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Energetically consistent Eddy-Diffusivity Mass-Flux convective schemes. Part I: Theory and Models.

M. Perrot^{1,*}, F. Lemarié¹, T. Dubos²

¹Univ. Grenoble Alpes, Inria, CNRS, Grenoble INP, LJK, Grenoble, France
²IPSL, Lab. Meteorologie Dynamique, Ecole Polytechnique, Palaiseau, France

Key Points:

- An Eddy-Diffusivity Mass-Flux parameterization is carefully derived from first principles, making the underlying assumptions explicit
- Closed bulk energy budgets between resolved and subgrid energy reservoirs are outlined using modern anelastic and Boussinesq energetics
- Energy budgets and mass-flux hypotheses motivates the consistent formulation of TKE equation, boundary conditions and transport of TKE

Corresponding author: Manolis Perrot, manolis.perrot@univ-grenoble-alpes.fr

Abstract

This paper provides a self-contained derivation from first principles of a convective vertical mixing scheme rooted in the Eddy-Diffusivity Mass-Flux (EDMF) approach. This type of closure involves separating vertical turbulent fluxes into two components: an eddy-diffusivity (ED) term that addresses local small-scale mixing in a near isotropic environment, and a mass-flux (MF) transport term that accounts for the non-local transport performed by vertically coherent plumes within the environment. Using the multi-fluid averaging underlying the MF concept, we review consistent energy budgets between resolved and subgrid scales for seawater and dry atmosphere, in anelastic and Boussinesq settings. We show that when using an EDMF scheme, closed energy budgets can be recovered if: (i) bulk production terms of turbulent kinetic energy (TKE) by shear, buoyancy and transport include MF contributions; (ii) boundary conditions are consistent with EDMF, to avoid spurious energy fluxes at the boundary. Moreover we show that lateral mixing due to either entrainment or detrainment induces a net production of TKE via the shear term, and such production is enhanced when horizontal drag increases. Throughout the theoretical development of the scheme, we maintain transparency regarding underlying assumptions. In a companion paper (Perrot and Lemarié (2024); hereafter Part II) we assess the validity of such hypotheses and the sensitivity of the scheme to modelling choices against Large Eddy Simulations (LES) and observational data of oceanic convection, detail an energy-conserving discretization, and quantify energy biases of inconsistent formulations.

Plain Language Summary

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

1 Introduction**1.1 Convection in the ocean and atmosphere and its parameterization in numerical models**

Boundary layer convection occurs in the atmosphere and the ocean due to buoyancy fluxes at the surface, which trigger gravitational instabilities. Buoyant plumes then tend to overturn and mix the fluid. When looking at the mean properties of the fluid, it leads to the formation of a well-mixed layer. The accurate representation of such boundary layers is of paramount importance for short-term forecasts as well as for climate projections in the atmosphere (Bony et al., 2015; Schneider et al., 2017) and the ocean (Martin et al., 2013; Piron et al., 2016; Moore et al., 2015; Fox-Kemper et al., 2019). Regarding current computational capacities, plumes are still unresolved in regional and global numerical models, and thus their effects require parameterization. Moreover in ocean modeling, beyond the requirement in terms of grid resolution, hydrostatic equations used in

63 the overwhelming majority of regional and global studies are not suitable for resolving
64 convective phenomena explicitly (Marshall et al., 1997).

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

82 To circumvent ED hypothesis, Deardorff (1966) proposed to introduce a constant
83 non-local term γ_X in the form $\overline{w'X'} = -K_X(\partial_z \overline{X} - \gamma_X)$. Later on, such a formula-
84 tion has been refined, where both K_X and γ_X were prescribed by a self-similar profile
85 function depending on external characteristics of the boundary layer such as surface forc-
86 ing, stratification at the atmospheric top (or oceanic base) of the mixed layer and im-
87 plicitly defined mixed layer height (see Troen and Mahrt (1986); Holtslag and Moeng
88 (1991) for atmospheric models, Large et al. (1994) for oceanic models). This approach
89 is still in use in some present-day ocean models (e.g. via the CVMIX library, Van Roekel
90 et al., 2018). Furthermore two other types of convective parameterization are sometimes
91 used: (i) a buoyancy sorting scheme (a.k.a. adjustment scheme or non-penetrative scheme),
92 in which static instabilities are eliminated in one time-step by mixing downward neigh-
93 boring vertical levels until a neutral buoyancy profile is attained (e.g. Madec et al., 1991)
94 (ii) an enhanced eddy-viscosity scheme in which the vertical diffusivity coefficient is ar-
95 tificially increased to a high value as soon as static instabilities are found on the den-
96 sity profiles (Madec et al., 2019). These two approaches are ad-hoc and cannot be de-
97 rived from first principles.

98 The present work builds on the combined Eddy-Diffusivity and Mass-Flux (EDMF)
99 parameterization schemes (Hourdin et al., 2002; Soares et al., 2004). The ED compo-
100 nent aims to represent turbulent transport in a nearly isotropic environment, in which
101 convective plumes -modeled by MF terms- support a non-local advective transport. The
102 MF concept was originally introduced in the atmospheric context to represent deep con-
103 vective clouds (Arakawa & Schubert, 1974), then it has been adapted to represent shal-
104 low and dry boundary layer convection in combination with ED schemes. It is intrin-
105 sically based on a multi-fluid averaging (Yano, 2014; Thuburn et al., 2018) of the fluid
106 equations. In ocean models the EDMF concept has been first introduced by Giordani
107 et al. (2020), and has been gaining increasing attention (e.g. Garanaik et al. (2024), or
108 a recent implementation in the code Oceananigans, Ramadhan et al. (2020)).

109 1.2 Parameterization development and physics dynamics coupling

110 The general objective of the proposed work is to approach the parameterization
111 problem in a “consistent” manner. Here the notion of consistency integrates various as-
112 pects: consistent dynamical and thermodynamical approximations between resolved and
113 subgrid models, energetic consistency at both continuous (e.g. Eden, 2016; Jansen et al.,

2019; Eden & Olbers, 2014) and discrete (e.g. Burchard, 2002) levels, consistency with a particular choice of scale-separation operator (Higgins et al., 2013; Lauritzen et al., 2022), and the rigorous reduction of a physical system to a scale-aware parametric representation based on well-identified approximations and hypotheses (Honnert et al., 2016; Tan et al., 2018).

Regarding boundary layer parameterizations, turbulent kinetic energy (TKE) or its budget can serve to compute viscous dissipation, which is key to close the total energy budget. Moreover some schemes use prognostic TKE to scale the intensity of eddy-diffusivity. By using energy arguments, we aim to remove ambiguity around three practical topics: how to interpret TKE in the model; whether to use ED or EDMF fluxes in the source terms of TKE; what are consistent boundary conditions? The question of the fluxes appears ambiguous in the literature. Some studies use ED fluxes (Giordani et al., 2020; Hourdin et al., 2019; Han et al., 2016). Other studies use explicitly the full EDMF fluxes (Han & Bretherton, 2019; Witek et al., 2011). However the majority of studies and documentations are ambiguous or not explicit about this point, and modelling choices are often motivated by simulation outputs rather than consistency. In this paper, we argue that energy conservation constraints can guide without ambiguity such choices. TKE represents a subgrid kinetic energy that exchanges energy with the resolved reservoirs. The use of mass-flux terms leads to energy transfers and redistributions that must be taken into account in the TKE equation to ensure energetic consistency between resolved and subgrid scales. In addition, the boundary conditions of the mass-flux equations must be consistent between ED and MF to avoid double-counting and subsequent artificial energy fluxes at the fluid boundary.

The aim of this paper is two-fold. First, we intend to provide an introductory, self-contained, and pedagogical derivation of EDMF schemes starting from first principles, to guide consistency considerations. Second, we derive theoretical energy budgets and provide guidelines to obtain energetically consistent EDMF models. Consequently, this paper is intended to both the oceanographic community as a comprehensive introduction to EDMF, and the atmospheric community seeking to reduce energy biases in EDMF models.

1.3 Organization of the paper

The paper is organized as follows. In section 2, we expose the derivation of an EDMF scheme from first principle, systematically discuss the successive assumptions at stake, provide closures according to state-of-the-art practice, and discuss consistent boundary conditions. In section 3, we recall the theoretical closure-agnostic resolved and subgrid energy budgets of a horizontally averaged anelastic (or Boussinesq) fluid, including radiative heating. In section 4, we expose analogous energy budgets when using an EDMF closure, including consistent TKE equation, and propose a new formulation for TKE transport. Furthermore, we derive vertically averaged energy budgets to reveal the net contribution of shear and the role of boundary conditions on the energy fluxes. In a companion paper (Perrot and Lemarié (2024); hereafter Part II) we assess the validity of hypotheses and the sensitivity of the scheme to modelling choices against Large Eddy Simulations (LES) and observational data of oceanic convection, detail an energy-conserving discretization, and quantify energy biases of inconsistent formulations.

2 Derivation of EDMF scheme

2.1 Formal derivation

We start from the unaveraged anelastic non-hydrostatic system in conservative form (e.g. eq. (76-80) of Tailleux & Dubos, 2024) in a cubic domain $L_x \times L_y \times H$, describ-

162 ing either a dry atmosphere or a salty ocean:

$$\partial_t \mathbf{u} = -\frac{1}{\rho_R} \nabla \cdot (\rho_R \mathbf{u} \otimes \mathbf{u}) - \nabla \left(\frac{p^\dagger}{\rho_R(z)} \right) + b \mathbf{e}_z + \frac{1}{\rho_R} \nabla \cdot (\rho_R \boldsymbol{\tau}) \quad (1)$$

$$\nabla \cdot (\rho_R(z) \mathbf{u}) = 0 \quad (2)$$

$$\partial_t \theta = -\frac{1}{\rho_R} \nabla \cdot (\rho_R \mathbf{u} \theta) + P_\theta \quad (3)$$

$$\partial_t S = -\frac{1}{\rho_R} \nabla \cdot (\rho_R \mathbf{u} S) \quad (4)$$

$$b = -g \frac{\rho_{\text{EOS}} - \rho_R(z)}{\rho_{\text{EOS}}} \quad (5)$$

$$\rho_{\text{EOS}} = \rho_{\text{EOS}}(\theta, S, p_R(z)) \quad (6)$$

163 where $\mathbf{u} = (u, v, w)$ denotes the velocity field in a local Cartesian frame of reference $(\mathbf{e}_x, \mathbf{e}_y, \mathbf{e}_z)$,
 164 z ranges from 0 to H in the atmosphere and $-H$ to 0 in the ocean, $\rho_R(z)$ is a reference
 165 density profile, the pressure has been decomposed as $p = p_R(z) + p^\dagger(x, y, z, t)$ with $\partial_z p_R =$
 166 $-\rho_R g$, b is the buoyancy acceleration, θ is potential temperature, S is the mass concen-
 167 tration of an additional component of the fluid (in kg/kg; typically salt in the ocean or
 168 any passive tracer in the atmosphere), P_θ is an additional source of potential temper-
 169 ature that will be specified in E3 via energy constraints, $\boldsymbol{\tau} = \nu \mathbf{1}/2(\nabla \mathbf{u} + \nabla \mathbf{u}^T)$ is the
 170 viscous stress tensor.

