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

M. Perrot^{1,*}, F. Lemarié¹ 3 ¹Univ Grenoble Alpes, Inria, CNRS, Grenoble INP, LJK, Grenoble, France 4 **Key Points:** 5 • An Eddy-Diffusivity Mass-Flux parameterization is carefully derived from first prin-6 ciples, making the underlying assumptions explicit 7 • Closed energy budgets between resolved and subgrid energy reservoirs are outlined, 8 including a new formulation of vertical TKE transport 9 • Comparisons with Large Eddy Simulations show that the new scheme successfully 10

reproduces TKE and its vertical transport

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12 Abstract

This study aims to introduce a new convective vertical mixing scheme rooted in the Eddy-13 Diffusivity Mass-Flux (EDMF) approach, itself derived from first principles. The inte-14 gration of the mass-flux (MF) concept with the Eddy-Diffusivity (ED) approach has long 15 been studied and applied in global and regional atmospheric models for parameterizing 16 convection, both dry and cloudy, and sees a growing interest in ocean models. This type 17 of closure involves separating vertical turbulent fluxes into two components: a diffusion 18 term that addresses local small-scale mixing in a near isotropic environment and a mass-19 flux transport term that accounts for the non-local transport due to vertically coherent 20 plumes within the environment. Here, we exploit the multi-fluid averaging technique un-21 derlying the MF concept to propose an original formulation of a scheme that possesses 22 properties not satisfied by most existing EDMF formulations. Consistent energy bud-23 gets between resolved and subgrid scales are derived for different multi-component flu-24 ids including seawater and dry atmosphere (in Boussinesq and anelastic cases). This guar-25 antees that all mean kinetic, potential, and internal energy sinks and sources as long as 26 turbulent kinetic energy (TKE) transport associated with EDMF terms are exactly added 27 or subtracted to the TKE budget, effectively rectifying energy biases existing in prior 28 EDMF schemes. Notably, this analysis facilitates a clear separation of convective and 29 turbulent small-scale energy reservoirs. In addition to bulk energy transfers, we provide 30 guidelines to avoid spurious energy fluxes at the fluid's boundary when using EDMF. 31 We illustrate the performance of the proposed *energetically consistent EDMF scheme* 32 in the context of oceanic convection. When compared with Large Eddy Simulations (LES) 33 of oceanic convection, our scheme can reproduce mean fields as well as higher-order mo-34 ments such as TKE, vertical fluxes, and turbulent transport of TKE. The energetic con-35 sistency is key to obtaining realistic TKE and turbulent transport of TKE profiles. To 36 further illustrate that the MF concept is a credible alternative to the traditional approaches 37 used in the oceanic context (using an enhanced vertical diffusion or a counter gradient 38 term \dot{a} la KPP) the proposed scheme is validated in a single-column configuration against 39 observational data of oceanic convection from the LION buoy. Last but not least, dur-40 ing the theoretical development of the scheme, we maintain transparency regarding un-41 derlying assumptions and systematically assess their validity in the light of LES data. 42

⁴³ Plain Language Summary

In Earth system models, various important processes occur on scales that are too 44 fine to be resolved with usual grid resolutions. Parameterizations have to be used to ap-45 proximate the average effect of such processes on the scales resolved by a numerical model. 46 The general objective of the proposed work is to approach the parameterization prob-47 lem for boundary-layer turbulence and convective plumes in a "consistent" manner. Here 48 the notion of consistency integrates various aspects: global energetic consistency, con-49 sistency with a particular averaging technique for the scale-separation, and the rigorous 50 reduction of a physical system to a scale-aware parametric representation based on well-51 identified and justifiable approximations and hypotheses. An originality is to jointly con-52 sider energy budgets including a subgrid energy reservoir on top of the resolved ener-53 gies allowing the proper coupling between the parameterization and the resolved fluid 54 dynamics. This research is fundamental to obtain an apt representation of mean fields 55 and higher-order turbulent moments and to pave the way toward an alternative method-56 ology to parameterize oceanic convection across scales. Numerical simulations demon-57 strate the adequacy of the proposed parameterization. 58

⁵⁹ 1 Introduction

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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 buoy-62 ancy fluxes at the surface, which trigger gravitational instabilities. Buoyant plumes then 63 tend to overturn and mix the fluid. When looking at the mean properties of the fluid, 64 it leads to the formation of a well-mixed layer. The accurate representation of such bound-65 ary layers is of paramount importance for short-term forecasts as well as for climate pro-66 jections in the atmosphere (Bony et al., 2015; Schneider et al., 2017) and the ocean (Martin 67 et al., 2013; Piron et al., 2016; Moore et al., 2015; Fox-Kemper et al., 2019). Regarding 68 current computational capacities, plumes are still unresolved in regional and global nu-69 merical models, and thus their effects require parameterization. Moreover in ocean mod-70 eling, beyond the requirement in terms of grid resolution, hydrostatic equations used in 71 the overwhelming majority of regional and global studies are not suitable for resolving 72 convective phenomena explicitly (Marshall et al., 1997). 73

For any quantity X, standard turbulent mixing models are based on the closure 74 of vertical turbulent fluxes $\overline{w'X'}$ proportional to the local mean gradient in the form $-K_X \partial_z \overline{X}$ 75 (which corresponds to the so-called Eddy-Diffusivity (ED) closure). Such a closure leads 76 to a diffusion of \overline{X} , which is often justified by considering that turbulent fluctuations re-77 semble Brownian motion (Vallis, 2017; Resseguier et al., 2017). Although the ED clo-78 sure has been widely used in many industrial and geophysical applications, it is known 79 to potentially predict incorrectly higher order moments and even mean fields for com-80 plex flows (e.g. Schmitt, 2007). For instance, the inadequacy of ED closures for atmo-81 spheric convection has long been highlighted (Deardorff, 1966). Indeed fluctuations are 82 carried by non-local structures, the buoyant plumes, that can be coherent over the whole 83 mixed layer. In particular, in such a layer, mean gradients are close to zero $(\partial_z X \simeq 0)$ 84 while transport is ensured at leading order by non-zero vertical fluxes $\overline{w'X'}$ which may 85 even be up-gradient. Indeed, using the assumption of a mixed-layer $\partial_z \overline{X} \simeq 0$ into a tur-86 bulent transport equation of the type $\partial_t \overline{X} + \partial_z \overline{w'X'} = 0$ implies that $\overline{w'X'}$ varies lin-87 early with z. Such linear variation of fluxes in the mixed layer is well-supported by ob-88 servations and numerical experiments (Garratt, 1994b; Denbo & Skyllingstad, 1996). 89

To circumvent ED hypothesis, Deardorff (1966) proposed to introduce a constant 90 non-local term γ_X in the form $\overline{w'X'} = -K_X(\partial_z \overline{X} - \gamma_X)$. Later on, such a formula-91 tion has been refined, where both K_X and γ_X were prescribed by a self-similar profile 92 function depending on external characteristics of the boundary layer such as surface forc-93 ing, stratification at the atmospheric top (or oceanic base) of the mixed layer and im-94 plicitly 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 96 is still in use in some present-day ocean models (e.g. via the CVMIX library, Van Roekel 97 et al., 2018). Furthermore, in the context of ocean models, two other types of convec-98 tive parameterization are sometimes used: (i) a buoyancy sorting scheme (a.k.a. adjust-99 ment scheme or non-penetrative scheme), in which static instabilities are eliminated in 100 one time-step by mixing downward neighboring vertical levels until a neutral buoyancy 101 profile is attained (e.g. Madec et al., 1991) (ii) an enhanced eddy-viscosity scheme in 102 which the vertical diffusivity coefficient is artificially increased to a high value as soon 103 as static instabilities are found on the density profiles. These two approaches are not grounded 104 on a physical derivation. 105

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 convective 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)).

