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# An "objective" definition of potential vorticity. Generalized evolution equation and application to the study of coastal upwelling instability.

Yves Morel<sup>1,2,\*</sup>, Guillaume Morvan<sup>1,\*</sup>, Rachid Benshila<sup>1,\*</sup>, Lionel Renault<sup>1,\*</sup>, Jonathan Gula<sup>2,\*</sup>, Francis Auclair<sup>3,\*</sup>

#### 6 Abstract

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In this paper, we propose a form for potential vorticity (PV), rescaled using the Lorenz's rearranged density profile, the novelty being that we here take 8 into account its time evolution. We argue this rescaled PV is more repre-9 sentative of the dynamics, in particular to evaluate the respective impact of 10 mixing and friction on the generation of geostrophic circulation. The im-11 pact of mixing at global scale, which only modifies the global stratification 12 at rest, is taken into account in the evolution equation of this "objective" 13 definition of PV, in the sense that it scales the PV changes with respect 14 to its effect on the circulation. Numerically, we show that all terms can be 15 calculated coherently using a single computation cell. 16

We illustrate our purpose by studying the instability of coastal upwelling 17 currents, using a numerical model at high resolution. The configuration is a 18 periodic flat channel on the f-plane with vertical walls at the southern and 19 northern boundaries. A constant wind is applied over a fluid at rest with 20 an initial linear stratification. An upwelling current forms at the northern 21 coast. After a few days, instabilities develop and vortices eventually emerge 22 with surface intensified cyclones and subsurface anticyclones. We show that 23 these instabilities and eddies are associated with (rescaled) PV anomalies, 24

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<sup>25</sup> triggered by mixing and friction.

We describe rescaled PV budgets in a layer bounded between the surface 26 and an isopycnal level. Eulerian and Lagrangian diagnostics allow to analyze 27 irreversible PV production terms, distinguishing the influence of advection, 28 friction (associated with wind stress) and mixing. We find that friction 29 plays the main role, generating negative PV anomalies, while mixing acts to 30 dampen this negative PV production. The association of this negative PV 31 anomaly with the outcropping front leads to the baroclinic destabilization 32 of the upwelling front, creating subsurface anticyclonic vortices and surface 33 intensified cyclonic vortices. Varying the strength of the wind forcing shows 34 that mixing is the most sensitive process, with a net effect that is strongly 35 reduced or even reversed with moderate to weak winds. 36

When the dynamics is fully turbulent, with filaments and vortices of small sizes, the PV production by mixing and friction is enhanced but the Lagrangian diagnostics are more difficult to analyze, since fluctuations at grid scale become significant and numerical effects – associated with imperfections of the numerical schemes – spoil the PV budget calculation.

37 Keywords: upwelling; instability; vortices; potential vorticity; mixing;

38 wind stress.

#### 39 1. Introduction

The ocean geostrophic circulation is strongly linked to the Potential Vorticity (PV) field. The most basic representation of the ocean dynamics is the quasigeostrophic (QG) model (Pedlosky, 1987; Cushman-Roisin and Beckers, 2011), based on the conservation of PV – in adiabatic evolution – and the PV inversion principle (the streamfunction, geostrophic velocity or vorticity fields can be inferred from the PV field and boundary conditions). The

QG model is based on a simplification of Ertel's general PV (Ertel, 1942). It 46 has been successfully used in numerous studies and helped to interpret many 47 aspects of ocean dynamics, from the ocean circulation at gyre scale (Rhines 48 and Young, 1982a,b; Luyten et al., 1983; Holland et al., 1984; Rhines, 1986; 49 Talley, 1988; Marshall and Nurser, 1992), to current instabilities (Charney 50 and Stern, 1962), geophysical turbulence (McWilliams, 1984), and isolated 51 vortices (McWilliams and Flierl, 1979; Sutyrin and Flierl, 1994; Morel and 52 McWilliams, 1997). 53

