_\phi &= K_u (\text{Pr}_t)^{-1} \end{aligned}$$

with  $l_m$  a mixing length scale,  $\text{Pr}_t$  the non-dimensional turbulent Prandtl number, and  $c_m$  is a constant ( $c_m = 0.1$  in NEMO). The mixing length  $l_m$  is calculated in two steps by considering separately the length scales  $l_{\text{up}}$  and  $l_{\text{dwn}}$  associated respectively to upward and downward movements : (1)  $l_{\text{up}}$  and  $l_{\text{dwn}}$  are initialized assuming  $l_{\text{up}} = l_{\text{dwn}} = \sqrt{2k}\tau_{\text{ed}}$  with  $\tau_{\text{ed}}$  a characteristic time equal to  $1/N = (\partial_z\bar{b})^{-1}$  (2) a physical limitation is used to guarantee that  $l_{\text{up}}$  and  $l_{\text{dwn}}$  do not exceed the distance to the top and the bottom, this limitation amounts to controlling the vertical gradients of  $l_{\text{up}}$  and  $l_{\text{dwn}}$  such that they are not larger than the variations of depth (*e.g.* Madec et al., 2019). Once  $l_{\text{up}}$  and  $l_{\text{dwn}}$  are computed the mixing length is taken as  $l_m = \min(l_{\text{up}}, l_{\text{dwn}})$ . The turbulent Prandtl number is modelled by  $\text{Pr}_t = \min(\text{Pr}_t^{\text{max}}, \max(\text{Ri}/\text{Ri}_c, 1))$  with  $\text{Ri} = N^2/\|\partial_z\bar{\mathbf{u}}_h\|^2$ ,  $\text{Pr}_t^{\text{max}} = 10$  and  $\text{Ri}_c = 0.2$ .

## Appendix C Boundary condition for plume equations

Near the surface, we linearize the plume and mean buoyancy in the form  $b \simeq b^0 + b'z$ . Then the plume equation for  $b_p$  reads at order  $O(z^0)$ :

$$a_p^0 w_p^0 b'_p = -E_0(b_p^0 - \bar{b}^0)$$

848 The boundary condition  $b_p^0 = \bar{b}^0$  implies that  $b'_p = 0$ . Thus we get

$$b_p(z) \simeq \bar{b}^0, \quad \bar{b} \simeq \bar{b}^0 + N_0^2 z$$

849 Then near the surface, the buoyancy force - which is a source of plume momentum and  
 850 kinetic energy  $1/2w_p^2$  - is at first order  $b_p - \bar{b} \simeq -N_0^2 z$ . Consequently, any static insta-  
 851 bility at the surface will result in the absolute growth of the plume vertical momentum  
 852 ( $-N_0^2 z > 0$  in the atmosphere and  $-N_0^2 z < 0$  in the ocean).

853 The boundary condition  $b_p(0) = \bar{b}(0)$  implies that at  $z = 0$ , all the surface flux is al-  
 854 located in the ED component. Consequently,  $N_0^2 = \overline{w'b'}(0)/(-K_b(0)) = \overline{w'b'}(0)/(c_b l_b(0)\sqrt{k(0)})$ .  
 855 The boundary condition  $b_p(0) = \bar{b}(0)$  thus implies that close to the surface

$$b_p(z) \simeq \bar{b}(z) + \frac{\overline{w'b'}(0)}{c_b l_b(0)\sqrt{k_0}} z$$

## 856 Appendix D EDMF Mean Variance Equation

857 Start from the mean and plume equations, and the turbulent flux decomposition

$$\partial_t \bar{X} = -\partial_z \overline{w'X'} + \bar{S}_X \quad (\text{D1})$$

$$\overline{w'X'} = -K_X \partial_z \bar{X} + a_p w_p (X_p - \bar{X}) \quad (\text{D2})$$

$$a_p w_p \partial_z X_p = -E(X_p - \bar{X}) + a_p S_{X,p} \quad (\text{D3})$$

858 Multiplying the mean equation (D1) by  $\bar{X}$  leads to

$$\begin{aligned} \frac{1}{2} \partial_t \bar{X}^2 &= -\partial_z (\bar{X} \overline{w'X'}) + \overline{w'X'} \partial_z \bar{X} + \bar{X} \bar{S}_X \\ &= -\partial_z (\bar{X} \overline{w'X'}) - K_X (\partial_z \bar{X})^2 + a_p w_p (X_p - \bar{X}) \partial_z \bar{X} + \bar{X} \bar{S}_X \end{aligned} \quad (\text{D4})$$