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1.2 Parameterization development and physics dynamics coupling

The general objective of the proposed work is to approach the parameterization 118 problem in a "consistent" manner. Here the notion of consistency integrates various as-119 pects: consistency with the laws of physics, energetic consistency at both continuous (e.g. 120 Eden, 2016; Jansen et al., 2019; Eden & Olbers, 2014) and discrete (e.g. Burchard, 2002) 121 levels, consistency with a particular choice of scale-separation operator (Higgins et al. 122 2013; Lauritzen et al., 2022), and the rigorous reduction of a physical system to a scale-123 aware parametric representation based on well-identified approximations and hypothe-124 ses (Honnert et al., 2016; Tan et al., 2018). 125

Regarding boundary layer parameterizations, eddy-diffusivity intensity often scales 126 with the turbulent kinetic energy (TKE) which is computed via a parameterized prog-127 nostic equation. TKE represents a subgrid kinetic energy that exchanges energy with 128 the resolved reservoirs. The use of mass-flux terms leads to energy transfers and redis-129 tributions that must be taken into account in the TKE equation to ensure energetic con-130 sistency between resolved and subgrid scales. In addition, the boundary conditions of 131 the mass-flux equations must be consistent between ED and MF to avoid double-counting 132 and artificial energy fluxes at the fluid boundary. Apart from a brief discussion in Tan 133 et al. (2018) for unsteady plume models, the energetically consistent coupling of TKE 134 and standard EDMF schemes has not been, to our knowledge, discussed in the litera-135 ture. Some modifications of the TKE equation when using a mass-flux model have been 136 proposed for the buoyancy production term (Witek et al., 2011b) and the vertical tur-137 bulent transport of TKE (Witek et al., 2011a; Han & Bretherton, 2019). However, these 138 studies are not motivated by considerations of energetic consistency. 139

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1.3 Goals and organisation of the paper

The aim of this paper is two-fold. First, we intend to provide an introductory, self-141 contained, and pedagogical derivation of EDMF schemes starting from first principles. 142 to guide consistency considerations. Second, we derive theoretical energy budgets and 143 provide guidelines to obtain energetically consistent EDMF models. Consequently, this 144 paper is intended to both the oceanographic community as a pedagogical introduction 145 to EDMF, and the atmospheric community seeking to reduce energy biases in EDMF 146 models. The paper is organized as follows. In section 2, we expose the derivation of an 147 EDMF scheme from first principle, systematically discuss the successive assumptions at 148 stake, provide closures according to state-of-the-art practice, and discuss consistent bound-149 ary conditions. In section 3, we recall the theoretical resolved and subgrid energy bud-150 gets of a horizontally averaged Boussinesq fluid without closures. In section 4, we ex-151 pose the necessary modification of the parameterized turbulent kinetic energy (TKE) 152 equation to obtain closed energy budgets when using EDMF. Furthermore, we derive ver-153 tically averaged energy budgets to reveal the role of boundary conditions on the energy 154 fluxes. In section 5, we analyze the assumptions used in the derivation of the scheme in 155 light of data from Large Eddy Simulation (LES) of idealized oceanic deep convection. 156 157 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, 158 we provide discretization details for interested model developers and energy budgets in 159 the anelastic setting which are more commonly used by the atmospheric community. 160

¹⁶¹ 2 Derivation of EDMF scheme

162 2.1 Formal derivation

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

$$\nabla \cdot \boldsymbol{u} = 0 \tag{1}$$

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

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

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

where $\boldsymbol{u} = (u, v, w)$ denotes the velocity field in a local Cartesian frame of reference $(\boldsymbol{e}_x, \boldsymbol{e}_y, \boldsymbol{e}_z)$, 165 z ranges from 0 to H in the atmosphere and -H to 0 in the ocean, ρ_0 is a constant ref-166 erence density, the pressure has been decomposed as $p = p_{ref}(z) + p^{\dagger}(x, y, z, t)$ with 167 $\partial_z p_{\rm ref} = -\rho_0 g, b$ is the buoyancy acceleration, ϕ is any entropic variable describing each 168 component of the fluid, S_{ϕ} is an additional source term (typically molecular diffusion). 169 For instance, in the context of a dry atmosphere modeled as an ideal gas, a simple choice¹ 170 would be $\phi = \theta$, where θ is the potential temperature, and $b_{eos}(\theta) = g(\theta - \theta_0)/\theta_0$. In 171 the context of ocean dynamics, one would choose conservative temperature and salin-172 ity $(\phi = \theta, S)$ and a linear equation of state, $b_{eos}(\theta, S) = g\alpha(\theta - \theta_0) - g\beta(S - S_0)$ where 173 α and β are thermal expansion and haline contraction coefficients, respectively, and θ_0 174 and S_0 are reference temperature and salinity. Details on source terms S_{ϕ} are given in 175 section 3. For the sake of simplicity, we do not include the Coriolis term in the present 176 study. Since the Coriolis force is energetically-neutral it does not interfere with the deriva-177 tions made throughout this paper. Next, we explicit the framework in which vertical mix-178 ing parameterizations are usually developed. We adopt a semi-discrete approach, where 179 the horizontal fluid domain is divided into a $N_x \times N_y$ mesh. Each horizontal grid cell 180 has length Δx_i and width Δy_j , and we denote (x_i, y_j) its center. Note that the time and 181 vertical coordinates z are kept *continuous*. The spatial domain can be thought of $N_x \times$ 182 N_{y} vertical columns stacked together. In a numerical model discretized on such a mesh, 183 the computed variables would be interpreted in a finite volume approach (LeVeque, 2002). 184 For any field $X = u, \phi$... one can define the following horizontal average and fluctua-185 186 tion

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

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

$$\partial_t \overline{X} + \partial_z \left(\overline{w} \overline{X} + \overline{w' X'} \right) + \frac{1}{\Delta x_i \Delta y_j} \oint_{\partial (\Delta x_i \times \Delta y_j)} X \boldsymbol{u}_h \cdot \mathrm{d}\boldsymbol{n} = \overline{S}_X \tag{5}$$

where $\boldsymbol{u}_h = (u, v, 0)$ denotes the horizontal velocity vector and d \boldsymbol{n} is an outward point-189 ing line integral element, i.e. $u_h \cdot dn = u dy - v dx$. The boundary integral in (5) is the 190 total (resolved and subgrid) horizontal flux of X. In a numerical model, X would be in-191 terpreted as the resolved variable, X' would be an unresolved fluctuation, the precise form 192 of the horizontal flux would depend on the numerical scheme (and possibly on param-193 eterizations), and the vertical subgrid flux $\overline{w'X'}$ has to be closed by a parameterization. 194 When focusing on the parameterization of vertical mixing processes, it is common to con-195 ceptually isolate one vertical column of fluid to work with a one-dimensional Single-Column 196

¹ 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

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

$$\partial_t \overline{\boldsymbol{u}}_h = -\partial_z \overline{\boldsymbol{w}' \boldsymbol{u}'_h} \tag{6}$$

$$\partial_t \overline{\phi} = -\partial_z \overline{w'\phi'} + \overline{S}_\phi \tag{7}$$

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

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

$$X_i = \frac{1}{\mathcal{A}_i(z,t)} \int_{\mathcal{A}_i(z,t)} X(x,y,z,t) \, \mathrm{d}x \mathrm{d}y$$
$$a_i = \mathcal{A}_i(z,t) / (\Delta x \times \Delta y)$$

Any mean field can then be decomposed as

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

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

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

222 where

$$\overline{w_i'X_i'} = \frac{1}{\mathcal{A}_i(z,t)} \int_{\mathcal{A}_i(z,t)} (X - X_i)(w - w_i) \, \mathrm{d}x \mathrm{d}y$$