171 Remark that by specifying $\rho_R(z) = \rho_0 = \text{cst}$, we obtain a Boussinesq system
 172 with buoyancy given by (5) instead of the more traditional form $-g(\rho_{\text{EOS}} - \rho_0)/\rho_0$ (Tailleux
 173 & Dubos, 2024; Eldred & Gay-Balmaz, 2021). This so-called Boussinesq-anelastic for-
 174 mulation has the advantage to possess "potential energy and thermodynamic potentials
 175 that are nearly identical to their exact counterparts so that their energetics is more easi-
 176 ly comparable to that of the fully compressible equations and do not require the intro-
 177 duction of artificial and ad-hoc thermodynamic potentials" (Tailleux & Dubos, 2024).
 178 For simplicity, we restrict to the case of a dry atmosphere and of seawater with a lin-
 179 earized equation of state¹. Moreover we do not include the Coriolis term in the present
 180 study. Since the Coriolis force is energetically-neutral it does not interfere with the deriva-
 181 tions made throughout this paper.

182 Next, we detail the framework in which vertical mixing parameterizations are usu-
 183 ally developed. We adopt a semi-discrete description, where the horizontal fluid domain
 184 is *discretized* into a $N_x \times N_y$ mesh whereas time and vertical coordinates z are kept as
 185 *continuous* variables. Each horizontal grid cell has length Δx_i and width Δy_j ($i = 1, \dots, N_x$;
 186 $j = 1, \dots, N_y$), and we denote (x_i, y_j) its center. The spatial domain can be thought
 187 of $N_x \times N_y$ vertical columns stacked together. In a numerical model discretized on such
 188 a mesh, the computed variables would be interpreted in a finite volume approach (LeVeque,
 189 2002): for any field $X = \mathbf{u}, \theta, S, \dots$ one can define the following horizontal average and
 190 fluctuation

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

191 If we recast (1)–(6) in the generic form $\partial_t X + \frac{1}{\rho_R} \nabla \cdot (\rho_R \mathbf{u} X) = P_X$, and then apply
 192 such a horizontal average, we obtain

$$\partial_t \bar{X} + \frac{1}{\rho_R} \partial_z (\rho_R \bar{w} \bar{X} + \rho_R \overline{w' X'}) + \frac{1}{\Delta x_i \Delta y_j} \oint_{\partial(\Delta x_i \times \Delta y_j)} X \mathbf{u}_h \cdot d\mathbf{n} = \bar{P}_X \quad (7)$$

¹ In both oceanic and atmospheric context, we use simple thermodynamic descriptions allowing convec-
 tion. Although these descriptions are inaccurate for real-world applications, they are sufficient to expose
 how to build energetically consistent EDMF parameterizations.

193 where $\mathbf{u}_h = (u, v, 0)$ denotes the horizontal velocity vector and $d\mathbf{n}$ is an outward point-
 194 ing line integral element, i.e. $\mathbf{u}_h \cdot d\mathbf{n} = udy - vdx$. In a numerical model, \bar{X} would be
 195 interpreted as the resolved variable, X' would be an unresolved fluctuation, the bound-
 196 ary integral in (7) would be interpreted as the divergence of the total (resolved and sub-
 197 grid) horizontal flux of X (precise form of the horizontal flux would depend on the nu-
 198 merical scheme and possibly on parameterizations), and the vertical subgrid flux $\overline{w'X'}$
 199 has to be closed via a parameterization.

200 When focusing on the parameterization of vertical mixing processes, it is common
 201 to conceptually isolate one vertical column of fluid to work with a one-dimensional Single-
 202 Column Model (SCM) (e.g. Zhang et al., 2016). Any quantity is assumed statistically
 203 invariant along the horizontal direction, meaning that in practice the horizontal fluxes
 204 and pressure gradients are neglected. We further simplify the problem with two addi-
 205 tional assumptions: First, the bottom (or top for the ocean) of the column is considered
 206 flat. Along with a non-penetration condition, this leads to $\overline{w}(z=0) = 0$. Now the hor-
 207 izontal homogeneity assumption implies that $\overline{\partial_x(\rho_R u)} + \overline{\partial_y(\rho_R v)} = 0$, thus mass con-
 208 servation reads $\partial_z(\rho_R \bar{w}) = 0$. Along with the non penetration condition it implies $\bar{w}(z) =$
 209 0 at any level z . Second, in the vertical momentum budget, the momentum flux diver-
 210 gence $\partial_z \overline{w'w'}$ is neglected, leading to the hydrostatic approximation $\partial_z \bar{p}^\dagger = b$. The re-
 211 sulting SCM equations are then

$$\partial_t \bar{\mathbf{u}}_h = -\frac{1}{\rho_R} \partial_z (\rho_R \overline{w' \mathbf{u}'_h}) \quad (8)$$

$$\partial_t \bar{\theta} = -\frac{1}{\rho_R} \partial_z (\rho_R \overline{w' \theta'}) + \bar{P}_\theta \quad (9)$$

$$\partial_t \bar{S} = -\frac{1}{\rho_R} \partial_z (\rho_R \overline{w' S'}) \quad (10)$$

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

219 We now *assume* a formal decomposition of the horizontal column area $\Delta x \times \Delta y$
 220 into two horizontal subdomains of areas $\mathcal{A}_e(z, t)$ and $\mathcal{A}_p(z, t)$ which also depend on depth
 221 and time (see fig. 1). Such decomposition is meant to isolate the coherent convective struc-
 222 tures usually referred to as *plumes* (occupying the subdomain of area $\mathcal{A}_p(z, t)$) from the
 223 rest of the flow, referred to as the *environment* (occupying the subdomain of area $\mathcal{A}_e(z, t)$).
 224 We introduce the following notations to characterize the subdomain averaged fields, fluc-
 225 tuations and *fractional* area ($i = e$ for environmental variables and $i = p$ for plume
 226 variables):

$$\begin{aligned} X_i &= \frac{1}{\mathcal{A}_i(z, t)} \int_{\mathcal{A}_i(z, t)} X(x, y, z, t) dx dy, & X'_i &= X - X_i \\ a_i &= \mathcal{A}_i(z, t) / (\Delta x \times \Delta y) \end{aligned}$$

227 Any mean field can then be decomposed as

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

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

$$\overline{w'X'} = a_e \overline{w'_e X'_e} + a_p \overline{w'_p X'_p} + a_e (w_e - \bar{w})(X_e - \bar{X}) + a_p (w_p - \bar{w})(X_p - \bar{X}) \quad (11)$$

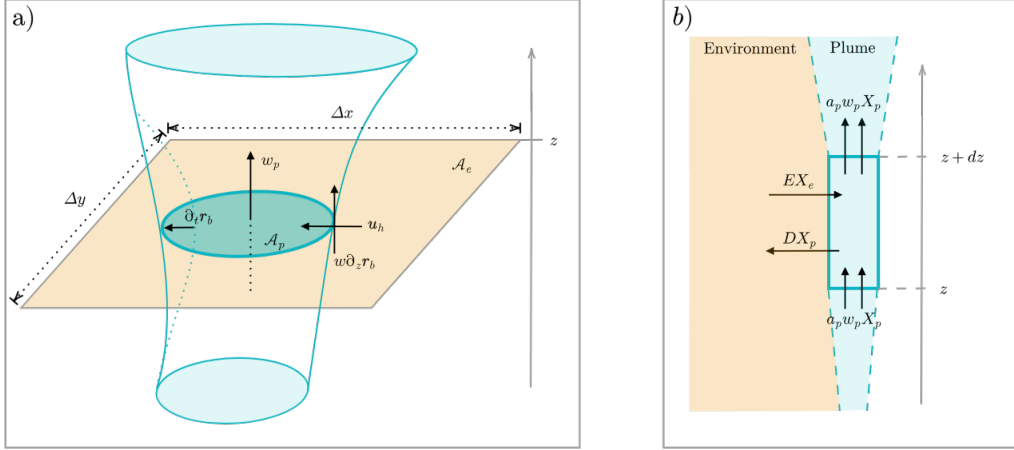


Figure 1: Schematic of representation of: (a) a 3D plume (blue volume) embedded into the environment. At a given level z , horizontal grid cell $\Delta x \times \Delta y$ is decomposed into plume area \mathcal{A}_p (blue shading) and environment area \mathcal{A}_e (orange shading). Fluxes of fluid and tracers across the boundary $\partial\mathcal{A}_p$ are due to horizontal velocity across the boundary \mathbf{u}_h , to (apparent) horizontal velocity of the boundary $\partial_t \mathbf{r}_b$ and to vertical velocity if the boundary of the 3D plume is vertically tilted ($\partial_z \mathbf{r}_b \neq 0$). (b) Horizontal and vertical fluxes of tracer X into the equivalent "single" plume, within the upstream approximation. See text for details.

230 where

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

231 Here we kept \bar{w} for generality, however as explained above the horizontal homogeneity
 232 assumption implies $\bar{w} = 0$. For each subdomain, the $a_i(w_i - \bar{w})(X_i - \bar{X})$ terms in (11)
 233 account for the "mass-flux" (i.e. the contribution of coherent structures to the flux), whereas
 234 the $a_i \overline{w'_i X'_i}$ terms are a contribution from internal variability within subdomain i . Ap-
 235 plying the subdomain average to any conservation law of the form $\partial_t X + \frac{1}{\rho_R} \nabla \cdot (\rho_R \mathbf{u} X) =$
 236 P_X and using Reynolds transport theorem leads to (see appendix A of Tan et al. (2018)
 237 and Yano (2014) for full derivation)

$$\partial_t (a_i X_i) + \frac{1}{\rho_R} \partial_z \left(\rho_R a_i w_i X_i + \rho_R a_i \overline{w'_i X'_i} \right) + \frac{1}{\mathcal{A}_i} \oint_{\partial\mathcal{A}_i} X \mathbf{u}_r \cdot d\mathbf{n} = a_i P_{X,i} \quad (12)$$

238 where the relative horizontal boundary velocity is $\mathbf{u}_r = \mathbf{u}_h - \partial_t \mathbf{r}_b - w \partial_z \mathbf{r}_b$ and $\mathbf{r}_b =$
 239 $(x_b(z, t), y_b(z, t))$ is the position vector of boundary elements. The three terms that con-
 240 stitute \mathbf{u}_r indicate that boundary fluxes can arise respectively due to horizontal veloc-
 241 ity across the boundary, to (apparent) horizontal velocity of the boundary, or to verti-
 242 cal velocity if the boundary of the 3D plume is vertically tilted (i.e. $\partial_z \mathbf{r}_b \neq 0$; see fig.
 243 1(a)).

244 2.2 Standard assumptions

245 2.2.1 Plume-Environment decomposition

246 The first standard assumption we have already made is to consider only two sub-
 247 domains, the convective plume and the environment. This is justified since in convec-
 248 tive situations the main contribution to the fluxes comes from the plumes. However, the
 249 framework is flexible enough to incorporate an arbitrary number of components, such

250 as multiple updrafts or downdrafts. In particular, several studies of the atmospheric con-
 251 vective boundary layer (CBL) underline the importance of returning coherent structures
 252 around the plumes, often referred to as CBL downdrafts (Schmidt & Schumann, 1989;
 253 Couvreux et al., 2007; Brient et al., 2023).