859 To rewrite the second term of the right-hand side, we use the plume equation (D2):

$$\begin{aligned} a_p w_p (X_p - \bar{X}) \partial_z \overbrace{\bar{X}}^{=X_p + (\bar{X} - X_p)} &= -E(X_p - \bar{X})^2 + (X_p - \bar{X}) a_p S_{X,p} \\ &\quad - a_p w_p \frac{1}{2} \partial_z (X_p - \bar{X})^2 \\ &= -E(X_p - \bar{X})^2 + (X_p - \bar{X}) a_p S_{X,p} \\ &\quad - \partial_z (a_p w_p \frac{1}{2} (X_p - \bar{X})^2) \\ &\quad + (E - D) \frac{1}{2} (X_p - \bar{X})^2 \\ &= -(E + D) \frac{1}{2} (X_p - \bar{X})^2 + (X_p - \bar{X}) a_p S_{X,p} \\ &\quad - \partial_z (a_p w_p \frac{1}{2} (X_p - \bar{X})^2) \end{aligned}$$

860 Using this expression into equation (D4), then vertically integrating the variance bud-  
 861 get leads to the desired equation (71).

## 862 Appendix E Anelastic energy budgets

863 In this appendix, we derive energy budgets for a general anelastic model commonly  
 864 used in atmospheric models. We start with the unaveraged anelastic mass and momen-  
 865 tum budgets:

$$\nabla \cdot (\rho_{\text{ref}} \mathbf{u}) = 0 \quad (\text{E1})$$

$$\partial_t \mathbf{u} = -\nabla \cdot (\mathbf{u} \otimes \mathbf{u}) - \mathbf{f} \times \mathbf{u} - \nabla \left( \frac{p^\dagger}{\rho_{\text{ref}}} \right) + b \mathbf{e}_z + \nu \nabla^2 \mathbf{u} \quad (\text{E2})$$

866 where  $\rho_{\text{ref}} = \rho_{\text{ref}}(z)$  is a reference density profile, and the total pressure is  $p(x, y, z, t) =$   
 867  $p_{\text{ref}}(z) + p^\dagger(x, y, z, t)$  where by definition  $\partial_z p_{\text{ref}}(z) = -\rho_{\text{ref}}g$ .

868 As in section 3, we keep the same notations for the specific mean kinetic energy  
 869  $E_k = (\bar{\mathbf{u}}_h \cdot \bar{\mathbf{u}}_h)/2$ , the turbulent kinetic energy  $k = (\overline{\mathbf{u}' \cdot \mathbf{u}'})/2$ , the potential energy  
 870  $E_p = gz$  and the mean internal energy  $E_i$ . Note however that these *specific energies*  
 871 have to be multiplied by  $\rho_{\text{ref}}$  to get corresponding energies.

## 872 E1 Kinetic energies

873 By using the SCM assumptions exposed in Sec. 2.1, we can derive budgets for the  
 874 resolved kinetic energy  $E_k$  and the turbulent kinetic energy  $k$ :

$$\partial_t E_k + \frac{1}{\rho_{\text{ref}}} \partial_z T_{E_k} = \overline{w' \mathbf{u}'_h} \cdot \partial_z \bar{\mathbf{u}}_h \quad (\text{E3})$$

$$\partial_t k + \frac{1}{\rho_{\text{ref}}} \partial_z T_k = -\overline{w' \mathbf{u}'_h} \cdot \partial_z \bar{\mathbf{u}}_h + \overline{w' b'} - \bar{\epsilon}_\nu \quad (\text{E4})$$

875 where  $\bar{\epsilon}_\nu = \overline{\nu \partial_z \mathbf{u}' \cdot \partial_z \mathbf{u}'}$  is the viscous dissipation of energy,  $T_{E_k} = \rho_{\text{ref}} \overline{w' \mathbf{u}'_h} \cdot \bar{\mathbf{u}}_h$  and  
 876  $T_k = \rho_{\text{ref}} \overline{w' \frac{\mathbf{u}' \cdot \mathbf{u}'}{2} + w' p^\dagger}$ . Exchanges between the resolved and subgrid reservoirs of ki-  
 877 netic energy are done via the mechanical shear term  $\overline{w' \mathbf{u}'_h} \cdot \partial_z \bar{\mathbf{u}}_h$ . To close the budgets,  
 878 we will provide in the following sections a budget of internal and potential energy.