More recently, a few studies have analyzed the influence of non-conservative 54 effects on the evolution of Ertel PV. Haynes and McIntyre (1987) and Haynes 55 and McIntyre (1990) have shown that there are specific constraints on the 56 evolution of PV and that the net PV content in a layer bounded by two isopy-57 cnic surfaces does not vary. The influence of non-conservative momentum 58 stress at boundaries on PV evolution has also been analyzed theoretically 59 (Thomas, 2005; Morel et al., 2006; Taylor and Ferrari, 2010; Benthuysen 60 and Thomas, 2012, 2013). Since then, several studies have investigated the 61 consequences of diabatic effects on the ocean dynamics from the prism of PV 62 modification, from basin scales (see for instance Hallberg and Rhines, 1996. 63 2000; Czaja and Hausmann, 2009) to meso and submesoscales<sup>4</sup> (see for in-64 stance Morel and McWilliams, 2001; Morel et al., 2006; Morel and Thomas, 65 2009; Rossi et al., 2010; Meunier et al., 2010; Thomas et al., 2013; Mole-66 maker et al., 2015; Gula et al., 2015, 2016, 2019; Vic et al., 2015; Giordani 67 et al., 2017). However, the link between Ertel PV and the dynamics (vor-68 ticity and velocity fields) is not straightforward, which makes the physical 69

<sup>&</sup>lt;sup>4</sup>Mesoscale refers to horizontal length scales close to the internal radius of deformation (10 to 100 km) and submesoscale to scales below (1 to 10 km).

<sup>70</sup> analysis inconvenient.

Morel et al. (2019) (see also Assene et al., 2020; Delpech et al., 2020; 71 Aguedjou et al., 2021; Napolitano et al., 2022; Ernst et al., 2023) proposed 72 a rescaled PV, which is calculated taking into account a reference density 73 profile "representative of the background stratification at rest". The inter-74 est of the rescaled PV is that it is a generalization of the QG PV. It scales 75 as a vorticity with a reference value at rest equal to the Coriolis parameter 76 (Morel et al., 2019; Assene et al., 2020; Napolitano et al., 2022) and devi-77 ations of the rescaled PV from its background value at each latitude (also 78 called PV anomalies) are the signature of the vortical geostrophic circulation 79 and can be linked to the dynamics following the QG framework (Morel and 80 McWilliams, 2001; Herbette et al., 2003, 2005; Morel and Thomas, 2009; 81 Le Hénaff et al., 2012). The rescaled PV is conserved for each fluid particle 82 in adiabatic dynamics, but its evolution under diabatic conditions follows 83 similar constraints as the classical Ertel PV (Morel et al., 2019). The gen-84 erated anomalies are therefore easier to link to the dynamics. Thanks to 85 these properties, the rescaled PV is very useful to analyze the importance of 86 adiabatic and diabatic processes on the generation and evolution of vortices 87 (Assene et al., 2020; Delpech et al., 2020; Aguedjou et al., 2021; Napolitano 88 et al., 2022; Ernst et al., 2023). 89

However, previous studies using rescaled PV have focused on the subsurface layers and have assumed that the reference density profile does not evolve. Surface layers are subject to strong diabatic processes, so that the reference profile, which is associated with the background stratification and used to define the rescaled PV, may change with time. In addition, outcropping must be taken into account to evaluate the PV budget of the surface layer (bounded by the ocean surface and a deeper isopycnic level). Indeed,

outcropping of isopycnic levels at the surface is dynamically equivalent to a 97 positive PV anomaly (Bretherton, 1966; Held et al., 1995; Schneider et al., 98 2003; Lapeyre et al., 2006; Lapeyre, 2017; Morel et al., 2019). We here pro-99 pose a new form for the rescaled PV, based on Lorenz's rearranged profile 100 (Lorenz, 1955) and taking into account its time evolution in case of diabatic 101 mixing. We argue it is the objective form to link PV to the dynamics and 102 measure the respective influence of friction and mixing on the circulation. 103 The evolution equation of this new PV formulation is derived as well as the 104 layer PV budget taking into account surface outcropping. We then illus-105 trate the use of this general rescaled PV by studying the development of 106 barotropic/baroclinic instabilities along coastal upwelling fronts in a simpli-107 fied configuration. 108

Coastal upwellings are of particular interest here, since it is known 109 that the developing coastal currents, starting from rest, are subject to 110 barotropic/baroclinic instabilities that generate vortices (Roed and Shi, 1999; 111 Marchesiello et al., 2003; Capet et al., 2004, 2008a,b). Barotropic/baroclinic 112 instabilities can only develop if the PV structure has opposite sign gradients 113 along isopycnic levels (Charney and Stern, 1962; Ripa, 1991). In addition, 114 (cyclo)geostrophic vortices can only exist if their core consists of a local 115 PV anomaly. Thus, Morel et al. (2006) argued that, since the initial PV 116 structure is homogeneous (the ocean is initially at rest), a non-conservative 117 process must be invoked to generate PV anomalies and explain the instabil-118 ity of upwelling currents and the generation of vortices. They also showed 119 that the friction associated with the wind stress acts differentially along an 120 isopycnic level, leading to a stress curl even with constant wind, which in this 121 case produces systematic negative isopycnal PV anomalies (see also Thomas, 122 2005; Morel and Thomas, 2009). The generated negative PV anomaly then 123

interacts with the surface outcropping, to produce instabilities and vortices
of both signs. However, Morel et al. (2006) used a layered model and did
not consider diapycnal mixing.