254 **2.2.2 Entrainment/Detrainment and Upstream approximation**

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

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

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

$$\frac{1}{\mathcal{A}_p} \oint_{\partial\mathcal{A}_p} X \mathbf{u}_r \cdot d\mathbf{n} = X_e E - X_p D \quad (13)$$

262 As a result of this approximation, the plume equation reads (fig. 1(b))

$$\partial_t(a_p X_p) + \frac{1}{\rho_R} \partial_z(\rho_R a_p w_p X_p) = -\frac{1}{\rho_R} \partial_z(\rho_R a_p \overline{w'_p X'_p}) + E X_e - D X_p + a_p P_{X,p} \quad (14)$$

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

$$\partial_t a_p + \frac{1}{\rho_R} \partial_z(\rho_R a_p w_p) = E - D \quad (15)$$

264 from which we can rewrite the plume equation in advective form,

$$a_p \partial_t X_p + a_p w_p \partial_z X_p = -\frac{1}{\rho_R} \partial_z(\rho_R a_p \overline{w'_p X'_p}) + E(X_e - X_p) + a_p P_{X,p} \quad (16)$$

265 **2.2.3 Steady plume hypothesis**

266 A common hypothesis is that the plume domain is in a quasi-steady regime, thus
 267 neglecting the temporal tendency compared to vertical advection. The relevance of this
 268 hypothesis is numerically tested in idealized LES cases in Part II. An *a priori* scaling
 269 estimation can also be performed. Let h be the boundary layer depth, which can also
 270 serve as a length scale for the mean plume. A characteristic time scale for the mean plume
 271 is $\tau_p = h/W$ where W is a plume vertical velocity scale. A time scale associated to the
 272 boundary layer growth and mean fields evolution is $\tau_{BL} = h/w_{\text{ent}}$ where $w_{\text{ent}} = dh/dt$
 273 is the boundary layer vertical entrainment velocity. In the limit of free convection trig-
 274 gered by a surface buoyancy loss $B_0 < 0$ into a fluid of constant stratification N_0^2 , the
 275 classical convective scalings $h \propto \sqrt{(-B_0/N_0^2)t}$ and $W = w_* = (-B_0 h)^{1/3}$ (Turner,
 276 1979; Deardorff, 1970) leads to

$$\frac{\tau_p}{\tau_{BL}} = \frac{w_{\text{ent}}}{W} \propto \frac{1}{(N_0 t)^{2/3}} \quad (17)$$

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

277 In a different context, that of the development of a shear-driven mixed layer forced by
 278 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
 279 such a layer $W \simeq u_*$, leading to a scaling similar to (17). These scalings suggest that
 280 as long as the surface forcings (represented here by u_* and B_0) are evolving slowly com-
 281 pared to $1/N_0$, the steady plume hypothesis remains valid. Under such a hypothesis, the
 282 plume equation for any field X and the plume area conservation now read

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

$$\partial_z (\rho_R a_p w_p X_p) = E - D \quad (19)$$

283 As a summary, we rewrite the coupled resolved/plume system in an advective form us-
 284 ing area conservation and $\overline{X} = (1-a_p)X_e + a_p X_p$ and the identity $(X_e - \overline{X}) = \frac{-a_p}{1-a_p}(X_p -$
 285 $\overline{X})$ (a summary of useful identities can be found in Appendix A):

$$\partial_t \overline{X} = -\frac{1}{\rho_R} \partial_z (\rho_R \overline{w' X'}) + \overline{P}_X \quad (20)$$

$$\overline{w' X'} = \frac{1}{1-a_p} a_p w_p (X_p - \overline{X}) + (1-a_p) \overline{w'_e X'_e} + a_p \overline{w'_p X'_p} \quad (21)$$

$$a_p w_p \partial_z X_p = -\frac{1}{1-a_p} E (X_p - \overline{X}) - \frac{1}{\rho_R} \partial_z (\rho_R a_p \overline{w'_p X'_p}) + a_p P_{X,p} \quad (22)$$

286 Several authors have recently proposed to relax the steady plume hypothesis (Tan et al.,
 287 2018; Thuburn et al., 2018). However, the overwhelming majority of mass flux schemes
 288 implemented in realistic models considers a plume domain in a quasi-steady regime.

289 **2.2.4 Small area limit**

290 A last standard hypothesis is that the fractional area of the plume is *small* com-
 291 pared to that of the environment (see Part II for a direct evaluation against LES). This
 292 generally means considering the formal limit $a_p \rightarrow 0$ and $a_e \rightarrow 1$ in the previous equa-
 293 tions while keeping non-zero mass-flux $a_p w_p$ and source terms. Yano (2014) proposes to
 294 assume $a_p w_p = O(w_e)$ and $a_p P_{X,p} = O(S_{X,e})$ to retain an order one contribution of
 295 $a_p w_p (X_p - \overline{X})$ in (21), to neglect subplume fluxes $\overline{w'_p X'_p}$ and to keep an order one con-
 296 tribution of advection and forcings in (22). In the small area limit, any environmental
 297 field X_e (except w_e) can be approximated by the mean field, the vertical turbulent flux
 298 (21) becomes

$$\overline{w' X'} = a_p w_p (X_p - \overline{X}) + \overline{w'_e X'_e} \quad (23)$$

299 and the plume equation (22) now reads

$$a_p w_p \partial_z X_p = -E (X_p - \overline{X}) + a_p P_{X,p} \quad (24)$$

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

308 **2.3 Standard Closures**

309 Thanks to the assumptions made so far, we have arrived at equations of the gener-
 310 al form (24) for the plume, and (23) for vertical turbulent fluxes. At this stage, addi-
 311 tional closure assumptions are required to express the entrainment and detrainment rates,
 312 the flux $\overline{w'_e X'_e}$, and the pressure gradients appearing in the $P_{w,p}$ and $P_{u_h,p}$ terms.

313 **2.3.1 Plume vertical pressure gradient**

314 Plume vertical pressure gradients are usually parameterized as the combination of
 315 a virtual mass term (e.g. Bretherton et al., 2004) – representing the reduction of plume
 316 buoyancy due to pushing and pulling on the environment –, a reduced entrainment term
 317 and a quadratic drag term (Simpson & Wiggert, 1969; Romps & Charn, 2015). Several
 318 formulations have been proposed (see Roode et al. (2012) for an intercomparison in the
 319 context of shallow cumulus convection). Alternatively several authors point out the im-
 320 portance of non-local (in height) effects (Peters, 2016; Kuo & Neelin, 2022), leading to
 321 recent formulations on e.g. velocity divergence (Weller et al., 2020), or adaptive updraft
 322 radius (He et al., 2021; Peters et al., 2021). A detailed intercomparison of these differ-
 323 ent closures is out of the scope of this paper. Here we adapt some usual practices in the
 324 atmospheric context (e.g. Pergaud et al., 2009; Rio et al., 2010) and consider

$$-a_p (\partial_z(p^\dagger/\rho_R))_p = (a-1)a_p B_p + (b-1)(-E w_p) + b' \frac{1}{h} a_p w_p^2 \quad (25)$$

325 leading to the plume vertical momentum budget

$$a_p w_p \partial_z w_p = a a_p B_p - b E w_p - \sigma_o^a b' \frac{1}{h} a_p w_p^2 \quad (26)$$

326 where a , b and b' are positive non-dimensional parameters, $\sigma_o^a = +1$ in the atmosphere
 327 and -1 in the ocean, and $B_p = b_p - \bar{b}$. The plume vertical extent $h = h(t)$ is com-
 328 puted as the height (or depth) at which the plume vertical velocity w_p goes to zero. Since
 329 plumes are structures of aspect ratio close to 1, h provides an acceptable scale to sub-
 330 stitute the constant plume radius classically used in the drag term (Simpson & Wiggert,
 331 1969; Romps & Charn, 2015; Tan et al., 2018; Weller et al., 2020). The main advantage
 332 of our formulation is to avoid the introduction of a constant *dimensional* radius coeffi-
 333 cient which would restrict parameterization universality. Note that in the case of dry at-
 334 mosphere or seawater with a linearized equation of state, we have $b_p - \bar{b} = b_{\text{eos}}(\theta_p, S_p, p_R(z)) -$
 335 $b_{\text{eos}}(\bar{\theta}, \bar{S}, p_R(z))$.

336 **2.3.2 Horizontal momentum budget**

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

$$-a_p \left(\nabla_h \frac{p^\dagger}{\rho_R} \right)_p = a_p w_p C_u \partial_z \bar{u}_h \quad (27)$$

340 where C_u is a parameter. It imposes a relaxation of the plume shear towards the grid-
 341 scale shear. We show in Section 4.4 that energy constraints impose $0 \leq C_u < 1$.

342 **2.3.3 Eddy-Diffusivity closure**

343 The environment is thought of as a subdomain where only small-scale turbulence
 344 occurs, thus supporting the hypothesis of a closure of the vertical flux with an eddy-diffusivity,
 345 $\overline{w'_e X'_e} = -K_X \partial_z X_e \underset{a_p \ll 1}{\simeq} -K_X \partial_z \bar{X}$. This leads to the eddy-diffusivity mass-flux clo-
 346 sure of subgrid fluxes

$$\overline{w' X'} = \underbrace{-K_X \partial_z \bar{X}}_{\text{ED}} + \underbrace{a_p w_p (X_p - \bar{X})}_{\text{MF}} \quad (28)$$

347 In order to compute the eddy-diffusivity coefficient K_X , various approaches relying ei-
 348 ther on self-similar empirical profiles (e.g. Siebesma et al., 2007; Han et al., 2016) or on
 349 prognostic turbulent kinetic energy (e.g. Hourdin et al., 2019) can be found in the lit-
 350 erature. However the practical choice of a closure do not directly affect energy budgets
 351 of the SCM.

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

Table 1: Summary of the vertical turbulent flux formulation and plume equations in the small area limit under the steady plume hypothesis detailed in sections 2.1, 2.2 and 2.3.

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

$$E = a_p \beta_1 \max(0, \partial_z w_p) \quad (29)$$

$$D = -a_p \beta_2 \min(0, \partial_z w_p) + \sigma_o^a a_p w_p \frac{\delta_0}{h} \quad (30)$$

where the two parameters β_1 and β_2 are positive, δ_0/h is a positive minimum detrainment (some authors also include a minimum "turbulent" entrainment, e.g. Cohen et al. (2020)).

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

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 \bar{X} must comply with the EDMF flux decomposition (28)

$$\overline{w'X'}(0) = -K_X \partial_z \bar{X}(0) + a_p(0)w_p(0)(X_p(0) - \bar{X}(0)) \quad (31)$$

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 for downdrafts and $+a_p w_p$ is the atmospheric mass-flux for updrafts.

371 Such a constraint should guide modeling choices concerning boundary conditions. In-
 372 deed, it systematically guarantees the correct partition of surface fluxes, and thus avoids
 373 double-counting biases linked to non-physical energy sources/sinks at the boundary (see
 374 Sec. 4.2). For instance, suppose the values of $\overline{w'X'}(0)$, $a_p(0)$, $w_p(0)$ and $X_p(0)$ are jointly
 375 specified. Then (31) would turn into a Robin (a.k.a type 3) boundary condition for the
 376 \overline{X} equation which arises naturally in advection-diffusion equations (e.g. Hahn and Özişik
 377 (2012), chapter 1-5). At the boundary $z = \sigma_o^a H$, a no-flux condition is imposed for the
 378 mean equation. For the specific case of oceanic convection reaching the ocean bottom,
 379 a possibility is to add a penalization term nudging the solution towards the condition
 380 $w_p(z = -H) = 0$.