## 879 E2 Internal and Potential energies

880 For a generic fluid, the unaveraged specific internal energy can be written as

$$\mathcal{E}_i = \mathcal{h}(p, \phi) - \frac{p}{\rho} \quad (\text{E5})$$

881 where  $\mathcal{h}$  is the specific enthalpy and  $\phi$  is any entropic variable describing each compo-  
 882 nent of the fluid. Within the context of anelastic approximation, internal energy becomes

$$\mathcal{E}_i = \mathcal{h}(p_{\text{ref}}, \phi) - \frac{p_{\text{ref}}}{\rho_{\text{ref}}} \quad (\text{E6})$$

883 In particular, it implies within the anelastic approximation that  $b(\phi) := -g(\rho(p_{\text{ref}}, \phi) -$   
 884  $\rho_{\text{ref}})/\rho(p_{\text{ref}}, \phi)$ , where the specific volume can be defined as  $1/\rho(p_{\text{ref}}, \phi) = \partial_p \mathcal{h}(p_{\text{ref}}, \phi)$ .  
 885 The unaveraged budget of internal and potential energy then reads

$$\partial_t (\mathcal{E}_i + E_p) + \frac{1}{\rho_{\text{ref}}} \nabla \cdot [\rho_{\text{ref}} (\mathcal{h}(p_{\text{ref}}, \phi) + gz) \mathbf{u}] = \epsilon_\nu - wb \quad (\text{E7})$$

886 Upon averaging and using the SCM assumptions, the budget of mean internal energy  
 887  $E_i = \bar{\mathcal{E}}_i$  and potential energy reads

$$\partial_t (E_i + E_p) + \frac{1}{\rho_{\text{ref}}} \partial_z (\rho_{\text{ref}} \overline{\partial_\phi \mathcal{h}_{\text{ref}} w' \phi'}) = \bar{\epsilon}_\nu - \frac{1}{\rho_{\text{ref}}} \partial_z (\rho_{\text{ref}} (\overline{\phi w' \partial_\phi \mathcal{h}'_{\text{ref}}} + \overline{\phi' w' \partial_\phi \mathcal{h}'_{\text{ref}}})) - \overline{w' b'} \quad (\text{E8})$$

888 where we introduced the notation  $\overline{\mathcal{h}_{\text{ref}}(\phi)} = \mathcal{h}(p_{\text{ref}}, \phi)$ . Remark that if  $\mathcal{h}(p_{\text{ref}}, \phi)$  is lin-  
 889 ear in  $\phi$ , we have closed relations  $\overline{\mathcal{h}(p_{\text{ref}}, \phi)} = \mathcal{h}(p_{\text{ref}}, \bar{\phi})$  and  $\overline{b(\phi)} = b(\bar{\phi})$ .

890 As a summary, the budgets of mean kinetic energy, turbulent kinetic energy and  
 891 the sum of mean internal and potential energy are

$$\begin{cases} \partial_t E_k + \partial_z T_{E_k} & = \overline{w' \mathbf{u}'_h} \cdot \partial_z \bar{\mathbf{u}}_h \\ \partial_t k + \partial_z T_k & = -\overline{w' \mathbf{u}'_h} \cdot \partial_z \bar{\mathbf{u}}_h + \overline{w' b'} - \bar{\epsilon}_\nu \\ \partial_t (E_i + E_p) + \frac{1}{\rho_{\text{ref}}} \partial_z (\rho_{\text{ref}} \overline{\partial_\phi \mathcal{h}_{\text{ref}} w' \phi'}) & = \bar{\epsilon}_\nu - \frac{1}{\rho_{\text{ref}}} \partial_z (\rho_{\text{ref}} \overline{\phi w' \partial_\phi \mathcal{h}'_{\text{ref}}} + \overline{\phi' w' \partial_\phi \mathcal{h}'_{\text{ref}}}) - \overline{w' b'} \end{cases} \quad (\text{E9})$$

892 where conversion of  $E_k$  into  $k$  occurs via mean shear, conversion of  $k$  into  $E_i$  occurs via  
 893 viscous dissipation, and conversion of  $k$  into  $E_i + E_p$  occurs via buoyancy fluxes.

894 For a *dry atmosphere* modeled as an ideal gas  $p = \rho R_d T$ , the specific enthalpy  
895 reads

$$h(p_{\text{ref}}, \theta) = c_p \left( \frac{p_{\text{ref}}}{p_0} \right)^{R_d/c_p} \theta \quad (\text{E10})$$

896 which is linear in the potential temperature  $\theta = T(p/p_0)^{-R_d/c_p}$ . and buoyancy is  $b(\bar{\theta}) =$   
897  $g(\bar{\theta} - \theta_{\text{ref}})/\theta_{\text{ref}}$ . The budget of  $E_i + E_p$  is

$$\partial_t(E_i + E_p) = c_p \left( \frac{p_{\text{ref}}}{p_0} \right)^{R_d/c_p} \partial_t \bar{\theta} = \bar{\epsilon}_\nu - \frac{1}{\rho_{\text{ref}}} \partial_z \left( \rho_{\text{ref}} c_p \left( \frac{p_{\text{ref}}}{p_0} \right)^{R_d/c_p} \overline{w' \theta'} \right) - \frac{g}{\theta_{\text{ref}}} \overline{w' \theta'} \quad (\text{E11})$$