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

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

where the relative horizontal boundary velocity is $\boldsymbol{u}_r = \boldsymbol{u}_h - \partial_t \boldsymbol{r}_b - w \partial_z \boldsymbol{r}_b$ and $\boldsymbol{r}_b = (x_b(z,t), y_b(z,t))$ is the position vector of boundary elements. The three terms that consitute \boldsymbol{u}_r indicate that boundary fluxes can arise respectively due to horizontal velocity across the boundary, to (apparent) horizontal velocity of the boundary, or to vertical velocity if the boundary of the 3D plume is vertically tilted (i.e. $\partial_z \boldsymbol{r}_b \neq 0$). 233 2.2 Standard assumptions

2.2.1 Plume-Environment decomposition

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

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2.2.2 Entrainment/Detrainment and Upstream approximation

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

$$\frac{1}{\mathcal{A}_p} \oint_{\partial \mathcal{A}_p} \boldsymbol{u}_r \cdot \mathrm{d}\boldsymbol{n} = \frac{1}{\mathcal{A}_p} \oint_{\partial \mathcal{A}_p, \boldsymbol{u}_r > 0} \boldsymbol{u}_r \cdot \mathrm{d}\boldsymbol{n} + \frac{1}{\mathcal{A}_p} \oint_{\partial \mathcal{A}_p, \boldsymbol{u}_r < 0} \boldsymbol{u}_r \cdot \mathrm{d}\boldsymbol{n}$$
$$= D - E$$

where E(>0) is called *entrainment rate* and D(>0) is called *detrainment rate*. We further assume that the value of X at the boundary is either equal to the mean value in the environment when entrainment is occurring, or the mean value in the plume when detrainment is occurring. This is the so-called *upstream approximation*, formulated as²

$$\frac{1}{\mathcal{A}_p} \oint_{\partial \mathcal{A}_p} X \boldsymbol{u}_r \cdot \mathrm{d}\boldsymbol{n} = X_e E - X_p D \tag{10}$$

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

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

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

$$\partial_t a_p + \partial_z (a_p w_p) = E - D \tag{12}$$

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2.2.3 Steady plume hypothesis

A common hypothesis is that the plume domain is in a quasi-steady regime, thus neglecting the temporal tendency compared to vertical advection. The relevance of this hypothesis is numerically tested using idealized cases in section 5.3. An *a priori* scaling estimation can also be performed. Introducing τ , h, and W the characteristic time, depth, and vertical velocity scales of the plume, the order of magnitude of the ratio between the temporal tendency and vertical advection can be estimated as follows

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

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

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

² 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 $\nabla_h \cdot (a_p \boldsymbol{u}_{h,p} X_p + a_p \overline{\boldsymbol{u}'_{h,p} X'_p})$ (see section 5.1 of Yano (2014)).

In a different context, that of the development of a shear-driven mixed layer forced by 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 such a layer $W \simeq u_*$, leading to a scaling similar to (14). These scalings suggest that as long as the surface forcings (represented here by u_* and B_0) are evolving slowly compared to $1/N_0$, the steady plume hypothesis remains valid. Under such a hypothesis, the plume equation for any field X now reads

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

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

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

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

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

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

274 2.2.4 Small area limit

A last standard hypothesis is that the fractional area of the plume is *small* compared to that of the environment (see section 5.3 for a direct evaluation against LES). This generally means considering the formal limit $a_p \to 0$ and $a_e \to 1$ in the previous equations while keeping non-zero mass-flux $a_p w_p$ and source terms. Yano (2014) proposes 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 of $a_p w_p (X_p - \overline{X})$ in (17), and to keep an order one contribution of advection and forcings in (18). In the small area limit, any environmental field X_e (except w_e) can be approximated by the mean field, the vertical turbulent flux (17) becomes

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

and the plume equation (18) now reads

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

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

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

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

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

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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.

311 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

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

leading to the plume vertical momentum budget

$$a_p w_p \partial_z w_p = a a_p B_p - b E w_p - \sigma_o^a b' a_p w_p^2 \tag{22}$$

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

323 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

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

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

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, $\overline{w'_e X'_e} = -K_X \partial_z X_e \underset{a_p \ll 1}{\simeq} -K_X \partial_z \overline{X}$. This leads to the eddy-diffusivity mass-flux closure of subgrid fluxes

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

In the present study, the eddy viscosity K_u and diffusivity K_{ϕ} in turbulent vertical fluxes are computed from a turbulence closure model based on a prognostic equation for the turbulent kinetic energy (TKE) $k = \overline{u' \cdot u'}/2$ and a diagnostic computation of appropriate length scales (a.k.a. 1.5-order turbulence closure). For the numerical tests in the oceanic context presented in Sec. 5, we use a formulation close to that of the Nucleus for European Modelling of the Ocean model (NEMO, Madec et al., 2019). The eddyviscosity and diffusivity are classically assumed to be related to TKE by

$$K_u = c_m l_m \sqrt{k}$$
$$K_\phi = K_u (\Pr_t)^{-1}$$

with l_m a mixing length scale, \Pr_t the non-dimensional turbulent Prandtl number, and c_m is a constant (further details on the computations of these quantities are given in Appendix B). Details of the prognostic equation for k, in connection with energetic consistency requirements, are given in Sec. 3. We acknowledge that since ED represents turbulence in the environment, one should use the environmental TKE $1/2\overline{u'_e} \cdot u'_e$ instead as it is done in Tan et al. (2018). Although no significant effect could be seen in preliminary idealized numerical tests, this point should be further explored.

2.3.4 Entrainment and detrainment closures

Entrainment and detrainment closures are still a topic of extensive research in the atmospheric modeling community. One difficulty is that a given closure can only be specific to a certain type of convection (de Rooy et al., 2013). To close entrainment and detrainment rates³, we adapt the formulation proposed by Rio et al. (2010), namely

$$E = a_p \beta_1 \max(0, \partial_z w_p) \tag{25}$$

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

where the two parameters β_1 and β_2 are positive, δ_0 is a positive minimum detrainment. In order to guarantee $0 \le a_p \le 1$, it is sufficient to impose $0 \le \beta_1 \le 1$ and $1 \le \beta_2 < 2$ (see Appendix F).

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

2.4 Consistent boundary conditions for mean and plume equations

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2.4.1 General concepts

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

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

Such a constraint should guide modeling choices concerning boundary conditions. Indeed, it systematically guarantees the correct partition of surface fluxes, and thus avoids double-counting biases linked to non-physical energy sources/sinks at the boundary (see

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

³ In the literature, closures are usually provided for *fractional* entrainment and detrainment rates, respectively $\epsilon = E/(\sigma_o^a a_p w_p)$ 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.

$rac{\overline{w'\phi'}}{w'oldsymbol{u}_h'}$	$= \frac{a_p w_p(\phi_p - \overline{\phi}) - K_{\phi} \partial_z \overline{\phi}}{= \frac{a_p w_p(u_{h,p} - \overline{u}_h) - K_u \partial_z \overline{u}_h}$	Vertical turbulent flux for component ϕ Vertical turbulent momentum flux
$egin{aligned} &\partial_z(a_pw_p)\ &a_pw_p\partial_z\phi_p\ &a_pw_p\partial_zoldsymbol{u}_{h,p}\ &a_pw_p\partial_zw_p \end{aligned}$	= E - D = $E(\overline{\phi} - \phi_p)$ = $E(\overline{u}_h - u_{h,p}) + a_p w_p C_u \partial_z \overline{u}_h$ = $-bEw_p + a_p \left\{ a \underline{B}_p - \sigma_o^a b'(w_p)^2 \right\}$	Plume area conservation equation Plume equation for component ϕ Plume horizontal momentum equation Plume vertical velocity equation
$egin{array}{c} B_p \ K_u \ K_\phi \end{array}$	$= b_{eos}(\phi_p) - b_{eos}(\phi)$ $= c_m l_m \sqrt{k}$ $= K_u (Pr_t)^{-1}$	Buoyancy forcing term Eddy-viscosity 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 \overline{u}_h and $\overline{\phi}$ 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 \overline{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

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

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

which can be easily integrated vertically to obtain

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

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

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

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

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

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

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

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

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

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2.4.3 Atmospheric context: consistency with Monin-Obukhov theory

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

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

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

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

At this stage, we have provided all the elements and underlying assumptions required to formulate an EDMF-type scheme (see Appendix F for the discretization aspects). Before studying the energetic impacts of using MF components, we derive theoretical horizontally averaged energy budgets.