381 **2.4.2 Oceanic context**

382 For oceanographic applications, we consider that a surface flux $\overline{w'X'}(0)$ is prescribed.
 383 The mass flux component becomes non-zero close to the surface as soon as the plume
 384 is accelerating and entrainment rate (29) is itself non-zero. For simplicity we consider
 385 here $\delta_0 = 0$. In this case the conservation of volume reads

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

386 which can be easily integrated vertically to obtain

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

387 Except for singular case $\beta_1 = 1$, non-trivial solutions are obtained if and only if non-
 388 zero boundary values for a_p and w_p are chosen. In the remainder, we adopt the follow-
 389 ing simple choice,

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

390 where a_p^0 and w_p^0 are parameters. According to (31), it implies that all the surface flux
 391 is allocated in the ED component, as advocated by Tan et al. (2018). This particular choice
 392 of boundary condition is also motivated by the fact that it implies that convection is trig-
 393 gered as soon as the surface Brünt-Väisälä frequency $\partial_z b(0)$ is negative (see Appendix
 394 C for further details). As a result, (31) turns into the Neumann boundary condition $-K_X \partial_z X(0) =$
 395 $\overline{w'X'}(0)$, which is standard practice for ED-only closures.

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

$$\theta_p(z) = \overline{\theta}(z) + \beta \frac{\overline{w'\theta'}(0)}{\sqrt{k(z)}} \quad (32)$$

398 where β is a constant. We show in Appendix C that our formulation is in fact equiva-
 399 lent to (32) for if $\beta = z/(c_b l_b(0))$ and $k(z) \simeq k(0)$ (where c_b is a constant and l_b a mix-
 400 ing length associated to buoyancy). Thus our simple choice is equivalent to a forcing of
 401 the plume by surface buoyancy loss. However, when using this type of boundary con-
 402 dition exactly at the surface (as in Pergaud et al., 2009), the boundary condition for $\overline{\theta}$
 403 must be modified in order to avoid double-counting of heat flux at the surface (see sec-
 404 tion 4.5).

405 **2.4.3 Atmospheric context: consistency with Monin-Obukhov theory**

406 For atmospheric applications, boundary conditions for the mean variables are com-
 407 monly imposed using Monin-Obukhov similarity theory (MOST), which assumes that
 408 in a surface layer located between $z = 0$ and $z = z_1$ fluxes are constant, and mean vari-
 409 ables obey a quasi-logarithmic profile. To properly include a surface layer obeying MOST,

410 then the EDMF flux decomposition must be imposed at the new model boundary $z =$
 411 z_1 , namely

$$\overline{w'X'}(z_1) = -K_X(z_1)\partial_z\overline{X}(z_1) + a_p(z_1)w_p(z_1)(X_p(z_1) - \overline{X}(z_1)) \quad (33)$$

412 At this stage, we can point the following ambiguity. When the MF term is non-zero, it
 413 is not clear whether the flux arising from MOST – which is an ED flux – should be al-
 414 located 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 con-
 415 stant flux assumption. Although not discussed transparently, it seems that the second
 416 option is a common practice. However, in such a case, special attention would be required
 417 to compute the total flux entering in energy budget computations.
 418 Although beyond the scope of this article, we would like to point out that MOST is known
 419 to fail in strongly unstable conditions (Johansson et al., 2001; Li et al., 2018). Recently,
 420 Li et al. (2021) proposed corrections to formulate departure from MOST in the form of
 421 an EDMF closure including updraft *and* downdraft contributions. This approach could
 422 potentially help provide physically consistent boundary conditions to EDMF models.

423 At this stage, we have provided all the elements and underlying assumptions re-
 424 quired to formulate an EDMF-type scheme (see Part II for the discretization aspects).
 425 Before studying the energetic impacts of using MF components, we derive theoretical
 426 horizontally averaged energy budgets.

427 3 Horizontally Averaged Energy Budgets

428 In this section, we derive horizontally averaged energy budgets regardless of flux
 429 parameterizations. As a starting point, we recall the closed energy budgets of the un-
 430 averaged anelastic system (or Boussinesq system if $\rho_R(z) = \rho_0$) derived for reference
 431 in Appendix E:

$$\begin{cases} \partial_t(\rho_R\mathcal{E}_k) + \nabla \cdot [\mathbf{u}(\rho_R E_k + p^\dagger) + \rho_R\nu\mathbf{u} \cdot \boldsymbol{\tau}] & = \rho_R w b - \rho_R \epsilon \\ \partial_t(\rho_R\mathcal{E}_i) + \nabla \cdot [\mathbf{u}(\rho_R\mathcal{E}_i + p_R)] + \nabla \cdot [\rho_R\mathbf{F}_h] & = -\rho_R g w - \rho_R b w + \rho_R(\epsilon + \dot{q}_{\text{rad}}) \\ \partial_t(\rho_R\mathcal{E}_p) + \nabla \cdot [\mathbf{u}\rho_R\mathcal{E}_p] & = \rho_R g w \end{cases} \quad (34)$$

432 where the (unaveraged) total material energy has been divided into kinetic energy $\rho_R(z)\mathcal{E}_k =$
 433 $\rho_R(z)\frac{1}{2}\mathbf{u} \cdot \mathbf{u}$, internal energy $\rho_R\mathcal{E}_i = \rho_R(\hat{h}(\eta, S, p_R(z)) - p_R(z)/\rho_R(z))$ –with \hat{h} the
 434 specific enthalpy–, and potential energy $\rho_R\mathcal{E}_p = \rho_R g z$ (see e.g. Tailleux and Dubos (2024),
 435 where these authors referred to $\mathcal{E}_i + \mathcal{E}_p$ as “potential energy”). Moreover, the viscous
 436 stress tensor and viscous dissipation of kinetic energy have been written $\boldsymbol{\tau}$ and $\epsilon := -\nabla\mathbf{u} : \boldsymbol{\tau} = \nu\|\nabla\mathbf{u}\|^2$. \mathbf{F}_h is the (molecular) diffusive flux of enthalpy. The radiative heating \dot{q}_{rad}
 437 is treated as an external energy source; consequently one would need to include the ra-
 438 diative energy \mathcal{E}_r to the material energy in order to close the energy budget (see Appendix
 439 E for details).
 440

441 Now, we will focus on the horizontal averages of these energies. First let us recall
 442 that the SCM assumptions (sec. 2.1) implies $\overline{w} = 0$. Then the averaged kinetic energy
 443 $\overline{\mathcal{E}_k}$ can be advantageously split into the kinetic energy of the horizontal resolved flow $E_k =$
 444 $(\overline{\mathbf{u}_h} \cdot \overline{\mathbf{u}_h})/2$ (usually referred as *mean* or *resolved kinetic energy*) and the residual tur-
 445 bulent (or subgrid) kinetic energy $k = (\overline{\mathbf{u}' \cdot \mathbf{u}'})/2$. We will denote also by $E_{i+p} = \overline{\mathcal{E}_i} + \overline{\mathcal{E}_p}$
 446 the sum of averaged internal energy and potential energy. Upon averaging and apply-
 447 ing the SCM assumptions, the budgets of the horizontally averaged energies E_k , k and
 448 E_{i+p} read

$$\begin{cases} \partial_t(\rho_R E_k) + \partial_z(\rho_R T_{E_k}) & = \rho_R \overline{w' \mathbf{u}'_h} \cdot \partial_z \overline{\mathbf{u}_h} \\ \partial_t(\rho_R k) + \partial_z(\rho_R T_k) & = -\rho_R \overline{w' \mathbf{u}'_h} \cdot \partial_z \overline{\mathbf{u}_h} + \rho_R \overline{w' b'} - \rho_R \bar{\epsilon} \\ \partial_t(\rho_R E_{i+p}) + \partial_z(\rho_R T_{E_{i+p}}) & = -\rho_R \overline{w' b'} + \rho_R(\bar{\epsilon} + \bar{q}_{\text{rad}}) \end{cases} \quad (35)$$

449 and the transport terms that redistribute energy on the vertical are

$$\begin{cases} T_{E_k} &= \overline{w' \mathbf{u}'_h \cdot \bar{\mathbf{u}}_h} \\ T_k &= \overline{w' \frac{\mathbf{u}' \cdot \mathbf{u}'}{2}} + \frac{1}{\rho_R} \overline{w' p'^{\dagger}} - \nu \partial_z k \\ T_{E_{i+p}} &= \overline{w' h'} \end{cases} \quad (36)$$

450 where we made the classical approximations that dissipation of mean KE is negligible,
451 i.e. $\nu \|\nabla \bar{\mathbf{u}}\|^2 \simeq 0$, $\nu \|\nabla \mathbf{u}'\|^2 \simeq \bar{\epsilon}$ and neglected the (molecular) diffusive flux of enthalpy.

452 Now we are going to specify temperature equation, heat flux $\overline{w' h'}$ and buoyancy
453 flux $\overline{w' b'}$ for two fluids with simplified thermodynamics.

454 3.1 Dry atmosphere

455 For dry air in the anelastic approximation, specific enthalpy and buoyancy reads

$$h(\theta, p_R(z)) = c_p T = c_p \theta \left(\frac{p_R(z)}{p_0} \right)^\kappa \quad (37)$$

$$b = -\partial_z (h + gz) = g \frac{\theta - \theta_R(z)}{\theta_R(z)} \quad (38)$$

456 where c_p is a constant specific heat capacity of dry air, p_0 is a constant pressure refer-
457 ence, θ is the potential temperature, $\theta_R(z) = p_R \left(\frac{p_R(z)}{p_0} \right)^{-\kappa} / (\rho_R R_d)$ is the reference
458 potential temperature profile, R_d is the specific dry air ideal constant, $\kappa = R_d / c_p$. We
459 straightforwardly obtain an equation for the unaveraged potential temperature using the
460 enthalpy budget (E13):

$$c_p \left(\frac{p_R}{p_0} \right)^\kappa \partial_t \theta + \frac{1}{\rho_R} \nabla \cdot \left(\rho_R c_p \left(\frac{p_R}{p_0} \right)^\kappa \theta \mathbf{u} + \rho_R \mathbf{F}_h \right) = -gw - g \frac{\theta - \theta_R(z)}{\theta_R(z)} w + \epsilon + \dot{q}_{\text{rad}} \quad (39)$$

461 which can be rewritten after some algebra as

$$\partial_t \theta + \frac{1}{\rho_R} \nabla \cdot (\rho_R \theta \mathbf{u}) + \frac{1}{c_p} \left(\frac{p_R}{p_0} \right)^{-\kappa} \nabla \cdot (\rho_R \mathbf{F}_h) = \frac{1}{c_p} \left(\frac{p_R}{p_0} \right)^{-\kappa} (\epsilon + \dot{q}_{\text{rad}}) \quad (40)$$