898 where  $\theta_{\text{ref}} = \left( \frac{p_{\text{ref}}}{p_0} \right)^{-R_d/c_p} \frac{p_{\text{ref}}}{\rho_{\text{ref}} R_d}$ . As a summary, the budgets of mean kinetic energy,  
899 turbulent kinetic energy and the sum of mean internal and potential energy for a *dry at-*  
900 *mosphere* within the anelastic approximation are

$$\begin{cases} \partial_t E_k + \partial_z T_{E_k} & = \overline{w' \mathbf{u}'_h} \cdot \partial_z \bar{\mathbf{u}}_h \\ \partial_t k + \partial_z T_k & = -\overline{w' \mathbf{u}'_h} \cdot \partial_z \bar{\mathbf{u}}_h + \frac{g}{\theta_{\text{ref}}} \overline{w' \theta'} - \bar{\epsilon}_\nu \\ c_p \left( \frac{p_{\text{ref}}}{p_0} \right)^{R_d/c_p} \partial_t \bar{\theta} & = \bar{\epsilon}_\nu - \frac{1}{\rho_{\text{ref}}} \partial_z \left( \rho_{\text{ref}} c_p \left( \frac{p_{\text{ref}}}{p_0} \right)^{R_d/c_p} \overline{w' \theta'} \right) - \frac{g}{\theta_{\text{ref}}} \overline{w' \theta'} \end{cases} \quad (\text{E12})$$

### 901 E3 EDMF-parameterized budget

902 Within the anelastic approximation, the budget of resolved kinetic energy, subgrid  
903 kinetic energy and resolved internal+potential energy for a *dry atmosphere* with EDMF  
904 closures is

$$\begin{cases} \partial_t E_k + \frac{1}{\rho_{\text{ref}}} \partial_z T_{E_k} & = -K_u (\partial_z \bar{\mathbf{u}}_h)^2 + a_p w_p (\mathbf{u}_{f,p} - \bar{\mathbf{u}}_h) \cdot \partial_z \bar{\mathbf{u}}_h \\ \partial_t k + \frac{1}{\rho_{\text{ref}}} \partial_z T_k & = \frac{g}{\theta_{\text{ref}}} [-K_\theta \partial_z \bar{\theta} + a_p w_p (\theta_p - \bar{\theta})] + K_u (\partial_z \bar{\mathbf{u}}_h)^2 - a_p w_p (\mathbf{u}_{f,p} - \bar{\mathbf{u}}_h) \cdot \partial_z \bar{\mathbf{u}}_h - \bar{\epsilon}_\nu \\ \partial_t \left[ c_p \left( \frac{p_{\text{ref}}}{p_0} \right)^{R_d/c_p} \bar{\theta} \right] & = -\frac{1}{\rho_{\text{ref}}} \partial_z T_{E_i + E_p} + \bar{\epsilon}_\nu - \frac{g}{\theta_{\text{ref}}} [-K_\theta \partial_z \bar{\theta} + a_p w_p (\theta_p - \bar{\theta})] \end{cases} \quad (\text{E13})$$

905 where the flux terms are

$$T_{E_k} = \rho_{\text{ref}} (-K_u \partial_z \bar{\mathbf{u}}_h + a_p w_p (\mathbf{u}_{f,p} - \bar{\mathbf{u}}_h)) \cdot \bar{\mathbf{u}}_h \quad (\text{E14})$$

$$T_k = -\rho_{\text{ref}} K_k \partial_z k + \rho_{\text{ref}} a_p w_p \left( k_p - k + \frac{1}{2} \|\mathbf{u}_p - \bar{\mathbf{u}}\|^2 \right) \quad (\text{E15})$$

$$T_{E_i + E_p} = \rho_{\text{ref}} c_p \left( \frac{p_{\text{ref}}}{p_0} \right)^{R_d/c_p} (-K_\theta \partial_z \bar{\theta} + a_p w_p (\theta_p - \bar{\theta})) \quad (\text{E16})$$