We here resume the study of Morel et al. (2006) in a configuration with 127 continuous stratification and taking into account mixing. The wind causes 128 mixing near the surface, so that a mixed layer develops. Since the wind 129 is constant, mixing occurs throughout the domain and modifies the global 130 stratification profile. Away from the coast, the evolution is 1D with an 131 Ekman spiral developing in a deepening mixed layer. The density profile and 132 PV structure evolve, but no isopycnal PV anomalies are generated, so no 133 instability vortices can be generated in this region. Near the coast, variations 134 in stratification and current structures, associated with the development 135 of the upwelling, locally modify the diapycnal mixing, so that isopycnal 136 anomalies can be created by mixing or friction. However, in order to assess 137 the dynamical significance of the generated anomalies, we need to calculate 138 the rescaled PV with a variable reference profile (representing the global 139 stratification at rest at any time). 140

The coastal upwelling configuration is thus a particularly interesting test 141 case for the rescaled PV evolution we propose here. It is also an interesting 142 test in terms of physics, and we will also compare the influence of the wind 143 stress intensity on the PV change and the characteristics of the generated 144 vortices. In section 2, we present the equations, the numerical model and the 145 configuration used in the study. The theoretical framework of the rescaled 146 PV is presented in section 3. We then analyze numerical simulations of 147 upwelling development and instabilities with the rescaled PV in section 4, 148 discussing the effect of friction and mixing with strong and moderate winds. 149 Our results are summarized and discussed in the final section. 150

#### 151 2. Equations, numerical model and configuration

#### 152 2.1. Equations

In this paper, we consider the Navier-Stokes equations with Boussinesq approximation:

$$\frac{d}{dt}\vec{U} + \vec{f} \times \vec{U} = -\frac{\vec{\nabla}P}{\rho_0} + \vec{g}\frac{\rho}{\rho_0} + \vec{F}$$
$$\vec{\nabla}.\vec{U} = 0$$
$$\frac{d}{dt}\rho = \dot{\rho}$$
(1)

where  $\vec{U} = (u, v, w)$  is the velocity field,  $\frac{d}{dt}\phi = \partial_t \phi + \vec{U} \cdot \vec{\nabla} \phi$ ,  $\vec{\nabla} \cdot \vec{V} = \partial_x V_x + \vec{U} \cdot \vec{\nabla} \phi$ 153  $\partial_y V_y + \partial_z V_z$  is the divergence of vector field  $\vec{V} = (V_x, V_y, V_z), \ \vec{f} = (0, f_y, f)$ 154 is the Coriolis vector (f, its vertical component, is the Coriolis parameter),155 P is the pressure,  $\rho$  is the potential density and  $\vec{F} = (F_x, F_y, F_z)$  and  $\dot{\rho}$  are 156 terms associated with non-conservative processes for momentum (here the 157 wind stress) and density fields (mixing). They are generally prescribed as 158 diffusive terms  $\partial_z(K_{\phi} \ \partial_z \ \phi)$ , where  $\phi$  is the velocity or the density field, and 159 the diffusion coefficient  $K_{\phi}$  is given by some parameterization. 160

#### 161 2.2. Numerical model

The oceanic simulations were performed with the Coastal and Regional 162 Ocean Community Model (CROCO, see Debreu et al., 2012), developed 163 around the kernel of the Regional Oceanic Modeling System (ROMS, see 164 Shchepetkin and McWilliams, 2005). CROCO is a free-surface, terrain-165 following coordinate model with split-explicit time stepping, used here with 166 the Boussinesq and hydrostatic approximations. There are several options 167 for the numerical schemes and here we have chosen a third-order, upstream-168 biased, dissipative advection scheme, with free slip conditions at lateral 169

<sup>170</sup> boundaries, for horizontal advection of momentum and tracers, (Shchep<sup>171</sup> etkin and McWilliams, 1998). There is no explicit lateral viscosity in the
<sup>172</sup> model.