462 unveiling the advantage of working with potential temperature. The linearity of enthalpy
463 with respect to θ allow to easily derive the following heat flux, buoyancy flux, internal
464 and potential energy and mean temperature equation (again neglecting (molecular) dif-
465 fusive fluxes),

$$\overline{w' h'} = c_p \left(\frac{p_R}{p_0} \right)^\kappa \overline{w' \theta'}, \quad \overline{w' b'} = \frac{g}{\theta_R} \overline{w' \theta'}, \quad E_{i+p} = c_p \bar{\theta} \left(\frac{p_R}{p_0} \right)^\kappa - \frac{p_R}{\rho_R} + gz \quad (41)$$

$$\partial_t \bar{\theta} + \frac{1}{\rho_R} \partial_z (\rho_R \overline{w' \theta'}) = \frac{1}{c_p} \left(\frac{p_R}{p_0} \right)^{-\kappa} (\bar{\epsilon} + \bar{q}_{\text{rad}}) \quad (42)$$

466 3.2 Boussinesq seawater with a linearized EOS

467 For seawater with a linearized EOS in Boussinesq approximation ($\rho_R(z) = \rho_0$)
468 buoyancy reads

$$b = -\partial_z (h + gz) = g\alpha(\theta - \theta_0) - \beta(S - S_0) \quad (43)$$

469 and a corresponding enthalpy can be formed as

$$h(\theta, S, p_R(z)) = c_p \theta + \overbrace{\frac{p_R(z) - p_0}{\rho_0}}^{-gz} (1 + \alpha(\theta - \theta_0) - \beta(S - S_0)) \quad (44)$$

470 where c_p is a constant specific heat capacity of seawater, p_0 and ρ_0 are constant pres-
 471 sure and density references, α is the thermal expansion coefficient and β is the haline
 472 contraction coefficient. For a linearized equation of state potential and conservative tem-
 473 perature coincide, and they are denoted by θ . We show in appendix E32 that the un-
 474 averaged energetically consistent temperature equation is

$$\frac{D}{Dt}\theta = \frac{\epsilon + \dot{q}_{\text{rad}}}{c_p - \alpha g z} + \frac{-\nabla \cdot \mathbf{F}_h + z g \beta \nabla \cdot \mathbf{F}_S}{c_p - \alpha g z} \quad (45)$$

475 where \mathbf{F}_S is the (molecular) diffusive salt flux. The energy increase due to viscous dis-
 476 sipation is small and usually neglected in the ocean (e.g. McDougall, 2003; Olbers et al.,
 477 2012). In appendix E32 we show that by doing so it leads to unclosed energy budgets
 478 but justifies the "standard" usage of $-zb$ as a Boussinesq potential energy by the oceanog-
 479 raphic community (e.g. sec. 2.4.3 of Vallis, 2017), because $E_{i+p} = c_p \bar{\theta} - z \bar{b} + g z$.
 480 However since viscous dissipation is an important quantity for turbulence modelling, we
 481 retain this dissipative heating in the temperature budget (45) to work with a properly
 482 closed energy budget.

483 We are now able to specify heat flux, buoyancy flux and mean temperature equa-
 484 tion (again neglecting (molecular) diffusive fluxes),

$$\overline{w' h'} = c_p \overline{w' \theta'} - g z (\alpha \overline{w' \theta'} - \beta \overline{w' S'}) = c_p \overline{w' \theta'} - z \overline{w' b'} \quad (46)$$

$$\overline{w' b'} = \alpha \overline{w' \theta'} - \beta \overline{w' S'} \quad (47)$$

$$\partial_t \bar{\theta} + \partial_z \overline{w' \theta'} = \frac{\bar{\epsilon} + \bar{q}_{\text{rad}}}{c_p - \alpha g z} \quad (48)$$

485 Remark that even with very simple thermodynamic modelling such as linearized EOS,
 486 the consistent inclusion of salinity as an active tracer lead to non-trivial expression of
 487 heat flux.

488 4 Energy budgets of the SCM

489 4.1 Consistency of TKE equation with EDMF closures

490 In this section, we discuss the energetic consistency of a parameterized TKE equa-
 491 tion based on the horizontally averaged TKE equation:

$$\partial_t k + \frac{1}{\rho_R} \partial_z (\rho_R T_k) = -\overline{w' \mathbf{u}'_h} \cdot \partial_z \bar{\mathbf{u}}_h + \overline{w' b'} - \bar{\epsilon} \quad (49)$$

492 By using energy arguments, we aim to remove ambiguity around three practical
 493 topics: how to interpret TKE in the model; whether to use ED or EDMF fluxes in the
 494 source terms of TKE; what boundary conditions should be used? Regarding the fluxes,
 495 some studies use ED fluxes (Giordani et al., 2020; Hourdin et al., 2019; Han et al., 2016).
 496 Other studies use explicitly the full EDMF fluxes (Han & Bretherton, 2019; Witek et
 497 al., 2011). However the majority of studies and documentations are ambiguous or not
 498 explicit about this point, and modelling choices are often motivated by realism of sim-
 499 ulation results based on few test cases. Here, we argue that energy conservation constraints
 500 can guide without ambiguity such choices.

501 If we aim to mimick the energy budgets of the averaged system (35), then k rep-
 502 represents the turbulent kinetic of the whole grid cell, *i.e.* $1/2 \overline{\mathbf{u}' \cdot \mathbf{u}'}$. We keep this choice
 503 to stay in line with previous practices. However note that Tan et al. (2018) made a dif-
 504 ferent choice by considering a budget for the *environmental* TKE, $k_e = 1/2 \overline{\mathbf{u}'_e \cdot \mathbf{u}'_e}$.

505 In (49) sources of TKE arise from the mean kinetic energy via mean shear $-\overline{w' \mathbf{u}'_h} \cdot$
 506 $\partial_z \bar{\mathbf{u}}_h$, or from internal and potential energies via buoyancy production $\overline{w' b'}$. When the
 507 EDMF approach is used to close fluxes in the diagnostic equations of $\bar{\mathbf{u}}_h$, $\bar{\theta}$ and \bar{S} , then

508 the same closures must be used in the TKE budget to ensure energetic consistency. As
 509 a consequence, the shear term must be closed as

$$-\overline{w'\mathbf{u}'_h} \cdot \partial_z \overline{\mathbf{u}}_h \stackrel{\text{EDMF}}{=} -[-K_u \partial_z \overline{\mathbf{u}}_h + a_p w_p (\mathbf{u}_{h,p} - \overline{\mathbf{u}}_h)] \cdot \partial_z \overline{\mathbf{u}}_h \quad (50)$$

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

$$\overline{w'b'} \stackrel{\text{EDMF}}{=} \frac{g}{\theta_R} [-K_\theta \partial_z \overline{\theta} + a_p w_p (\theta_p - \overline{\theta})] \quad (51)$$

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

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

512 The flux of TKE T_k is of great importance in convective conditions where non-local trans-
 513 port dominates (Witek et al., 2011). Within the framework exposed in section 2.1, we
 514 can apply the two-domain decomposition of the horizontal average to get the exact rela-
 515 tion

$$\begin{aligned} \overline{w' \frac{\mathbf{u}' \cdot \mathbf{u}'}{2}} &= \sum_{i=e,p} a_i \underbrace{\frac{1}{2} \overline{\mathbf{u}'_i \cdot \mathbf{u}'_i w'_i}}_{\text{I}_i} + \underbrace{a_i (\mathbf{u}_i - \overline{\mathbf{u}}) \cdot \overline{\mathbf{u}'_i w'_i}}_{\text{II}_i} \\ &\quad + \underbrace{a_i (w_i - \overline{w}) \frac{1}{2} \overline{\mathbf{u}'_i \cdot \mathbf{u}'_i}}_{\text{III}_i} + \underbrace{a_i \frac{1}{2} \|\mathbf{u}_i - \overline{\mathbf{u}}\|^2 (w_i - \overline{w})}_{\text{IV}_i} \end{aligned} \quad (52)$$

516 Based on a conditional sampling of plumes on LES, we derive in Part II a simplified EDMF
 517 parameterization of T_k encompassing previous approaches existing in the literature, namely

$$\overline{w' \frac{\mathbf{u}' \cdot \mathbf{u}'}{2}} = \underbrace{-K_k \partial_z k}_{\text{ED}} + \underbrace{a_p w_p (k_p - k)}_{\text{Han \& Bretherton 2019}} + \underbrace{a_p w_p^3}_{\text{Witek et al. 2011}} + \underbrace{\frac{a_p w_p}{2} \|\mathbf{u}_{h,p} - \overline{\mathbf{u}}_h\|^2}_{\text{new EDMF}} \quad (53)$$

518 4.2 EDMF-parameterized budgets

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

$$\begin{cases} \partial_t E_k + \frac{1}{\rho_R} \partial_z (\rho_R T_{E_k}) & = -K_u (\partial_z \overline{\mathbf{u}}_h)^2 + a_p w_p (\mathbf{u}_{h,p} - \overline{\mathbf{u}}_h) \cdot \partial_z \overline{\mathbf{u}}_h \\ \partial_t k + \frac{1}{\rho_R} \partial_z (\rho_R T_k) & = \frac{g}{\theta_R} [-K_\theta \partial_z \overline{\theta} + a_p w_p (\theta_p - \overline{\theta})] + K_u (\partial_z \overline{\mathbf{u}}_h)^2 - a_p w_p (\mathbf{u}_{h,p} - \overline{\mathbf{u}}_h) \cdot \partial_z \overline{\mathbf{u}}_h - \bar{\epsilon} \\ \partial_t E_{i+p} + \frac{1}{\rho_R} \partial_z (\rho_R T_{E_{i+p}}) & = -\frac{g}{\theta_R} [-K_\theta \partial_z \overline{\theta} + a_p w_p (\theta_p - \overline{\theta})] + \bar{\epsilon} + \bar{q}_{\text{rad}} \end{cases} \quad (54)$$

522 where the flux terms are

$$T_{E_k} = (-K_u \partial_z \overline{\mathbf{u}}_h + a_p w_p (\mathbf{u}_{h,p} - \overline{\mathbf{u}}_h)) \cdot \overline{\mathbf{u}}_h \quad (55)$$

$$T_{E_{i+p}} = -c_p K_\theta \partial_z \overline{\theta} + c_p a_p w_p (\theta_p - \overline{\theta}) \quad (56)$$

523 and the associated consistent potential temperature equation is

$$\partial_t \overline{\theta} + \frac{1}{\rho_R} \partial_z [\rho_R (-K_\theta \partial_z \overline{\theta} + a_p w_p (\theta_p - \overline{\theta}))] = \frac{1}{c_p} \left(\frac{p_R}{p_0} \right)^{-\kappa} (\bar{\epsilon} + \bar{q}_{\text{rad}}) \quad (57)$$