## 906 Appendix F Discretization of energetically consistent EDMF equa- 907 tions

908 We start from the standard grid arrangement used in oceanic models which are usu-  
909 ally discretized on a Lorenz grid in the vertical (density is located in the center of the  
910 cells on the vertical). We consider  $N$  grid cells in the vertical with thickness  $\Delta z_j = z_{j+1/2} -$   
911  $z_{j-1/2}$  ( $z_{1/2} = -H$  and  $z_{N+1/2} = 0$  the surface) such that  $\sum_{j=1}^N \Delta z_j = -H$ . Tradi-  
912 tionally, the turbulent quantities like turbulent kinetic energy  $k$  and eddy diffusivities  
913  $K_X$  are naturally located on the interfaces at  $z_{j+1/2}$  to avoid interpolations when com-  
914 puting the vertical gradients of the turbulent fluxes (Burchard, 2002). For the discrete  
915 values, not to interfere with the grid indices, the subscript  $p$  for the plume quantities is  
916 now a superscript such that plume quantities are now noted  $X_{j+1/2}^p = X_p(z = z_{j+1/2})$ .  
917 In the following, we consider that the plume quantities and  $k$  are discretized at cell in-  
918 terfaces and the mean quantities  $\bar{X}$  are discretized at cell centers and are interpreted in  
919 a finite-volume sense (i.e.  $\bar{X}_j = \frac{1}{\Delta z_j} \int_{z_{j-1/2}}^{z_{j+1/2}} \bar{X}(z) dz$ ). In the remainder, we consider  
920 the oceanic case with  $\sigma_o^a = -1$ .

921

## F1 Discretization of mass-flux equations

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We consider here the mass-flux equations given in Tab. 1 but in conservative form (except for the vertical velocity and TKE plume equations) :

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$$\partial_z(a_p w_p) = E - D \quad (\text{F1})$$

$$\partial_z(a_p w_p \phi_p) = E \bar{\phi} - D \phi_p \quad (\text{F2})$$

$$\partial_z(a_p w_p \mathbf{U}_p) = E \bar{\mathbf{U}} - D \mathbf{U}_p \quad (\text{F3})$$

$$w_p \partial_z w_p = -(E/a_p)(b w_p) + a B_p + b' w_p^2 \quad (\text{F4})$$

$$a_p w_p \partial_z k_p = E \left( k - k_p + \frac{1}{2} (\bar{\mathbf{u}}_p - \bar{\mathbf{u}})^2 \right) - a_p (\epsilon_\nu)_p \quad (\text{F5})$$

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where the equation for horizontal momentum has been manipulated to have the same form as the  $\phi_p$  equation by taking  $\mathbf{U}_p = \mathbf{u}_{h,p} - C_u \bar{\mathbf{u}}_h$  and  $\bar{\mathbf{U}} = (1 - C_u) \bar{\mathbf{u}}_h$ . The advective form is used for the  $w_p$  equation to make the computation of  $w_p$  independent of  $a_p$  (with the closure hypothesis (25) for  $E$ ,  $E/a_p$  is independent of  $a_p$ ); the motivations for this will become clearer later. The mass-flux equations correspond to a first-order nonlinear set of ODEs. There are a whole lot of methods for solving such initial value problems. We present here a simple method combining explicit (Euler) and semi-implicit (Crank-Nicolson) steps as the use of more advanced methods did not produce significantly different results. In the following, we describe the different steps for the resolution starting from known initial values  $X_{N+1/2}^p$  at the surface and advancing downward.

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### F11 Initial conditions

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The discrete form of the initial conditions given in 2.4 are obtained by a linear extrapolation of  $\bar{\phi}_N$  and  $(\bar{\mathbf{u}}_h)_N$  toward the surface.

$$\begin{aligned} w_{N+1/2}^p &= -w_{\min}^p \\ \phi_{N+1/2}^p &= \frac{(2\Delta z_N + \Delta z_{N-1})\bar{\phi}_N - \Delta z_N \bar{\phi}_{N-1}}{\Delta z_N + \Delta z_{N-1}} \\ \mathbf{U}_{N+1/2}^p &= (1 - C_u) \frac{(2\Delta z_N + \Delta z_{N-1})(\bar{\mathbf{u}}_h)_N - \Delta z_N (\bar{\mathbf{u}}_h)_{N-1}}{\Delta z_N + \Delta z_{N-1}} \end{aligned} \quad (\text{F6})$$

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Since the TKE  $k$  is already discretized at cell interfaces the boundary condition for  $k_p$  does not require an extrapolation. In particular the condition on  $\phi_p$  leads to the following value of the  $B_p$  term in the topmost grid cell :

$$B_N^p = \Delta z_N \left( \frac{\bar{b}_N - \bar{b}_{N-1}}{\Delta z_N + \Delta z_{N-1}} \right) = \frac{\Delta z_N}{2} (N^2)_{N-1/2}$$

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meaning that using the condition (F6) allows to trigger convection as soon as the Brunt-Väisälä frequency is negative. Indeed a negative value of  $B_N^p$  in the RHS of the  $w_p$ -equation (F4) leads to a positive value of  $(\partial_z w_p)_N$  and thus larger negative values of  $w_p$  when going downward.