Vertical mixing of momentum and tracers is given by the K-profile parameterization (Large et al., 1994) with a critical Richardson number of 0.3. This closure scheme gives vertical diffusion coefficients for momentum and tracers as a function of wind stress and interior shear (other mixing processes, associated with internal waves or double diffusion, can be taken into account but are not considered here).

#### 179 2.3. Upwelling configuration

The configuration is a periodic East-West channel with a flat bottom and 180 vertical walls at the Northern and Southern boundaries (Fig. 1). The chan-181 nel depth is H = 1000 m and its width and length are similar  $L_x = L_y = 250 km$ . 182 The stratification is initially uniform with a Brundt-Vaisala frequency  $N = 5.2 \, 10^{-3} s^{-1}$ . 183 The theory, presented in sections 3.1, 3.2 and 3.3, is valid in general con-184 figurations taking into account the full Navier-Stokes equations (1), with 185 variable Coriolis parameter and winds, but to simplify the analysis, in the 186 numerical simulations presented here, the Coriolis parameter f and the wind 187 are chosen constant. We fix  $f = 7 \ 10^{-5} \ s^{-1}$  which gives a first internal radius 188 of deformation  $Rd \simeq 23 \ km$ . The grid step is  $\Delta x = 1 \ km$ . The vertical 189 sigma grid follows Song and Haidvogel (1994) with stretching parameters 190  $\theta_s~=~5,\,\theta_b~=~0$  and hc~=~30~m. We use 80 vertical sigma levels and the 191 vertical resolution ranges from  $\Delta z \simeq 1 m$  at the surface to  $\Delta z \simeq 50 m$  at 192 the bottom. There are 50 layers in the upper 150 m where the dynamics is 193 analyzed. 194

195

The ocean is initially at rest and we apply a constant West/East wind

W (see Fig. 1). The West/East surface stress associated with the wind 196 is calculated using the bulk formulae  $\tau_x = \rho_a \ C_d \ |W|W$  (and  $\tau_y = 0$ ), 197 where  $\rho_a \simeq 1.225 \ kg.m^{-3}$  is the air density and  $C_d = 0.0012$  the turbulent 198 momentum transfer parameter. Two different wind velocities are considered, 199 strong with W = 8 m/s, and moderate with W = 2 m/s, corresponding 200 respectively to  $\tau = 0.1 \ N/m^2$  and  $\tau = 0.006 \ N/m^2$ . Buoyancy (heat 201 and freshwater) fluxes are not considered here. A quadratic bottom drag, 202 with a drag coefficient  $rdrg2 = 2.10^{-3}$ , is used, but it plays no role in 203 the transformation of PV in the upper layer. We focus on the Northern side 204 where the upwelling takes place. The downwelling occurring at the Southern 205 boundary is not studied (PV is also modified in the downwelling area, but 206 does not lead to instabilities. See Morel et al., 2006, for more details). For 207 each simulation, we record hourly outputs of all physical fields (velocity 208  $\vec{U}=(u,v,w)$  and density  $\rho)$  but also of the parameterized non-conservative 209 terms  $(\vec{F} = (F_x, F_y, F_z)$  and  $\dot{\rho})$ . 210

#### 211 3. Potential Vorticity

If the domain was infinite (without Southern and Northern boundaries), 212 the evolution would be 1D. Indeed, in this case an Ekman spiral devel-213 ops and the upper part of the water column undergoes mixing (see Fig. 2) 214 a). The stratification and Ertel PV are modified, with a homogenized up-215 per layer overlying a pycnocline with stronger stratification than the initial 216 stratification. However, there are no horizontal variations of this structure, 217 and no geostrophic motion is associated with this homogeneous stratifica-218 tion change, so the Ertel PV change is not significant in terms of geostrophic 219 dynamics. 220



Figure 1: Configuration characteristics, horizontal view (panel a) and vertical section (panel b).



Figure 2: Vertical section of the stratification evolution (panel b). In the open ocean the modifications are close to 1D (panel a), with an Ekman spiral developing in the mixed layer. A pycnocline forms but the stratification below is unchanged. Close to the vertical boundary, where the upwelling develops (panel c), the stratification and current structures are very different. Mixing is modified.