524 Equivalently, in the case of *seawater* with linearized equation of state within the Boussi-
 525 nesq approximation ($\rho_R(z) = \rho_0$),

$$\begin{cases} \partial_t E_k + \partial_z T_{E_k} & = -K_u (\partial_z \overline{\mathbf{u}}_h)^2 + a_p w_p (\mathbf{u}_{h,p} - \overline{\mathbf{u}}_h) \cdot \partial_z \overline{\mathbf{u}}_h \\ \partial_t k + \partial_z T_k & = -K_b \partial_z \overline{b} + a_p w_p (b_p - \overline{b}) + K_u (\partial_z \overline{\mathbf{u}}_h)^2 - a_p w_p (\mathbf{u}_{h,p} - \overline{\mathbf{u}}_h) \cdot \partial_z \overline{\mathbf{u}}_h - \bar{\epsilon} \\ \partial_t E_{i+p} + \partial_z T_{E_{i+p}} & = -(-K_b \partial_z \overline{b} + a_p w_p (b_p - \overline{b})) + \bar{\epsilon} + \bar{q}_{\text{rad}} \end{cases} \quad (58)$$

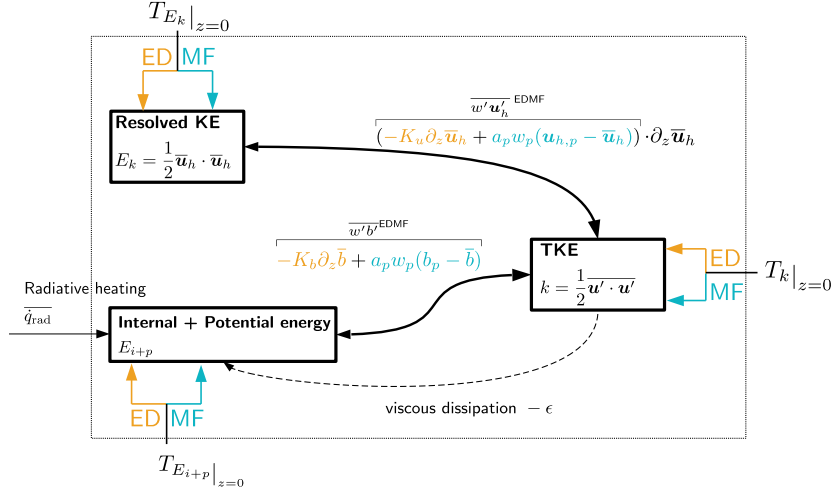


Figure 2: Schematic representation of bulk and boundary energy fluxes within EDMF closure (KE: kinetic energy, TKE: turbulent kinetic energy).

526 where the flux of internal and potential energy is

$$T_{E_{i+p}} = -\partial_z (c_p (-K_\theta \partial_z \bar{\theta} + a_p w_p (\theta_p - \bar{\theta}))) - z (-K_b \partial_z \bar{b} + a_p w_p (b_p - \bar{b})) \quad (59)$$

527 and the conservative temperature equation is

$$\partial_t \bar{\theta} = \frac{\bar{\epsilon} + \bar{q}_{\text{rad}}}{c_p - \alpha g z} - \partial_z (-K_\theta \partial_z \bar{\theta} + a_p w_p (\theta_p - \bar{\theta}))$$

528 A schematic of EDMF energy budgets is provided in Fig. 2.

529 4.3 Viscous dissipation and eddy-diffusivity

530 In order to conserve energy we have seen in the previous section that viscous dis-
 531 sipation must be converted into heating. It can be computed in two manners. Either by
 532 implementing in the SCM the TKE equation of (54) and using the closure

$$\bar{\epsilon} = \frac{c_\epsilon}{l_\epsilon} k^{3/2}$$

533 where c_ϵ is a numerical constant and l_ϵ an appropriate length scale. This approach is usu-
 534 ally used when eddy-diffusivity is computed as $K_X = c_X l_X \sqrt{k}$ (with c_X a constant and
 535 l_X a mixing length). Alternatively dissipation can be computed by assuming a station-
 536 ary TKE equation and neglecting the transport term, leading to

$$\bar{\epsilon} = \overline{w'b'} - \overline{w'u'_h} \cdot \partial_z \bar{u}_h \quad (60)$$

537 which is commonly done in SCM using empirical K-profiles (e.g. Han et al., 2016).

538 4.4 Vertically integrated energy budgets

539 In this section, we provide global energy budgets to highlight the role of mass-flux
 540 terms in bulk energy exchange as well as sinks/sources at boundaries. Let us introduce

541 the vertical average $\langle X \rangle_z = 1/(\sigma_o^a H) \int_0^{\sigma_o^a H} X dz$, and the boundary operator $[X]_0^{\sigma_o^a H} =$
 542 $1/(\sigma_o^a H)(X(z = \sigma_o^a H) - X(z = 0))$ (with $\sigma_o^a = 1$ in the atmosphere and -1 in the
 543 ocean). Then for any advected field X with source term P_X , we have (see Appendix D
 544 for a detailed derivation):

$$\begin{aligned} \frac{1}{2} \partial_t \langle \rho_R \bar{X}^2 \rangle_z &= \overbrace{-\langle \rho_R K_X (\partial_z \bar{X})^2 \rangle_z}^{<0} - \overbrace{\left\langle \rho_R \frac{E+D}{2} (X_p - \bar{X})^2 \right\rangle_z}^{<0} \\ &+ \langle \rho_R \bar{X} \bar{P}_X \rangle_z + \langle \rho_R a_p (S_X)_p (X_p - \bar{X}) \rangle_z \\ &- \left[\rho_R \bar{X} \overline{w'X'} + \rho_R a_p w_p \frac{(X_p - \bar{X})^2}{2} \right]_0^{\sigma_o^a H} \end{aligned} \quad (61)$$

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

552 We use (61) and the specific source of plume momentum budget (see Appendix D)
 553 to get the vertically integrated mean kinetic energy budget,

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

554 Vertically integrating the TKE equation (58) leads to

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

555 where again the MF contribution to shear has been reformulated into a sign-definite bulk
 556 production and a boundary term (Appendix D). It allows a clear interpretation: lateral
 557 mixing due to either entrainment or detrainment induces a net production of TKE via
 558 the shear term, and this production is hyperbolically enhanced if the horizontal drag co-
 559 efficient C_u is increased. Moreover this provides an energy constraint on C_u , namely $0 \leq$
 560 $C_u < 1$. Additionally, the vertically integrated potential energy and resolved internal
 561 energy budget reads

$$\partial_t \langle \rho_R E_{i+p} \rangle_z = \langle \rho_R K_b \partial_z \bar{b} \rangle_z - \langle \rho_R a_p w_p (b_p - \bar{b}) \rangle_z + \left\langle \rho_R (\bar{\epsilon} + \bar{q})_{\text{rad}} \right\rangle_z - [T_{E_i + \epsilon_p}]_0^{\sigma_o^a H} \quad (62)$$

562 In the three budgets presented above, two different types of source terms appear. The
 563 terms in angle bracket $\langle \cdot \rangle_z$ corresponds to bulk conversions of different type of energy
 564 and must compensate within each other (excepted for radiative transfer), since no to-
 565 tal energy can be created inside the fluid. The terms in square brackets $[\cdot]_0^{\sigma_o^a H}$ are in-
 566 puts of energy at the boundaries of the fluid which are a net source/sink of total energy
 567 (e.g. bottom heating of the atmosphere or surface wind work in the ocean).

568 4.5 Inconsistent boundary conditions and spurious energy fluxes

569 In this section, based on the choices made in Pergaud et al. (2009) we provide an
 570 example of inconsistent boundary conditions for the plume temperature and the mean
 571 temperature resulting in spurious surface heat fluxes in the system.

572 If we assume that the boundary condition for the mean temperature equation is
 573 $-K_\theta \partial_z \bar{\theta}(0) = \overline{w'\theta'}_{\text{sfc}}$ (where $\overline{w'\theta'}_{\text{sfc}}$ is a prescribed surface flux), and that the plume
 574 boundary condition is prescribed following Soares et al. (2004)

$$\theta_p(0) = \bar{\theta}(0) + \beta \frac{\overline{w'\theta'}_{\text{sfc}}}{\sqrt{k(0)}} \quad (63)$$

575 then using (56) the resulting surface flux of E_{i+p} is

$$\begin{aligned} T_{E_{i+p}}(0) &= -c_p K_\theta \partial_z \bar{\theta}(0) + c_p a_p(0) w_p(0) (\theta_p(0) - \bar{\theta}(0)) \\ &= c_p \overline{w'\theta'}_{\text{sfc}} + c_p \overline{w'\theta'}_{\text{sfc}} \frac{a_p(0) w_p(0) \beta}{\sqrt{k(0)}} \end{aligned}$$

576 where the second term of the r.h.s. is an unphysical source of energy. This bias is due
 577 to an inconsistent partitioning of the physical boundary flux $c_p \overline{w'\theta'}_{\text{sfc}}$ into ED and MF
 578 fluxes. In Pergaud et al. (2009), $w_p(0) = \sqrt{2/3k(0)}$ and $\beta = 0.3$ leading to biases from
 579 a few percents up to 25 % depending on the surface value of a_p . In order to correct this
 580 bias, one can start from imposing the physical energy flux $T_{E_{i+p}}(0) = c_p \overline{w'\theta'}_{\text{sfc}}$, then
 581 by using its EDMF decomposition (56) and Soares-type plume boundary condition we
 582 obtain the consistent Neumann boundary condition for mean temperature

$$\begin{aligned} -K_b(0) \partial_z \bar{\theta}(0) &= \overline{w'\theta'}_{\text{sfc}} - a_p(0) w_p(0) (\theta_p(0) - \bar{\theta}(0)) \\ &= \left(1 - \frac{a_p(0) w_p(0) \beta}{\sqrt{k(0)}} \right) \overline{w'\theta'}_{\text{sfc}} \end{aligned}$$

583 5 Discussion and conclusion

584 In this work, we have presented the theoretical derivation of an EDMF scheme with
 585 special attention paid to energetic aspects for both dry atmosphere and seawater with
 586 linearized equation of state in the anelastic and modernized Boussinesq approximations
 587 (Tailleux & Dubos, 2024). Moreover, we provide energy budgets of the scheme, includ-
 588 ing radiative processes. The derivation systematically reviews approximations used and
 589 provides *a priori* scaling estimations. We also documented all necessary subsequent clo-
 590 sures necessary to obtain a mass-flux scheme, in order to propose a self-contained intro-
 591 duction to EDMF for oceanographers. Closed energetics at the SCM level is a necessary
 592 step to obtain energetically consistent 3D models and thus reduce spurious energy bi-
 593 ases. Theoretical horizontally averaged energy budgets are guiding the derivation of con-
 594 sistent energy budgets for SCM with EDMF closure. Besides taking into account MF
 595 terms in shear and buoyancy terms, we propose a new MF parameterization of TKE trans-
 596 port. It generalizes previous formulations and implies the consideration of a subplume
 597 TKE (Han & Bretherton, 2019). We also show that boundary conditions on both mean
 598 and plume variables should be consistent with the EDMF decomposition to avoid spu-
 599 rious energy fluxes at the boundary. Finally we provide a clear interpretation of MF con-
 600 tribution to shear: lateral mixing due to either entrainment or detrainment induces a
 601 net production of TKE via the shear term, and such production is enhanced when hor-
 602 izontal drag increases. In a companion paper (Part II, Perrot & Lemarié, 2024), we eval-
 603 uate EDMF hypotheses in the light of LES of oceanic convection, detail an energy-conserving
 604 discretization of the SCM, quantify energy biases of inconsistent formulations.