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### F12 $w_p$ -equation

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The  $w_p$ -equation (F4) using the entrainment  $E$  given in (25) can be formulated as

$$\partial_z w_p^2 + b \beta_1 \min(\partial_z w_p^2, 0) = 2a B_p + 2b' w_p^2$$

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which can be discretized in a straightforward way as

$$\begin{aligned} \tilde{\beta} \left[ (w^p)_{j+1/2}^2 - (w^p)_{j-1/2}^2 \right] &= 2a \Delta z_j B_j^p - \sigma_o^a (b' \Delta z_j) \left[ (w^p)_{j+1/2}^2 + (w^p)_{j-1/2}^2 \right] \\ B_j^p &= b_{\text{eos}}(\phi_{j+1/2}^p) - b_{\text{eos}}(\bar{\phi}_j) \end{aligned} \quad (\text{F7})$$

947 where  $\tilde{\beta} = 1 + b\beta_1$  if  $aB_j^p - \sigma_o^a b'(w^p)_{j+1/2}^2$  is negative and  $\tilde{\beta} = 1$  otherwise. Knowing  
 948  $w_{j+1/2}^p$ , it is easily found that

$$(w^p)_{j-1/2}^2 = \frac{(\tilde{\beta} - b'\Delta z_j)(w^p)_{j+1/2}^2 - 2a\Delta z_j B_j^p}{\tilde{\beta} + b'\Delta z_j}$$

949 Once this quantity falls below a certain threshold  $(w_{\min}^p)^2$ , the plume is considered evanes-  
 950 cent. In the oceanic context we consider  $w_{j-1/2}^p = -\sqrt{(w^p)_{j-1/2}^2}$  for the rest of the cal-  
 951 culations to guarantee that  $w_{j-1/2}^p$  is strictly negative. The upwinding used to compute  
 952  $B_p$  in (F7) in addition to the fact that the  $w_p$ -equation does not depend on  $a_p$  avoid the  
 953 need for an iterative process to solve the mass-flux equations.

### 954 **F13 Continuity and tracer equations**

955 The entrainment  $E_j$  and detrainment  $D_j$  rates given in (25) and (26) discretized  
 956 on a grid cell  $j$  correspond to

$$\begin{aligned}\Delta z_j E_j &= \frac{1}{2} \left( a_{j+1/2}^p + a_{j-1/2}^p \right) \beta_1 (\delta_z w^p)_j^+ \\ \Delta z_j D_j &= \frac{1}{2} \left( a_{j+1/2}^p + a_{j-1/2}^p \right) \left[ -\beta_2 (\delta_z w^p)_j^- - \frac{\delta_0 \Delta z_j}{2} (w_{j+1/2}^p + w_{j-1/2}^p) \right]\end{aligned}$$

957 where  $(\delta_z w^p)_j^+ = \max(w_{j+1/2}^p - w_{j-1/2}^p, 0)$  and  $(\delta_z w^p)_j^- = \min(w_{j+1/2}^p - w_{j-1/2}^p, 0)$ .  
 958 Integrating from  $z_{j-1/2}$  to  $z_{j+1/2}$  the continuity equation and  $\phi_p$  equations we obtain

$$\begin{aligned}(a^p w^p)_{j+1/2} - (a^p w^p)_{j-1/2} &= \Delta z_j (E_j - D_j) \\ (a^p w^p \phi^p)_{j+1/2} - (a^p w^p \phi^p)_{j-1/2} &= \Delta z_j E_j \bar{\phi}_j - (\Delta z_j D_j / 2) (\phi_{j+1/2}^p + \phi_{j-1/2}^p)\end{aligned}$$

959 which can also be extended to the horizontal momentum equation formulated using  $U_p$ .  
 960 Since at this stage  $w_{j+1/2}^p$  and  $w_{j-1/2}^p$  are known, the continuity equation is used to com-  
 961 pute  $a_{j-1/2}^p$  through

$$\begin{aligned}a_{j-1/2}^p &= a_{j+1/2}^p \left\{ \frac{2w_{j+1/2}^p - \text{Em}D_j}{2w_{j-1/2}^p + \text{Em}D_j} \right\} \\ \text{Em}D_j &= \beta_1 (\delta_z w^p)_j^+ + \beta_2 (\delta_z w^p)_j^- + \min \left\{ \frac{\delta_0 \Delta z_j}{2} (w_{j+1/2}^p + w_{j-1/2}^p), -2(w_{\min}^p) \right\} \quad (\text{F8})\end{aligned}$$

962 Note that  $a_p$  is subject to a boundedness requirement as  $0 \leq a_p \leq 1$ . Assuming  $0 \leq$   
 963  $a_{j+1/2}^p \leq 1$ , sufficient conditions to guarantee that  $a_{j-1/2}^p \leq 1$  are  $\beta_1 \leq 1$  and  $\beta_2 \geq$   
 964  $1$  and a sufficient condition to guarantee that  $a_{j-1/2}^p \geq 0$  is  $\beta_2 < 2$ . Moreover a con-  
 965 straint is added on the background detrainment  $\delta_0$  in (F8) to guarantee that  $a_{j-1/2}^p =$   
 966  $0$  as soon as  $w_{j+1/2}^p = w_{j-1/2}^p = -w_{\min}^p$  which occurs once outside the plume.