⁴¹⁸ **3** Horizontally Averaged Energy budgets

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

425 **3.1 Kinetic energies**

Under the SCM assumptions exposed in Sec. 2.1, we can derive budgets for the resolved kinetic energy E_k and the turbulent kinetic energy k:

$$\partial_t E_k + \partial_z T_{E_k} = \overline{w' u'_h} \cdot \partial_z \overline{u}_h \tag{30}$$

$$\partial_t k + \partial_z T_k = -\overline{w' u'_h} \cdot \partial_z \overline{u}_h + \overline{w' b'} - \overline{\epsilon}_\nu \tag{31}$$

where $\overline{\epsilon}_{\nu} = \nu \overline{\partial_z u'} \cdot \overline{\partial_z u'}$ is the viscous dissipation of energy, whereas $T_{E_k} = \overline{w' u'_h} \cdot \overline{u}_h$ and $T_k = \overline{w' \frac{u' \cdot u'}{2}} + \frac{1}{\rho_0} \overline{w' p^{\dagger \prime}} - \nu \overline{\partial_z k}$ resdistribute energy on the vertical. Exchanges between the resolved and subgrid reservoirs of kinetic energy are done via the mechanical shear term $w'u'_h \cdot \partial_z \overline{u}_h$. To close the budgets, we provide in the following sections a budget for internal and potential energy.

3.2 Internal and Potential energies

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

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

where h is the specific enthalpy and ϕ is any entropic variable describing components of the fluid. Under the Boussinesq approximation, internal energy is (Tailleux & Dubos, 2023)

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

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

$$\mathcal{E}_{i} + E_{p} = z(g-b) + \hbar(p_{0},\phi) - \frac{p_{0}}{\rho_{0}}$$
(34)

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

$$\partial_t (\mathcal{E}_i + E_p) + \nabla \cdot \left(\left[\left(\hbar(p_0, \phi) + gz \right] \boldsymbol{u} \right) = \epsilon_\nu - wb$$
(35)

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

$$\partial_t (E_i + E_p) + \partial_z (\overline{\partial_\phi h_0} \,\overline{w'\phi'}) = \overline{\epsilon}_\nu - \partial_z (\overline{\phi} \,\overline{w'\partial_\phi h_0'} + \overline{\phi'w'\partial_\phi h_0'}) - \overline{w'b'} \tag{36}$$

where we introduced the notation $h_0(\phi) := h(p_0, \phi)$. Remark that if $h(p_0, \phi)$ is linear in ϕ , we have closed relations $\overline{h(p_0, \phi)} = h(p_0, \overline{\phi})$ and $\overline{b(\phi)} = b(\overline{\phi})$.

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

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

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

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

3.2.1 Dry atmosphere

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

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

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

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

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

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

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

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

3.2.2 Seawater with linearized equation of state

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

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

462 and specific enthalpy is

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

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

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

⁴⁶⁴ The budgets of mean kinetic energy, turbulent kinetic energy, and the sum of mean in-

ternal and potential energy for *seawater* with a linearized equation of state are

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

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

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

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

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

471 4 Consistency of TKE equation with EDMF closures

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

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

where k represents the turbulent kinetic of the whole grid cell, *i.e.* $1/2\overline{u' \cdot u'}$. In (48), turbulent fluxes have been closed using ED. However, we argue that if an EDMF closure is used in the mean equations (for momentum, temperature, and salinity or humidity), the TKE equation should be modified by MF terms to ensure energetic consistency as shown below. Note that Tan et al. (2018) made a different choice by considering a budget for the *environmental* TKE, $k_e = 1/2\overline{u'_e \cdot u'_e}$. 482 4.1 Shear and Buoyancy terms

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

486 When the EDMF approach is used to close fluxes in the diagnostic equations of \overline{u}_h 487 and $\overline{\phi}$, then the same closures must be used in turbulent kinetic energy budget to en-488 sure energetic consistency. As a consequence, the shear term must be closed as

$$-\overline{w'\boldsymbol{u}_{h}'} \cdot \partial_{z}\overline{\boldsymbol{u}}_{h} \stackrel{=}{}_{\text{EDMF}} - \left[-K_{u}\partial_{z}\overline{\boldsymbol{u}}_{h} + a_{p}w_{p}(\boldsymbol{u}_{h,p} - \overline{\boldsymbol{u}}_{h})\right] \cdot \partial_{z}\overline{\boldsymbol{u}}_{h}$$
(49)

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

$$\overline{w'b'} \underset{\text{EDMF}}{=} \frac{g}{\theta_0} \left[-K_\theta \partial_z \overline{\theta} + a_p w_p (\theta_p - \overline{\theta}) \right]$$
(50)

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

$$\overline{w'b'} = g\alpha \left[-K_{\theta}\partial_{z}\overline{\theta} + a_{p}w_{p}(\theta_{p} - \overline{\theta}) \right] - g\beta \left[-K_{S}\partial_{z}\overline{S} + a_{p}w_{p}(S_{p} - \overline{S}) \right]$$
$$= -K_{\phi}\partial_{z}\overline{b} + a_{p}w_{p}(b_{p} - \overline{b})$$

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.

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

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

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 mod-

els, TKE transport is usually parameterized via K-diffusion, namely

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

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

$$\overline{w'\frac{u'\cdot u'}{2}} = \sum_{i=e,p} \underbrace{a_i \frac{1}{2} \overline{u'_i \cdot u'_i w'_i}}_{I_i} + \underbrace{a_i (u_i - \overline{u}) \cdot \overline{u'_i w'_i}}_{II_i} + \underbrace{a_i (w_i - \overline{w}) \frac{1}{2} \overline{u'_i \cdot u'_i}}_{III_i} + \underbrace{a_i \frac{1}{2} (u_i - \overline{u})^2 (w_i - \overline{w})}_{IV_i}$$
(53)

where: I_i is an intra-subdomain turbulent TKE transport; II_i is a transport of Reynolds stress by the coherent velocities; III_i is a transport of subdomain TKE by the coherent velocities (*i.e.* transport of TKE by mass-flux); IV_i is a transport of convective kinetic energy by coherent velocities. Based on LES simulations (see Sec. 5.3), we found that: (*i*) I_p can be neglected, consistently with the small area limit; (*ii*) II_e and II_p are almost compensating, thus the sum $II_e + II_p$ can be neglected. Using $a_p w_p = -a_e w_e$, we can conveniently reformulate the remaining terms:

$$\operatorname{III}_{e} + \operatorname{III}_{p} + \operatorname{IV}_{e} + \operatorname{IV}_{p} = a_{p}w_{p}\frac{1}{1-a_{p}}\left(k_{p} + \frac{1}{2}\|\boldsymbol{u}_{p} - \overline{\boldsymbol{u}}\|^{2} - k\right)$$
(54)