In the current configuration, far from the boundaries, the evolution is 221 close to 1D as depicted above. However, the stratification varies close to the 222 boundary, where the upwelling develops. Isopycnic levels bend towards the 223 surface and a vertically sheared geostrophic current develops. Both processes 224 locally modify the mixing characteristics (Fig. 2 c). As discussed in Morel 225 et al. (2006), even though the wind stress is constant, the momentum stress 226 varies vertically, so that a stress curl is created along isopycnic levels bending 227 towards the surface<sup>5</sup> (see also section 4.1.2 and Fig. 10). 228

The stress curl and differential mixing create PV anomalies in the up-229 welling region and an associated dynamical signal, in particular leading to 230 destabilization of the upwelling current (Morel et al., 2006). It is therefore 231 interesting to isolate the PV anomalies generated by diabatic processes that 232 are truly associated with geostrophic dynamics, and to measure the respec-233 tive influence of mixing and friction on the observed dynamics. But such a 234 measure depends on the definition of PV and the latter has to be carefully 235 defined to get objective diagnostics. This is a delicate issue that we now 236 discuss. 237

#### 238 3.1. An objective definition of Potential Vorticity

As shown by Ertel (1942) (see also Muller, 2006), vorticity is not conserved, but a quantity combining vorticity and stratification can be defined that is conserved for each particle for adiabatic motions:

$$PV_{Ertel} = (\vec{\nabla} \times \vec{U} + \vec{f}) \cdot \vec{\nabla}\rho \tag{2}$$

<sup>&</sup>lt;sup>5</sup>Note that the stress parameterization is generally sensitive to the vertical structure of mixing and thus also varies horizontally in the present case, even though the wind stress at the surface is constant.

All dynamical fields (vorticity, velocity and stratification) can be calculated from PV under the simple assumption of (cyclo)geostrophic equilibrium and given boundary conditions. Most studies, using Navier-Stokes or Primitive Equations, invoking PV are based on Ertel PV, including recent studies analyzing the influence of mixing and/or friction. In fact, as already noticed by Ertel, PV is not uniquely defined in the sense that any form of the type

$$PV_{Gene} = (\vec{\nabla} \times \vec{U} + \vec{f}).\vec{\nabla}G(\rho)$$
(3)

-where G can be an arbitrary function- is still a Lagrangian tracer for adiabatic motions. So one may wonder which choice for G is the most objective to define PV. This is particularly important since in case mixing and friction are considered, the evolution equation for  $PV_{Gene}$  is

$$\frac{d}{dt}PV_{Gene} = \vec{\nabla}.[ (\vec{\nabla} \times \vec{F}) G(\rho) + (\vec{\nabla} \times \vec{U} + \vec{f}) \partial_{\rho}G(\rho) \dot{\rho} ]$$
(4)

This equation clearly shows that the strength of the PV fluxes associated with friction (first term on the right hand side) or mixing (second term) strongly depend on the choice of G. The form of Ertel PV (Eq. 2) with  $G(\rho) = \rho$  has no objective justification apart from its simplicity. In fact, the interest of PV being its link with the circulation, the adequate form has to be quantitatively representative of the dynamics, that is to say directly invertible to estimate the vorticity field. This is not the case of Ertel PV.

The proper choice for G can be defined considering a purely barotropic circulation. Indeed, in this case the dynamics is independent of the vertical position z (oriented upward), and the background stratification is horizontally homogeneous:  $\rho(x, y, z) = \rho^*(z)$  and is also the stratification at rest. To be representative of the dynamics, PV should correspond to the