967 Once  $a_{j-1/2}^p$  is known, it is possible to compute  $\phi_{j-1/2}^p$  (as well as  $U_{j-1/2}^p$ ). The  
 968 proposed discretization ensures that the compatibility between the continuity and the  
 969 tracer equations is maintained at the discrete level (*i.e.* we recover the continuity equa-  
 970 tion for  $\phi_{j+1/2}^p = \phi_{j-1/2}^p = 1$  and  $\bar{\phi}_j = 1$ ).

971 The same reasoning can be applied to solve the  $k_p$  equation, which presents no ad-  
 972 ditional difficulties as all necessary quantities  $w_{j\pm 1/2}^p$ ,  $a_{j\pm 1/2}^p$  and  $u_{j\pm 1/2}^p$  are known.

973 In summary, the proposed discretization guarantees that  $w_p$  is strictly negative, that  
 974  $a_p$  is bounded between 0 and 1, and that the continuity and tracer equations are com-  
 975 patible, without the need for an iterative solution procedure.



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## F2 Energy consistent discretization of turbulent kinetic energy

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In Burchard (2002) an energetically consistent discretization of the turbulent shear and buoyancy production terms for the TKE equation in the ED case is derived. Such methodology can be extended in the EDMF case to discretize the MF-related TKE production terms given in magenta and cyan in Tab. 2. Starting from a simple Euler-upwind discretization of mass-flux terms in the  $\bar{\mathbf{u}}_h$  and  $\bar{\phi}$  equations which can be written generically for a variable  $X$

$$\frac{\bar{X}_j^{n+1} - \bar{X}_j^n}{\Delta t} = \frac{F_{j+1/2}^{\text{MF}} - F_{j-1/2}^{\text{MF}}}{\Delta z_j}$$

$$F_{j+1/2}^{\text{MF}} = (a^p w^p)_{j+1/2} (\bar{X}_{j+1/2}^p - \bar{X}_j^n)$$

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the kinetic and potential energy budgets can be derived by multiplying the velocity equations (*i.e.*  $\bar{X} = u$ ) by  $(\bar{u}_j^{n+1} + \bar{u}_j^n)/2$  and the buoyancy equation by  $-z_j$ . After some simple algebra, we obtain that

$$(a_p w_p (\mathbf{u}_{h,p} - \bar{\mathbf{u}}_h) \cdot \partial_z \bar{\mathbf{u}}_h)_{j+1/2} = (a_p w_p)_{j+1/2} \left( (\mathbf{u}_h)_{j+1/2}^p - (\mathbf{u}_h)_j^n \right) \cdot \left( \frac{(\mathbf{u}_h)_{j+1}^{n+1} + (\mathbf{u}_h)_{j+1}^n - (\mathbf{u}_h)_j^{n+1} - (\mathbf{u}_h)_j^n}{2\Delta z_{j+1/2}} \right)$$

$$(a_p w_p (b_p - \bar{b}))_{j+1/2} = (a_p w_p)_{j+1/2} B_j^p$$

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where  $B_j^p$  is given in (F7). Using these discrete forms for the MF-related TKE production terms combined with the discretization of the turbulent shear and buoyancy production terms derived in Burchard (2002) ensure the proper energy flux between resolved and subgrid energies.

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## F3 Coupling ED and MF schemes

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In the EDMF approach, the usual vertical diffusion/viscous subgrid terms are completed by an advective term so that the following equation must be advanced in time:

$$\partial_t \bar{X} = \partial_z (K_X \partial_z \bar{X}) - \partial_z (a_p w_p (X^p - \bar{X})) \quad (\text{F9})$$

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This amounts to couple a boundary layer scheme which provides  $K_X$  and a convection scheme which provides  $a_p w_p$  and  $X^p$ . The numerical treatment of such coupling is rarely discussed in the literature. This problem can be approached in 2 ways: either by integrating the 2 schemes sequentially or in parallel. For the numerical experiments discussed in Sec. 5 we chose a *boundary layer-then-convection* strategy corresponding to the following temporal integration for the single-column model (leaving aside the Coriolis and solar penetration terms)