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

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

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

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

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

Finally, one still needs to provide a value for k_p . Without any assumption, its prognostic equation reads (Tan et al., 2018, eq. (11))

$$\partial_t (a_p k_p) + \partial_z (a_p w_p k_p) = -a_p \overline{w'_p u'_{h,p}} \cdot \partial_z u_{h,p} + a_p \overline{w'_p b'_p} \\ + E \left(k_e + \frac{1}{2} \| u_e - u_p \|^2 \right) - Dk_p \\ - \partial_z \left(a_p \overline{w'_p \frac{u'_p \cdot u'_p}{2}} + a_p \overline{u'_p \cdot \frac{1}{\rho_0} (\nabla p^{\dagger})'_p} \right) \\ - a_p (\epsilon_{\nu})_p$$

As a first attempt, we propose to retain advection, entrainment, detrainment and dissipation terms, which lead to the simplified form of the previous equation:

$$\partial_{z}(a_{p}w_{p}k_{p}) = E\left(k_{e} + \frac{1}{2}\|\boldsymbol{u}_{e} - \boldsymbol{u}_{p}\|^{2}\right) - Dk_{p} - a_{p}(\epsilon_{\nu})_{p}$$
(57)
$$= E\left(\frac{1}{1-a_{p}}k - \frac{a_{p}}{1-a_{p}}k_{p} + \frac{1}{1-a_{p}}\frac{1}{2}(\boldsymbol{u}_{p} - \overline{\boldsymbol{u}})^{2}\right) - Dk_{p} - a_{p}(\epsilon_{\nu})_{p}$$
(58)

where we have used the identity $(\boldsymbol{u}_e - \boldsymbol{u}_p)^2 = \frac{1}{(1-a_p)^2} (\boldsymbol{u}_p - \overline{\boldsymbol{u}})^2$ and substituted k_e using (55). Using area conservation, we get the advective form

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

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

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

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

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

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

4.3 Viscous dissipation

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

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

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

538 4.4 Boundary conditions

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

543 4.4.1 Generic constraint

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

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

In general if plume variables are specified at z = 0, then (63) is again a Robin boundary condition for the TKE equation.

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4.4.2 Oceanic context

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

$$\overline{w'\frac{\boldsymbol{u'}\cdot\boldsymbol{u'}}{2}} = 0, \qquad k_p(0) = k(0)$$

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

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

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

553 4.4.3 Atmospheric context

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

559 4.5 EDMF-parameterized budgets

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

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

$$\tag{65}$$

⁵⁶³ where the flux terms are

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

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

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

⁵⁶⁴ Equivalently, in the case of *seawater* with linearized equation of state

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

$$\tag{69}$$

⁵⁶⁵ where the flux of internal and potential energy is

$$T_{E_i+E_p} = -\partial_z \left(c_p \left(-K_\phi \partial_z \overline{\theta} + a_p w_p(\theta_p - \overline{\theta}) \right) - z \left(-K_\phi \partial_z \overline{b} + a_p w_p(b_p - \overline{b}) \right) \right)$$
(70)

⁵⁶⁶ and the conservative temperature equation is

$$\partial_t \overline{\theta} = \frac{\overline{\epsilon}_{\nu}}{c_p - \alpha g z} - \partial_z \left(-K_{\phi} \partial_z \overline{\theta} + a_p w_p (\theta_p - \overline{\theta}) \right)$$

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

4.6 Vertically integrated energy budgets

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):

$$\frac{1}{2}\partial_t \left\langle \overline{X}^2 \right\rangle_z = \underbrace{-\left\langle K_X(\partial_z \overline{X})^2 \right\rangle_z}^{\leq 0} \underbrace{-\left\langle \frac{E+D}{2} (X_p - \overline{X})^2 \right\rangle_z}_{+\left\langle \overline{X} \, \overline{S}_X \right\rangle_z + \left\langle a_p (S_X)_p (X_p - \overline{X}) \right\rangle_z}_{-\left[\overline{X} \, \overline{w'X'} + a_p w_p \frac{(X_p - \overline{X})^2}{2}\right]_0^{\sigma_o^a H}}$$

⁵⁷⁴ Consequently, the entrainment and detrainment processes contribute on average to de-⁵⁷⁵ creasing the mean variance, similar to eddy-diffusivity terms. Although not sufficient in ⁵⁷⁶ the context of nonlinear equations, monotonically decreasing variance is usually a nec-⁵⁷⁷ essary property to ensure analytical well-posedness of transport partial differential equa-⁵⁷⁸ tions (e.g. Evans, 2010). Interestingly, the last term of the budget implies that a non-⁵⁷⁹ zero MF flux at the boundary leads to an additional sink of resolved variance (which is ⁵⁸⁰ exactly compensated by an equal and opposite boundary source for $\overline{X'^2}$).



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

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

$$\partial_t \langle E_k \rangle_z = -\left\langle K_u (\partial_z \overline{\boldsymbol{u}}_h)^2 \right\rangle_z - \left\langle \frac{E+D}{2(1-C_u)} (\boldsymbol{u}_{h,p} - \overline{\boldsymbol{u}}_h)^2 \right\rangle_z - \left[\overline{\boldsymbol{u}}_h \cdot \overline{w' \boldsymbol{u}'_h} \right]_0^{\sigma_o^a H} - \left[\frac{a_p w_p}{2(1-C_u)} (\boldsymbol{u}_{h,p} - \overline{\boldsymbol{u}}_h)^2 \right]_0^{\sigma_o^a H}$$

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

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

587 get reads

581

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

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

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

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

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

$\partial_t E_k + \partial_z T_{E_k}$	$= -K_u(\partial_z \overline{\boldsymbol{u}}_h)^2 + a_p w_p(\boldsymbol{u}_{h,p} - \overline{\boldsymbol{u}}_h) \cdot \partial_z \overline{\boldsymbol{u}}_h$	Resolved kinetic energy budget
$\partial_t \left(E_i + E_p \right) + \partial_z T_{E_i + E_p}$	$= -\left(-K_{\phi}\partial_{z}\overline{b} + a_{p}w_{p}(b_{p} - \overline{b})\right) + \overline{\epsilon}_{\nu}$	Internal and potential energy budget
$\partial_t k - \partial_z \left(K_k \partial_z k \right)$	$=K_u(\partial_z \overline{\boldsymbol{u}}_h)^2 - K_\phi \partial_z \overline{\boldsymbol{b}}$	ED related TKE production terms
	$-a_p w_p (\boldsymbol{u}_{h,p} - \overline{\boldsymbol{u}}_h) \cdot \partial_z \overline{\boldsymbol{u}}_h + a_p w_p (b_p - b)$	MF related TKE production terms
	$-\partial_{oldsymbol{z}}\left(a_{p}w_{p}\left k_{p}-k+rac{1}{2}\ oldsymbol{u}_{p}-oldsymbol{u}\ ^{2} ight ight)$	MF related TKE transport term
	$-\overline{\epsilon}_{ u}$	TKE dissipation
$a_p w_p \partial_z k_p$	$= E\left(k - k_p + \frac{1}{2}\ \boldsymbol{u}_p - \boldsymbol{u}\ ^2\right) - a_p(\epsilon_{\nu})_p$	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.