605 The development of energetically consistent EDMF schemes can be continued in
 606 several ways. First, for real-world applications, the present work has to be extended to
 607 more complex thermodynamics models (i.e. moist atmosphere, Pauluis (2008), and sea-
 608 water with a non-linear equation of state). The proposed framework is flexible enough
 609 to be readily extended to other coherent structures of the boundary layer contributing
 610 to transport, such as atmospheric downdraft (Han & Bretherton, 2019; Brient et al., 2023).

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

Table B1: Same as table 1, but with a relaxation of the small area limit. The small area limit is recovered if $\sigma \equiv 1$ and $\tilde{\sigma} \equiv 0$.

611 For atmospheric models, the ED-based Monin-Obukhov similarity theory should be re-
 612 conciled with the EDMF representation of fluxes (Li et al., 2021) to provide unambigu-
 613 ous and consistent boundary conditions and thus avoid potential spurious boundary en-
 614 ergy fluxes.

615 Appendix A Useful identities

$$a_p w_p = -a_e w_e \quad (\text{A1})$$

$$X_p - X_e = \frac{1}{1 - a_p} (X_p - \overline{X}) \quad (\text{A2})$$

$$= \frac{1}{-a_p} (X_e - \overline{X}) \quad (\text{A3})$$

$$a_p (w_p - \overline{w})(X_p - \overline{X}) + a_e (w_e - \overline{w})(X_e - \overline{X}) = a_p (1 - a_p) (w_p - w_e) (X_p - X_e) \quad (\text{A4})$$

$$= \frac{a_p}{1 - a_p} (w_p - \overline{w})(X_p - \overline{X}) \quad (\text{A5})$$

616 Appendix B Relaxing the small-area assumption

617 The small-area assumption can be relaxed with no additional complexity if the sub-
 618 plume fluxes $\overline{w'_p X'_p}$ ($X = \theta, S, u, v$) are still neglected. A summary of the EDMF-Energy
 619 parameterization in such a regime is presented in Tab. B1.

Appendix C Boundary condition for plume equations

Near the surface, we linearize the plume and mean buoyancy in the form $b_p \simeq b_p^0 + b'_p z$, $\bar{b} \simeq \bar{b}^0 + N_0^2 z$. Then the plume equation for b_p reads at order $O(z^0)$:

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

The boundary condition $b_p^0 = \bar{b}^0$ implies that $b'_p = 0$. Thus close to the surface we have

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

Then near the surface, the buoyancy force - which is a source of plume momentum and kinetic energy $1/2 w_p^2$ - is at first order $b_p - \bar{b} \simeq -N_0^2 z$. Consequently, any static instability 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 $b_p(0) = \bar{b}(0)$ implies that at $z = 0$, all the surface flux is allocated 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 $b_p(0) = \bar{b}(0)$ thus implies that close to the surface

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

which has the same form as the Soares-type boundary condition (63).

Appendix D EDMF Mean Variance Equation

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

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

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

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

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

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

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

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

636 Using this expression into equation (D4), then vertically integrating the variance bud-
 637 get leads to the desired equation (61).

638 We can adapt these computations to deduce the MF contribution to shear produc-
 639 tion of TKE, knowing that $P_{\mathbf{u}_{h,p}} = C_u w_p \partial_z \bar{\mathbf{u}}$. Thus the first equality of the compu-
 640 tation is

$$\begin{aligned} a_p w_p (\mathbf{u}_{h,p} - \bar{\mathbf{u}}_h) \partial_z \bar{\mathbf{u}}_h &= -E(\mathbf{u}_{h,p} - \bar{\mathbf{u}}_h)^2 + C_u a_p w_p (\mathbf{u}_{h,p} - \bar{\mathbf{u}}_h) \partial_z \bar{\mathbf{u}}_h \\ &\quad - a_p w_p \frac{1}{2} \partial_z (\mathbf{u}_{h,p} - \bar{\mathbf{u}}_h)^2 \\ \implies (1 - C_u) a_p w_p (\mathbf{u}_{h,p} - \bar{\mathbf{u}}_h) \partial_z \bar{\mathbf{u}}_h &= -E(\mathbf{u}_{h,p} - \bar{\mathbf{u}}_h)^2 \\ &\quad - a_p w_p \frac{1}{2} \partial_z (\mathbf{u}_{h,p} - \bar{\mathbf{u}}_h)^2 \end{aligned}$$

641 and the rest of the computation follows similarly, justifying the factor $1/(1-C_u)$ in (62).

642 Appendix E Anelastic energy budgets

643 In this section, we recall how to derive energy budgets of the anelastic system, fol-
 644 lowing the derivation for compressible fluids of Tailleux (2010) (sec. 2.2), including ra-
 645 diative heating (Weiss, 1994). We then derive temperature equations from the energet-
 646 ically consistent enthalpy budget. Let us start again from the anelastic non-hydrostatic
 647 system in advective form coupled to a budget for the specific energy of radiation \mathcal{E}_r :

$$\frac{D}{Dt} \mathbf{u} = -\nabla \left(\frac{p^\dagger}{\rho_R(z)} \right) + b \mathbf{e}_z + \frac{1}{\rho_R} \nabla \cdot (\rho_R \boldsymbol{\tau}) \quad (\text{E1})$$

$$\nabla \cdot (\rho_R(z) \mathbf{u}) = 0 \quad (\text{E2})$$

$$\frac{D}{Dt} \eta = \dot{\eta}_{\text{irr}} - \frac{1}{\rho_R} \nabla \cdot (\rho_R \mathbf{F}_\eta) \quad (\text{E3})$$

$$\frac{D}{Dt} S = -\frac{1}{\rho_R} \nabla \cdot (\rho_R \mathbf{F}_S) \quad (\text{E4})$$

$$b = -g \frac{\rho_{\text{EOS}} - \rho_R(z)}{\rho_{\text{EOS}}} \quad (\text{E5})$$

$$\rho_{\text{EOS}} = \rho_{\text{EOS}}(\eta, S, p_R(z)) \quad (\text{E6})$$

$$\frac{D}{Dt} \mathcal{E}_r = -\frac{1}{\rho_R} \nabla \cdot (\rho_R \mathbf{F}_r) - \dot{q}_{\text{rad}} \quad (\text{E7})$$

648 where $\boldsymbol{\tau}$ is the viscous stress, η is the specific entropy of the fluid (not including entropy
 649 of radiation), $\dot{\eta}_{\text{irr}}$ is the irreversible production of entropy, \mathbf{F}_η is the (molecular) diffu-
 650 sive flux of entropy, S is the concentration of an additional component in the fluid (typ-
 651 ically salt in the ocean), \mathbf{F}_S is the (molecular) diffusive flux of S , $\rho_R(z)$ is a reference
 652 density profile, $p_R(z)$ is an associated hydrostatic pressure, i.e. $dp_R/dz = -\rho_R g$, \mathbf{F}_r
 653 is a non-advective radiative flux and \dot{q}_{rad} is an energy transfer term due emission and
 654 absorption of radiation, $D/Dt = \partial_t + \mathbf{u} \cdot \nabla$ is the Lagrangian derivative.

655 In contrast with section 2.1 we use specific entropy η instead of potential temperature
 656 θ as a state variable. This is motivated by the fact that thermodynamic relationship are
 657 written more naturally using η ; a consistent equation for θ will be further derived.

658 The total energy of this system can be advantageously divided into kinetic energy
 659 $\rho_R \mathcal{E}_k = \rho_R \frac{1}{2} \mathbf{u} \cdot \mathbf{u}$, internal energy $\rho_R \mathcal{E}_i = \rho_R (\hat{h}(\eta, S, p_R(z)) - p_R(z)/\rho_R(z))$ –with \hat{h} the
 660 specific enthalpy–, and potential energy $\rho_R \mathcal{E}_p = \rho_R g z$ (in Tailleux and Dubos (2024)
 661 the sum $\mathcal{E}_i + \mathcal{E}_p$ is referred as potential energy), and radiation energy $\rho_R \mathcal{E}_r$. Kinetic en-
 662 ergy budget can be derived straightforwardly by taking the scalar product of (E1) with
 663 $\rho_R \mathbf{u}$, namely

$$\rho_R \frac{D}{Dt} \mathcal{E}_k = -\nabla \cdot (\mathbf{u} p^\dagger) + \rho_R w b + \nabla \cdot (\rho_R \mathbf{u} \cdot \boldsymbol{\tau}) - \underbrace{\rho_R \boldsymbol{\tau} : \nabla \mathbf{u}}_{\rho_R \epsilon} \quad (\text{E8})$$

664 where ϵ is the viscous dissipation.

665 **E1 Enthalpy budget**

 666 Let $F_h(x_\eta, x_S, x_p)$ be the mathematical function defining the enthalpy of a fluid,
 667 i.e. if x_η, x_S, x_p are respectively equal to the parcel's entropy, mass of component S and
 668 pressure then $F_h(x_\eta, x_S, x_p)$ is the parcel's enthalpy. Since enthalpy, entropy and mass
 669 of component S are extensive variables, we have by definition that for any scalar λ ,

$$F_h(\lambda x_\eta, \lambda x_S, x_p) = \lambda F_h(x_\eta, x_S, x_p) \quad (\text{E9})$$

670 which in turn implies that by virtue of Euler's homogeneous function theorem,

$$F_h(x_\eta, x_S, x_p) = x_\eta \frac{\partial F_h}{\partial x_\eta} + x_S \frac{\partial F_h}{\partial x_S} \quad (\text{E10})$$

 671 Now let η^V and S^V be respectively entropy and mass of component S per unit volume
 672 of the fluid, i.e. $h^V = \rho_R(z)\hat{h}$, $\eta^V = \rho_R(z)\eta$, $S^V = \rho_R(z)S$. Previous properties on
 673 F_h allow to define the enthalpy per unit volume,

$$\hat{h}^V = F_h(\eta^V, S^V, p) = \rho_R \hat{h} = \eta^V \frac{\partial F_h}{\partial x_\eta}(\eta^V, S^V, p) + S^V \frac{\partial F_h}{\partial x_S}(\eta^V, S^V, p) \quad (\text{E11})$$

 674 Finally, equating the gradient of $h^V = F_h(\eta^V, S^V, p)$ and of $\hat{h}^V = \eta^V \frac{\partial F_h}{\partial x_\eta}(\eta^V, S^V, p) +$
 675 $S^V \frac{\partial F_h}{\partial x_S}(\eta^V, S^V, p)$, we derive the useful relation:

$$\frac{\partial F_h}{\partial x_p}(\eta^V, S^V, p) \nabla p = \eta^V \nabla \frac{\partial F_h}{\partial x_\eta}(\eta^V, S^V, p) + S^V \nabla \frac{\partial F_h}{\partial x_S}(\eta^V, S^V, p) \quad (\text{E12})$$