ED step

$$\phi^{n+1,*} = \phi^n + \Delta t \partial_z (K_\phi (k^n, b^n) \partial_z \phi^{n+1,*})$$

$$\mathbf{u}_h^{n+1,*} = \mathbf{u}_h^n + \Delta t \partial_z (K_u (k^n, b^n) \partial_z \mathbf{u}_h^{n+1,*})$$

$$b^{n+1,*} = b_{\text{eos}}(\phi^{n+1,*})$$

MF step

$$[a_p, w_p, \phi_p, \mathbf{u}_{h,p}, k_p, B_p] = \text{MF}(b^{n+1,*}, \mathbf{u}_h^{n+1,*})$$

$$\phi^{n+1} = \phi^{n+1,*} - \Delta t \partial_z (a_p w_p (\phi_p - \phi^{n+1,*}))$$

$$\mathbf{u}_h^{n+1} = \mathbf{u}_h^{n+1,*} - \Delta t \partial_z (a_p w_p (\mathbf{u}_{h,p} - \mathbf{u}_h^{n+1,*}))$$

TKE update

$$k^{n+1} = k^n + \Delta t \partial_z (K_k (k^n, b^n) \partial_z k^{n+1}) + \mathcal{F}_k(b^{n+1}, \mathbf{u}_h^{n+1}, \mathbf{u}_h^n, a_p, w_p, \mathbf{u}_{h,p}, k_p, B_p)$$

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where the MF(.) function represents the computation of mass-flux quantities as described previously and  $\mathcal{F}_k$  contains the TKE transport and forcing terms. The "ED step" is clas-

1002 sically computed using an Euler backward scheme. With the proposed approach, the con-  
 1003 vection scheme sees a state already updated by the boundary layer scheme (and by the  
 1004 solar penetration and non-solar surface heat flux which are applied during the "ED step")  
 1005 The convection scheme thus sees a state whose static stability is representative of the  
 1006 current time-step and external forcing.

1007 Ultimately, with the proposed approach, the various stages can be expressed di-  
 1008 rectly as follows

$$\begin{aligned}\phi^{n+1} &= \phi^n + \Delta t \partial_z (K_\phi \partial_z \phi^{n+1,*} - a_p w_p (\phi_p - \phi^{n+1,*})) \\ [a_p, w_p, \phi_p] &= \text{MF}(\phi^{n+1,*})\end{aligned}$$

1009 which reflects the fact that we have good synchronization between the ED part and the  
 1010 MF part, which see the same mean fields. On the other hand, the approach of simulta-  
 1011 neously considering the ED and MF parts in a single tridiagonal problem would lead to

$$\begin{aligned}\phi^{n+1} &= \phi^n + \Delta t (K_\phi \partial_z \phi^{n+1} - a_p w_p (\phi_p - \phi^{n+1})) \\ [a_p, w_p, \phi_p] &= \text{MF}(\phi^n)\end{aligned}$$

1012 In this case, the mass flux is applied to the mean fields at time  $n$  thus breaking the syn-  
 1013 chronization between the ED and MF parts. Indeed  $\phi_p$  has been computed using  $\phi^n$  while  
 1014 it is applied at time  $n + 1$ .

## 1015 Open Research

### 1016 Data Availability Statement

1017 Data from the Lion mooring (located in the Gulf of Lion; Mediterranean sea) are  
 1018 freely accessible from Bosse et al. (2023). The output from LES simulations and the ini-  
 1019 tial and surface boundary conditions for the Hymex/ASICS-MED experiments are avail-  
 1020 able at [Zenodo link here](#).

### 1021 Software Availability Statement

1022 All the numerical codes used in this study have been made available and can be  
 1023 found at [Zenodo link here](#). It includes the single-column model with Eddy-Diffusivity  
 1024 Mass-Flux turbulent closure developed from scratch. The latter consists of low-level code  
 1025 written in Fortran interfaced with Python using F2PY (Peterson, 2009). The single-column  
 1026 simulations analyzed in this study can be executed from a high-level Python driver code  
 1027 without any intervention on the Fortran code. The high-level Python driver code and  
 1028 scripts to reproduce the figures are available in the Zenodo archive. The Fortran code  
 1029 contains inline documentation following the FORD (Fortran Documenter) format.

## 1030 Acknowledgments

1031 This work was supported by the *institut des Mathématiques pour la Planète Terre* (iMPT)  
 1032 through the project "Coherent sub-grid scale modeling for ocean climate models". This  
 1033 study was carried out as part of the technological defense project PROTEVS2 under the  
 1034 auspices of the French Ministry of the Armies / DGA. MP was supported by a PhD fel-  
 1035 lowship from Ecole Normale Supérieure Paris. The authors are extremely grateful to Jean-  
 1036 Luc Redelsperger for his essential contributions to the MESO-NH model and Thomas  
 1037 Dubos for constructive comments on an earlier version of this paper. This research was  
 1038 funded in part by l'Agence Nationale de la Recherche (ANR), project ANR-23-CE01-  
 1039 0009.

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