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

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

600

5.1 Description of idealized cases

The two idealized cases considered are reminiscent of typical deep convective con-601 ditions in the ocean (e.g. Marshall & Schott, 1999), where convection into a initially rest-602 ing ocean of constant stratification $\Delta \theta = 1 \text{ K}/1000 \text{ m}$ (corresponding $N_0^2 = 1.962 \times 10^{-6} \text{ s}^{-2}$) is triggered by a surface cooling of $Q_0 = -500 \text{ Wm}^{-2}$ (corresponding to a surface buoyancy loss of $B_0 = -2.456 \times 10^{-7} \text{ m}^2 \text{s}^{-3}$). In both cases, salinity is kept 603 604 605 uniform at S = 32.6 psu. The first case (FC500) consists of free convection, where no 606 wind stress is applied. In the second idealized case (W005_C500) a uniform wind stress 607 along the meridional direction, of magnitude $(u_*^a)^2 = 0.05 \,\mathrm{m}^2 \,\mathrm{s}^{-2}$, is applied. A sum-608 mary of the parameters for each case can be found in table 3. To characterize wind-shear 609 effects, we introduce the Froude number (Haghshenas & Mellado, 2019) 610

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

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

Table 3: Idealized cases parameters

Case	$Q_0 \; ({\rm W}{\rm m}^{-2})$	$(u^a_*)^2 (\mathrm{m}^2 \mathrm{s}^{-2})$	$N_0^2 ~({ m s}^{-2})$	t_f (h)	Fr_*
FC500	-500	0	1.962×10^{-6}	72	0
$W005_{-}C500$	-500	0.05	1.962×10^{-6}	72	0.56

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

Case	h/L_{Ob}	Ri_h	Ri_*
FC500	∞	∞	97
$W05_{-}C500$	5.7	310	97

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

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

is an estimate of the depth at which the production of TKE by turbulent shear is of the 619 same order of magnitude as the production of TKE by buoyancy fluxes. Noting $w_* =$

620

 $(-B_0h)^{1/3}$ the convective velocity scale (Deardorff, 1970), we get 621

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

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

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

measures the destabilization by surface shear stresses of a stably stratified water column. 624 At $t_f = 72$ h, the case W005_C500 can be described by $h/L_{Ob} \simeq 5.7$ and $Ri_h \simeq 310$, 625 which corresponds to a regime of strong deepening of the MLD according to Legay et 626 al. (2023). Finally, for free convection cases (no wind) a convective Richardson number 627 can be built as 628

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

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

$$h \propto h_{\rm enc}$$
 (74)

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

$$\frac{w_e}{w_*} \propto R i_*^{-1} \tag{75}$$

633

5.2 LES model description and conditional sampling

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



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.

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

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

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

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

661

5.3 Validity of the steady plume hypothesis and small area limit

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



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).

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

678

All the previous findings are also verified for the W005_C500 case (not shown).

5.4 SCM evaluation

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

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

The examination of mean temperature and flux of temperature profiles shows that 697 ED fails to reproduce the so-called vertical entrainment zone (e.g. Garcia & Mellado, 698 2014), in which penetrative convection generates negative temperature flux and sharp-699 ens the temperature gradients at the base of the mixed layer. The lack of penetrative 700 convection is known to reduce the deepening rate (e.g. chap. 6, Garratt, 1994a), thus 701 producing an important bias of a hundred meters regarding the mixed layer depth com-702 pared to LES. On the other hand, EDMF and EDMF-energy equally perform in repre-703 senting these profiles. The absence of a noticeable effect of the energetic consistency on 704 the temperature mean and flux profiles is a consequence of the small value of the ED fluxes 705 (dashed lines) in the mixed layer. When considering the TKE profile, ED can model the 706 correct order of magnitude, however, the TKE does not penetrate enough. EDMF fails 707 to reproduce TKE due to energetic inconsistency. Indeed, looking at temperature and 708 velocity fluxes allows us to infer that the losses of resolved energy due to buoyancy and 709 shear are dominated by the MF contributions. However, such contributions are not in-710 cluded as sources of TKE for the EDMF scheme, leading to the very low levels of TKE 711 observed in the simulation. EDMF-energy can reproduce accurate profiles of TKE. The 712 main discrepancies arise close to the surface and at the base of the mixed layer. Neither 713 ED nor EDMF can reproduce the vertical transport of TKE, whereas EDMF-energy re-714 produces well the profile. Similar conclusions are drawn from the WC005_C500 case (see 715 Fig. 5). 716

In Fig. 6, we represent the vertically integrated energy budget of the SCM for the case W005_C500 (FC500 is similar), namely the quantity

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

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

$$\int_{-H}^{0} \left(-a_p w_p(b_p - \overline{b}) + a_p w_p(\boldsymbol{u}_{h,p} - \overline{\boldsymbol{u}}_h) \cdot \partial_z \overline{\boldsymbol{u}}_h \right) \,\mathrm{d}z \tag{78}$$

and scales with B_0h .

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5.5 Realistic case: Hymex/ASICS-MED campaign

We now move to more realistic situations corresponding to a sequence of strong convective events which were documented in the Northwestern Mediterranean during the winter 2013 of the HyMeX/ASICS-MED experiment at the LION buoy. This experiment was also carried out by Giordani et al. (2020) and we use a similar setup here (similar 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).

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

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

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

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



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 72*h* of simulation. LES data (black dots), ED-only scheme (grey line), standard EDMF scheme (blue line) and energetically-consistent EDMF (or-ange 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_{\star} (m s⁻¹, top panel) and surface buoyancy flux B_0 (m² s⁻³, middle panel) computed from atmospheric forcings. Time series of mixed layer depth h_{mxl} (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 (≈ -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

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



Figure 8: Temperature (°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.

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

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

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

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

To implement and then assess the impact of this energetically consistent parameterization on realistic 3D oceanic simulations a calibration of the remaining "free" parameters must be achieved (Hourdin et al., 2017; Couvreux et al., 2021). It should be performed on parameters whose universality can sometimes be statistically assessed (Souza et al., 2020), and should be mathematically and physically constrained as much as possible (see e.g. section 4.6). We believe that designing energetically consistent parameterization is a way to achieve more realistic models before their tuning.

Appendix A Relaxing the small area limit

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

$$\begin{split} \widetilde{\boldsymbol{\alpha}} &= \frac{1}{1-a_p} \\ \overline{\boldsymbol{w}'\boldsymbol{\phi}'} &= \widetilde{\alpha}a_p w_p(\phi_p - \overline{\phi}) - K_{\phi} \partial_z \overline{\phi} \\ \overline{\boldsymbol{w}'\boldsymbol{u}'_h} &= \widetilde{\alpha}a_p w_p(\boldsymbol{u}_{h,p} - \overline{\boldsymbol{u}}_h) - K_m \partial_z \overline{\boldsymbol{u}}_h \\ \partial_z(a_p w_p) &= E - D \\ a_p w_p \partial_z \phi_p &= \widetilde{\alpha} E(\overline{\phi} - \phi_p) \\ a_p w_p \partial_z w_p &= \widetilde{\alpha} E(\overline{\boldsymbol{u}}_h - \boldsymbol{u}_{h,p}) + a_p w_p C_u \partial_z \overline{\boldsymbol{u}}_h \\ B_p &= \delta cos(\phi_p) - \delta cos(\overline{\phi}) \\ \partial_t k - \partial_z (K_k \partial_z k) &= K_m (\partial_z \overline{\boldsymbol{u}}_h)^2 - K_{\phi} \partial_z \overline{b} \\ -\widetilde{\alpha}a_p w_p ((\boldsymbol{u}_{h,p} - \overline{\boldsymbol{u}}_h) \cdot \partial_z \overline{\boldsymbol{u}}_h - (b_p - \overline{b})) \\ -\partial_z \left(\widetilde{\alpha}a_p w_p \left[k_p - k + \frac{1}{2} \|\boldsymbol{u}_p - \boldsymbol{u}\|^2\right]\right) \\ -\overline{\epsilon}_\nu \\ a_p w_p \partial_z k_p &= \widetilde{\alpha} E\left(((k - k_p) + \frac{1}{2} \|\boldsymbol{u}_p - \boldsymbol{u}\|^2\right) - a_p(\epsilon_\nu)_p \end{split}$$
Rescaling coefficient
Vertical turbulent flux for component ϕ
Vertical turbulent momentum flux
Plume area conservation equation
Plume horizontal momentum equation
Plume vertical velocity equation
Buoyancy forcing term
ED related TKE production terms
MF related TKE transport term
TKE dissipation
Plume related TKE transport term
TKE dissipation
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