 676 Now, one can compute the evolution of \hat{h}^V ,

$$\begin{aligned} \partial_t \hat{h}^V + \nabla \cdot (\hat{h}^V \mathbf{u}) &= \frac{\partial F_h}{\partial x_\eta} \partial_t \eta^V + \frac{\partial F_h}{\partial x_S} \partial_t S^V + \frac{\partial F_h}{\partial x_p} \partial_t p \\ &\quad + \nabla \cdot \left(\left(\eta^V \frac{\partial F_h}{\partial x_\eta} + S^V \frac{\partial F_h}{\partial x_S} \right) \mathbf{u} \right) \\ &= \frac{\partial F_h}{\partial x_\eta} (\partial_t \eta^V + \nabla \cdot (\eta^V \mathbf{u})) \\ &\quad + \frac{\partial F_h}{\partial x_S} (\partial_t S^V + \nabla \cdot (S^V \mathbf{u})) \\ &\quad + \frac{\partial F_h}{\partial x_p} (\partial_t p + \mathbf{u} \cdot \nabla p) \\ &\quad + \underbrace{\eta^V \mathbf{u} \cdot \left(\frac{\partial F_h}{\partial x_\eta} \right) + S^V \mathbf{u} \cdot \left(\frac{\partial F_h}{\partial x_S} \right) - \frac{\partial F_h}{\partial x_p} \mathbf{u} \cdot \nabla p}_{=0, (\text{E12})} \end{aligned}$$

 677 Now using $d\hat{h}^V = \rho_R V dp + T d\eta^V + \mu dS^V$ (where μ is the chemical potential of S)
 678 and $V = 1/\rho_{\text{EOS}}$, we obtain $\frac{\partial F_h}{\partial x_\eta}(\eta^V, S^V, p) = T$, $\frac{\partial F_h}{\partial x_S}(\eta^V, S^V, p) = \rho_R/\rho_{\text{EOS}} = 1 +$
 679 b/g , $\frac{\partial F_h}{\partial x_p}(\eta^V, S^V, p)$. Evaluating the enthalpy equation at $p = p_R$, using η and S bud-
 680 gets and integrating by part leads to

$$\begin{aligned} \partial_t (\rho_R \hat{h}) + \nabla \cdot (\rho_R \hat{h} \mathbf{u}) &= (1 + b/g)(-\rho_R g w) \\ &\quad + \rho_R (T \dot{\eta}_{\text{irr}} + \mathbf{F}_\eta \cdot \nabla T + \mathbf{F}_S \cdot \nabla \mu) \\ &\quad - \nabla \cdot (\rho_R [T \mathbf{F}_\eta + \mu \mathbf{F}_S]) \end{aligned} \quad (\text{E13})$$

 681 where the first source on the right-hand side corresponds to the work of pressure forces,
 682 the second one is a production of enthalpy due to irreversible production of entropy and
 683 diffusion of entropy and S , and the last term is the divergence of a diffusive flux of en-
 684 thalpy. In the remainder of this section, we will denote it $\mathbf{F}_\hat{h} = T \mathbf{F}_\eta + \mu \mathbf{F}_S$.

685

E2 Total energy conservation and entropy production

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687

Using relation $\mathcal{E}_i = \hat{h} - p_R/\rho_R$, we can combine the previous expression to obtain the total energy budget in advective form

$$\rho_R \frac{D}{Dt} (\mathcal{E}_k + \mathcal{E}_i + \mathcal{E}_p + \mathcal{E}_r) = \nabla \cdot (\rho_R \mathbf{F}_{\text{tot}}) + \rho_R \dot{\mathcal{E}}_{\text{tot}} \quad (\text{E14})$$

688

where the non-advective flux of total energy and the net production of total energy are

$$\rho_R \mathbf{F}_{\text{tot}} = -\mathbf{u}(p^\dagger + p_R) + \rho_R [\mathbf{u} \cdot \boldsymbol{\tau} - T \mathbf{F}_\eta - \mu \mathbf{F}_S - \mathbf{F}_r] \quad (\text{E15})$$

$$\rho_R \dot{\mathcal{E}}_{\text{tot}} = \rho_R (T \dot{\eta}_{\text{irr}} + \mathbf{F}_\eta \cdot \nabla T + \mathbf{F}_S \cdot \nabla \mu - \epsilon - \dot{q}_{\text{rad}}) \quad (\text{E16})$$

689

Thus total energy is conserved if and only if $\dot{\mathcal{E}}_{\text{tot}}$ vanishes, leading to the constraint

$$\dot{\eta}_{\text{irr}} = \underbrace{\frac{\epsilon - \mathbf{F}_\eta \cdot \nabla T - \mathbf{F}_S \cdot \nabla \mu}{T}}_{\text{material prod.}} + \underbrace{\frac{\dot{q}_{\text{rad}}}{T}}_{\text{radiative prod.}} \quad (\text{E17})$$

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691

In order to illustrate the energy conversion between the different energy reservoirs, one can write

$$\begin{cases} \rho_R \frac{D}{Dt} \mathcal{E}_k = \nabla \cdot (-\mathbf{u}p^\dagger + \rho_R \mathbf{u} \cdot \boldsymbol{\tau}) + \rho_R w b - \rho_R \epsilon \\ \rho_R \frac{D}{Dt} \mathcal{E}_i = \nabla \cdot (-\mathbf{u}p_R + \rho_R [-T \mathbf{F}_\eta - \mu \mathbf{F}_S]) - \rho_R g w - \rho_R w b + \rho_R \epsilon + \rho_R \dot{q}_{\text{rad}} \\ \rho_R \frac{D}{Dt} \mathcal{E}_p = \rho_R g w \\ \rho_R \frac{D}{Dt} \mathcal{E}_r = -\nabla \cdot (\rho_R \mathbf{F}_r) - \rho_R \dot{q}_{\text{rad}} \end{cases} \quad (\text{E18})$$

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E3 Temperature equation

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The constraint on entropy production derived above ensures that the enthalpy budget (E13) is energetically consistent. It is more convenient to work with temperature than enthalpy, since enthalpy is not observable. In this section, we will derive temperature equations from enthalpy budgets, which ensures that temperature budgets remain energetically consistent.

698

E31 Anelastic dry air

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For dry air in the anelastic approximation, specific enthalpy and buoyancy reads

$$\hat{h}(\theta, p_R(z)) = c_p T = c_p \theta \left(\frac{p_R(z)}{p_0} \right)^\kappa \quad (\text{E19})$$

$$b = -\partial_z(\hat{h} + gz) = g \frac{\theta - \theta_R(z)}{\theta_R(z)} \quad (\text{E20})$$

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where c_p is a constant specific heat capacity of dry air, p_0 is a constant pressure reference, θ is the potential temperature, $\theta_R(z) = p_R \left(\frac{p_R(z)}{p_0} \right)^{-\kappa} / (\rho_R R_d)$ is the reference potential temperature profile, R_d is the specific dry air ideal constant, $\kappa = R_d/c_p$. We straightforwardly obtain an equation for potential temperature using the enthalpy budget (E13):

$$c_p \left(\frac{p_R}{p_0} \right)^\kappa \partial_t \theta + \frac{1}{\rho_R} \nabla \cdot \left(\rho_R c_p \left(\frac{p_R}{p_0} \right)^\kappa \theta \mathbf{u} + \rho_R \mathbf{F}_\hat{h} \right) = -g w - g \frac{\theta - \theta_R(z)}{\theta_R(z)} w + \epsilon + \dot{q}_{\text{rad}} \quad (\text{E21})$$

705

which can be rewritten after some algebra as

$$\partial_t \theta + \frac{1}{\rho_R} \nabla \cdot (\rho_R \theta \mathbf{u}) + \frac{1}{c_p} \left(\frac{p_R}{p_0} \right)^{-\kappa} \nabla \cdot (\rho_R \mathbf{F}_\hat{h}) = \frac{1}{c_p} \left(\frac{p_R}{p_0} \right)^{-\kappa} (\epsilon + \dot{q}_{\text{rad}}) \quad (\text{E22})$$

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707

The elimination of the buoyancy flux $-wb$ on the r.h.s of the budget unveils the advantage of working with potential temperature instead of in situ temperature.

708 **E32 Boussinesq seawater with a linearized EOS**

709 For seawater with a linearized EOS in Boussinesq approximation ($\rho_R(z) = \rho_0$)
 710 buoyancy reads

$$b = -\partial_z(\hat{h} + gz) = g\alpha(\theta - \theta_0) - \beta(S - S_0) \quad (\text{E23})$$

711 and the corresponding enthalpy can be formed as

$$\hat{h}(\theta, S, p_R(z)) = c_p\theta + \overbrace{\frac{p_R(z) - p_0}{\rho_0}}^{-gz} (1 + \alpha(\theta - \theta_0) - \beta(S - S_0)) \quad (\text{E24})$$

712 where c_p is a constant specific heat capacity of seawater, p_0 and ρ_0 are constant pres-
 713 sure and density references, α is the thermal expansion coefficient and β is the haline
 714 contraction coefficient. For a linearized equation of state potential and conservative tem-
 715 perature coincide, and they are denoted by θ . They are related to in-situ temperature
 716 T by the formula

$$T = \left(1 + \alpha \frac{p_R - p_0}{\rho_0 c_p}\right) \theta \quad (\text{E25})$$

717 Inserting the enthalpy expression (E24) into the enthalpy budget (E13) leads to

$$c_p \frac{D}{Dt} \theta + \frac{D}{Dt}(-zg) + \frac{D}{Dt}(-zb) = -wg - wb + \epsilon + \dot{q}_{\text{rad}} - \nabla \cdot \mathbf{F}_{\hat{h}} \quad (\text{E26})$$

$$\implies c_p \frac{D}{Dt} \theta - z \frac{D}{Dt} b = \epsilon + \dot{q}_{\text{rad}} - \nabla \cdot \mathbf{F}_{\hat{h}} \quad (\text{E27})$$

718 Since $\frac{D}{Dt} S = -\nabla \cdot \mathbf{F}_S$, we have $\frac{D}{Dt} b = g\alpha \frac{D}{Dt} \theta + g\beta \nabla \cdot \mathbf{F}_S$. Thus using (E27) we obtain
 719 the energetically consistent conservative temperature equation

$$\frac{D}{Dt} \theta = \frac{\epsilon + \dot{q}_{\text{rad}} - \nabla \cdot \mathbf{F}_{\hat{h}} + zg\beta \nabla \cdot \mathbf{F}_S}{c_p - \alpha gz} \quad (\text{E28})$$

720 Again the elimination of the buoyancy flux in the r.h.s of the budget unveils the advan-
 721 tage of using conservative temperature. It can be use to compute the budget of the "pseudo"-
 722 potential energy $-zb$,

$$\frac{D}{Dt}(-zb) = -wb - z\alpha g \frac{\epsilon + \dot{q}_{\text{rad}} - \nabla \cdot \mathbf{F}_{\hat{h}} + zg\beta \nabla \cdot \mathbf{F}_S}{c_p - \alpha gz} + z\beta g \nabla \cdot \mathbf{F}_S \quad (\text{E29})$$

723 Let us remark that the sum of potential and internal energy is $\mathcal{E}_i + \mathcal{E}_p = \hat{h} - p_R/\rho_R +$
 724 $gz = c_p\theta - zb + gz$. Neglecting molecular diffusion, viscous dissipation and radiative
 725 heating, this splitting justifies the common use of $-zb$ as a proxy for "potential" energy
 726 in oceanography (e.g. Olbers et al., 2012). We nevertheless retain these terms in the tem-
 727 perature budget (E28) to work with a properly closed energy budget.

728 **Open Research**

729 Figures were created with Mathcha (www.mathcha.io/). No data were used for this
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