$$K_u = c_m l_m \sqrt{k}$$

$$K_\phi = K_u (\Pr_t)^{-1}$$

with l_m a mixing length scale, \Pr_t the non-dimensional turbulent Prandtl number, and 834 c_m is a constant ($c_m = 0.1$ in NEMO). The mixing length l_m is calculated in two steps 835 by considering separately the length scales l_{up} and l_{dwn} associated respectively to up-836 ward and downward movements : (1) l_{up} and l_{dwn} are initialized assuming $l_{up} = l_{dwn} =$ 837 $\sqrt{2k\tau_{\rm ed}}$ with $\tau_{\rm ed}$ a characteristic time equal to $1/N = (\partial_z \bar{b})^{-1}$ (2) a physical limitation 838 is used to guarantee that l_{up} and l_{dwn} do not exceed the distance to the top and the bot-839 tom, this limitation amounts to controlling the vertical gradients of l_{up} and l_{dwn} such 840 that they are not larger that the variations of depth (e.g. Madec et al., 2019). Once l_{up} 841 and l_{dwn} are computed the mixing length is taken as $l_m = \min(l_{up}, l_{dwn})$. The turbu-842 lent Prandtl number is modelled by $\Pr_t = \min(\Pr_t^{\max}, \max(\operatorname{Ri}/\operatorname{Ri}_c, 1))$ with $\operatorname{Ri} = N^2 / \|\partial_z \overline{\mathbf{u}}_h\|^2$, 843 $Pr_{t}^{max} = 10 \text{ and } Ri_{c} = 0.2.$ 844

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 $O(z^0)$:

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

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

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

Then near the surface, the buoyancy force - which is a source of plume momentum and

- kinetic energy $1/2w_p^2$ is at first order $b_p \overline{b} \simeq -N_0^2 z$. Consequently, any static insta-
- bility at the surface will result in the absolute growth of the plume vertical momentum
- ($-N_0^2 z > 0$ in the atmosphere and $-N_0^2 z < 0$ in the ocean).
- The boundary condition $b_p(0) = \overline{b}(0)$ implies that at z = 0, all the surface flux is al-
- located in the ED component. Consequently, $N_0^2 = \overline{w'b'}(0)/(-K_b(0)) = \overline{w'b'}(0)/(c_b l_b(0)\sqrt{k(0)}).$
- The boundary condition $b_p(0) = \overline{b}(0)$ thus implies that close to the surface

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

⁸⁵⁶ Appendix D EDMF Mean Variance Equation

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

$$\partial_t \overline{X} = -\partial_z \overline{w'X'} + \overline{S}_X \tag{D1}$$

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

$$a_p w_p \partial_z X_p = -E(X_p - \overline{X}) + a_p S_{X,p} \tag{D3}$$

Multiplying the mean equation (D1) by \overline{X} leads to

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$$\frac{1}{2}\partial_t \overline{X}^2 = -\partial_z (\overline{X} \, \overline{w'X'}) + \overline{w'X'} \partial_z \overline{X} + \overline{X} \, \overline{S_X} \\
= -\partial_z (\overline{X} \, \overline{w'X'}) - K_X (\partial_z \overline{X})^2 + a_p w_p (X_p - \overline{X}) \partial_z \overline{X} + \overline{X} \, \overline{S_X} \tag{D4}$$

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

$$a_{p}w_{p}(X_{p}-\overline{X})\partial_{z} \xrightarrow{=X_{p}+(\overline{X}-X_{p})} = -E(X_{p}-\overline{X})^{2} + (X_{p}-\overline{X})a_{p}S_{X,p}$$
$$-a_{p}w_{p}\frac{1}{2}\partial_{z}(X_{p}-\overline{X})^{2}$$
$$= -E(X_{p}-\overline{X})^{2} + (X_{p}-\overline{X})a_{p}S_{X,p}$$
$$-\partial_{z}(a_{p}w_{p}\frac{1}{2}(X_{p}-\overline{X})^{2})$$
$$+(E-D)\frac{1}{2}(X_{p}-\overline{X})^{2}$$
$$= -(E+D)\frac{1}{2}(X_{p}-\overline{X})^{2} + (X_{p}-\overline{X})a_{p}S_{X,p}$$
$$-\partial_{z}(a_{p}w_{p}\frac{1}{2}(X_{p}-\overline{X})^{2})$$

Using this expression into equation (D4), then vertically integrating the variance budget leads to the desired equation (71).

⁸⁶² Appendix E Anelastic energy budgets

In this appendix, we derive energy budgets for a general anelastic model commonly used in atmospheric models. We start with the unaveraged anelastic mass and momentum budgets:

$$\nabla \cdot (\rho_{\rm ref} \boldsymbol{u}) = 0 \tag{E1}$$

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

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

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

872 E1 Kinetic energies

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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:

$$\partial_t E_k + \frac{1}{\rho_{\text{ref}}} \partial_z T_{E_k} = \overline{w' \boldsymbol{u}'_h} \cdot \partial_z \overline{\boldsymbol{u}}_h \tag{E3}$$

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

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

E2 Internal and Potential energies

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

$$\mathcal{E}_i = \hbar(p,\phi) - \frac{p}{\rho} \tag{E5}$$

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

$$\mathcal{E}_i = \hbar(p_{\rm ref}, \phi) - \frac{p_{\rm ref}}{\rho_{\rm ref}} \tag{E6}$$

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

$$\partial_t (\mathcal{E}_i + E_p) + \frac{1}{\rho_{\rm ref}} \nabla \cdot \left[\rho_{\rm ref} (\hbar(p_{\rm ref}, \phi) + gz) \boldsymbol{u} \right] = \epsilon_\nu - wb \tag{E7}$$

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

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

where we introduced the notation $\underline{h}_{ref}(\phi) = h(p_{ref}, \phi)$. Remark that if $h(p_{ref}, \phi)$ is linear in ϕ , we have closed relations $\overline{h}(p_{ref}, \phi) = h(p_{ref}, \overline{\phi})$ and $\overline{b(\phi)} = b(\overline{\phi})$.

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

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

where conversion of E_k into k occurs via mean shear, conversion of k into E_i occurs via viscous dissipation, and conversion of k into $E_i + E_p$ occurs via buoyancy fluxes. For a *dry atmosphere* modeled as an ideal gas $p = \rho R_d T$, the specific enthalpy reads

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

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

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

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, turbulent kinetic energy and the sum of mean internal and potential energy for a *dry atmosphere* within the anelastic approximation are

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

E3 EDMF-parameterized budget

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

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

⁹⁰⁵ where the flux terms are

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$$T_{E_k} = \rho_{\text{ref}} \left(-K_u \partial_z \overline{\boldsymbol{u}}_h + a_p w_p (\boldsymbol{u}_{h,p} - \overline{\boldsymbol{u}}_h) \right) \cdot \overline{\boldsymbol{u}}_h$$
(E14)

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

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

Appendix F Discretization of energetically consistent EDMF equa tions

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

F1 Discretization of mass-flux equations

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

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

$$\partial_z (a_p w_p \phi_p) = E \overline{\phi} - D \phi_p \tag{F2}$$

$$\partial_z (a_p w_p \boldsymbol{U}_p) = E \overline{\boldsymbol{U}} - D \boldsymbol{U}_p \tag{F3}$$

$$w_p \partial_z w_p = -(E/a_p)(bw_p) + aB_p + b'w_p^2 \tag{F4}$$

$$a_p w_p \partial_z k_p = E\left(k - k_p + \frac{1}{2}(\overline{\boldsymbol{u}}_p - \overline{\boldsymbol{u}})^2\right) - a_p(\epsilon_\nu)_p \tag{F5}$$

where the equation for horizontal momentum has been manipulated to have the same 924 form as the ϕ_p equation by taking $U_p = u_{h,p} - C_u \overline{u}_h$ and $U = (1 - C_u) \overline{u}_h$. The ad-925 vective form is used for the w_p equation to make the computation of w_p independent of 926 a_p (with the closure hypothesis (25) for $E, E/a_p$ is independent of a_p); the motivations 927 for this will become clearer later. The mass-flux equations correspond to a first-order 928 nonlinear set of ODEs. There are a whole lot of methods for solving such initial value 929 problems. We present here a simple method combining explicit (Euler) and semi-implicit 930 (Crank-Nicolson) steps as the use of more advanced methods did not produce significantly 931 different results. In the following, we describe the different steps for the resolution start-932 ing from known initial values $X_{N+1/2}^p$ at the surface and advancing downward. 933

934 F11 Initial conditions

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

$$w_{N+1/2}^{p} = -w_{\min}^{p}$$

$$\phi_{N+1/2}^{p} = \frac{(2\Delta z_{N} + \Delta z_{N-1})\overline{\phi}_{N} - \Delta z_{N}\overline{\phi}_{N-1}}{\Delta z_{N} + \Delta z_{N-1}}$$

$$U_{N+1/2}^{p} = (1 - C_{u})\frac{(2\Delta z_{N} + \Delta z_{N-1})(\overline{u}_{h})_{N} - \Delta z_{N}(\overline{u}_{h})_{N-1}}{\Delta z_{N} + \Delta z_{N-1}}$$
(F6)

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 ϕ_p leads to the following value of the B_p term in the topmost grid cell :

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

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 go-

- ⁹⁴³ ing downward.
- 944 $F12 w_p$ -equation
- 945

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

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

⁹⁴⁶ which can be discretized in a straightforward way as

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

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 $w_{j+1/2}^p$, it is easily found that

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

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

954 F13 Continuity and tracer equations

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

$$\Delta z_j E_j = \frac{1}{2} \left(a_{j+1/2}^p + a_{j-1/2}^p \right) \beta_1 (\delta_z w^p)_j^+$$

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

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

$$(a^{p}w^{p})_{j+1/2} - (a^{p}w^{p})_{j-1/2} = \Delta z_{j}(E_{j} - D_{j})$$
$$(a^{p}w^{p}\phi^{p})_{j+1/2} - (a^{p}w^{p}\phi^{p})_{j-1/2} = \Delta z_{j}E_{j}\overline{\phi}_{j} - (\Delta z_{j}D_{j}/2)\left(\phi_{j+1/2}^{p} + \phi_{j-1/2}^{p}\right)$$

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

$$a_{j-1/2}^{p} = a_{j+1/2}^{p} \left\{ \frac{2w_{j+1/2}^{p} - \operatorname{EmD}_{j}}{2w_{j-1/2}^{p} + \operatorname{EmD}_{j}} \right\}$$

$$\operatorname{EmD}_{j} = \beta_{1}(\delta_{z}w^{p})_{j}^{+} + \beta_{2}(\delta_{z}w^{p})_{j}^{-} + \min\left\{ \frac{\delta_{0}\Delta z_{j}}{2}(w_{j+1/2}^{p} + w_{j-1/2}^{p}), -2(w_{\min}^{p}) \right\}$$
(F8)

Note that a_p is subject to a boundedness requirement as $0 \le a_p \le 1$. Assuming $0 \le a_{j+1/2}^p \le 1$, sufficient conditions to guarantee that $a_{j-1/2}^p \le 1$ are $\beta_1 \le 1$ and $\beta_2 \ge 1$ and a sufficient condition to guarantee that $a_{j-1/2}^p \ge 0$ is $\beta_2 < 2$. Moreover a constraint is added on the background detrainment δ_0 in (F8) to guarantee that $a_{j-1/2}^p = 0$ 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 $\overline{\phi}_j = 1$).

The same reasoning can be applied to solve the k_p equation, which presents no additional 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.

In summary, the proposed discretization guarantees that w_p is strictly negative, that a_p is bounded between 0 and 1, and that the continuity and tracer equations are compatible, without the need for an iterative solution procedure.

⁹⁷⁶ F2 Energy consistent discretization of turbulent kinetic energy

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 \overline{u}_h and $\overline{\phi}$ equations which can be written generically for a variable X

$$\frac{\overline{X}_{j}^{n+1} - \overline{X}_{j}^{n}}{\Delta t} = \frac{F_{j+1/2}^{\rm MF} - F_{j-1/2}^{\rm MF}}{\Delta z_{j}}$$
$$F_{j+1/2}^{\rm MF} = (a^{p}w^{p})_{j+1/2} \left(\overline{X}_{j+1/2}^{p} - \overline{X}_{j}^{n}\right)$$

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

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

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

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.

F3 Coupling ED and MF schemes

⁹⁹¹ In the EDMF approach, the usual vertical diffusion/viscous subgrid terms are com-⁹⁹² pleted by an advective term so that the following equation must be advanced in time:

$$\partial_t \overline{X} = \partial_z \left(K_X \partial_z \overline{X} \right) - \partial_z \left(a_p w_p (X^p - \overline{X}) \right) \tag{F9}$$

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

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

$$\boldsymbol{u}_h^{n+1,\star} = \boldsymbol{u}_h^n + \Delta t \partial_z \left(K_{\boldsymbol{u}}(k^n, b^n) \partial_z \boldsymbol{u}_h^{n+1,\star} \right)$$

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

MF step

$$\begin{split} [a_p, w_p, \phi_p, \boldsymbol{u}_{h,p}, k_p, B_p] &= \mathrm{MF}(b^{n+1,\star}, \boldsymbol{u}_h^{n+1,\star}) \\ \phi^{n+1} &= \phi^{n+1,\star} - \Delta t \partial_z \left(a_p w_p(\phi_p - \phi^{n+1,\star}) \right) \\ \boldsymbol{u}_h^{n+1} &= \boldsymbol{u}_h^{n+1,\star} - \Delta t \partial_z \left(a_p w_p(\boldsymbol{u}_{h,p} - \boldsymbol{u}_h^{n+1,\star}) \right) \\ \mathrm{TKE} \text{ update} \\ k^{n+1} &= k^n + \Delta t \partial_z \left(K_k(k^n, b^n) \partial_z k^{n+1} \right) + \mathcal{F}_k(b^{n+1}, \boldsymbol{u}_h^{n+1}, \boldsymbol{u}_h^n, a_p, w_p, \boldsymbol{u}_{h,p}, k_p, B_p) \end{split}$$

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

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

$$\phi^{n+1} = \phi^n + \Delta t \partial_z \left(K_{\phi} \partial_z \phi^{n+1,\star} - a_p w_p (\phi_p - \phi^{n+1,\star}) \right)$$
$$[a_p, w_p, \phi_p] = \mathrm{MF}(\phi^{n+1,\star})$$

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

$$\phi^{n+1} = \phi^n + \Delta t \left(K_{\phi} \partial_z \phi^{n+1} - a_p w_p (\phi_p - \phi^{n+1}) \right)$$
$$[a_p, w_p, \phi_p] = \mathrm{MF}(\phi^n)$$

In this case, the mass flux is applied to the mean fields at time n thus breaking the synchronization between the ED and MF parts. Indeed ϕ_p has been computed using ϕ^n while it is applied at time n + 1.

1015 Open Research

1016 Data Availability Statement

Data from the Lion mooring (located in the Gulf of Lion; Mediterranean sea) are freely accessible from Bosse et al. (2023). The output from LES simulations and the initial and surface boundary conditions for the Hymex/ASICS-MED experiments are available at Zenodo link here.

¹⁰²¹ Software Availability Statement

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

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