barotropic vorticity in this case and be independent of z. The only choice 251 is then that  $G(\rho) = Z(\rho)$  where Z is defined using the profile  $\rho^*(z)$  so that 252  $Z(\rho^*(z)) = z$  (the function  $Z(\rho)$  corresponds to the vertical position of den-253 sity  $\rho$  along the reference profile  $\rho^*$ ). In this case  $PV = \partial_x v - \partial_y u + f$  is the 254 expected absolute vertical vorticity with a value at rest corresponding to the 255 Coriolis parameter. As argued in previous studies (Delpech et al., 2020; As-256 sene et al., 2020; Aguedjou et al., 2021; Napolitano et al., 2022; Ernst et al., 257 2023), in the general case,  $\rho^*$  should correspond to the stratification at rest, 258 obtained from the Lorenz's (Lorenz, 1955) rearranged stratification (see also 259 Nakamura, 1995; Winters and D'Asaro, 1996). Indeed, in this case only, the 260 rescaled PV at rest is still given by the Coriolis parameter  $PV_{rescaled}^{rest} = f$ 261 and, at first order, the anomaly from this reference corresponds to the quasi-262 geostrophic PV, which is again directly linked to the geostrophic circulation. 263 The link between the geostrophic circulation and rescaled PV is rigorous if 264 the reference density profile chosen for rescaling correspond to the stratifica-265 tion at rest at each time, indicating the necessity to take into account time 266 evolution of the reference profile. Indeed, Lorenz's rearranged profile can be 267 modified by large scale diabatic processes, so that  $\rho^* = \rho^*(z, t)$  also depends 268 on time. For instance, considering again a barotropic circulation for which 269 large scale ocean/atmosphere fluxes uniformly modify the stratification but 270 not the dynamics (vertical mixing of momentum does not modify barotropic 271 circulation), PV should remain equal to the absolute vorticity whatever the 272 evolution of the background stratification. In addition, in general circum-273 stances, mixing and ocean/atmosphere fluxes can destroy or create density 274 classes in a domain, which can cause problems to evaluate rescaled PV if no 275 time evolution is considered for the reference profile. 276

To achieve these properties and be representative of the dynamics at all

times, the objective form for the definition of PV is

$$PV_{rescaled} = \vec{\nabla}.( (\vec{\nabla} \times \vec{U} + \vec{f}) Z(\rho, t) )$$
(5)

where  $Z(\rho, t)$  is a function of both potential density and time and is defined 277 using the time evolving rearranged Lorenz's profile  $\rho^*(z, t)$ : Z is chosen 278 so that at all times  $Z(\rho^*(z, t), t) = z$ . This is what is chosen in the 279 present study to compare effects of mixing and friction on the dynamics, 280 through their associated PV fluxes terms. In our numerical simulations, 281 the calculation of the reference profile is based on previous work (Tseng and 282 Ferziger, 2001) with an adaptation associated with the present configuration 283 (see Appendix A). 284

Interestingly, previous studies, to our knowledge only using non-evolving 285 Lorenz's profiles, have identified other interesting properties of the rescaled 286 PV. The PV anomaly proposed by Morel and McWilliams (2001) (see also 287 Herbette et al., 2003, 2004, 2005; Morel et al., 2006; Morel and Thomas, 288 2009) is similar to the rescaled PV for adiabatic evolution, but written in 289 isopycnic coordinate (or for multi-layer shallow water models). This quan-290 tity was already shown to be a generalization of the QGPV for primitive 291 equations (written in isopycnic coordinates) and was used instead of the 292 classical form because it allows a direct inversion of PV to calculate the 293 (cyclo)geostrophic circulation. The available potential vorticity, proposed 294 by Wagner and Young (2015) (see also Early et al., 2021) for the filtering of 295 internal gravity waves, is similar to the rescaled PV. Gravity waves have no 296 PV signature along isopycnic surfaces, but in a Eulerian framework when 297 using the classical form of Ertel PV, the signature of the pycnocline induces 298 PV variations that are difficult to attribute to geostrophic dynamics or the 299 displacement of the pycnocline by gravity waves. The use of a rescaled PV 300

for which the PV at rest is uniform (on the f-plane) allows to filter out the dynamical signature of gravity waves in a Eulerian framework. Finally Morel and McWilliams (2001) showed that isolated vortices can only have finite kinetic energy provided the net PV budget is zero in a QG framework. This theory can be generalized to the Navier-Stokes equations and to frontal currents (Morel et al., 2019) again provided the rescaled PV is used.

#### 307 3.2. Generalized evolution equation for the rescaled Potential Vorticity

The evolution equation of the rescaled PV defined by Eq. 5 is obtained from Eq. 1 following Muller (2006), and we show in Appendix B that it is given by

$$\frac{d}{dt}PV_{rescaled} = \vec{\nabla}.( (\vec{\nabla} \times \vec{F}) Z(\rho, t) + (\vec{\nabla} \times \vec{U} + \vec{f}) \partial_{\rho}Z(\rho, t) (\dot{\rho} - \partial_{t}\rho^{*} |_{\rho,t}) )$$
(6)

or in Eulerian form

$$\partial_t P V_{rescaled} = \vec{\nabla}.(\vec{U} \ P V_{rescaled} + (\vec{\nabla} \times \vec{F}) \ Z(\rho, \ t) + (\vec{\nabla} \times \vec{U} + \vec{f}) \ \partial_\rho Z(\rho, \ t) \ (\dot{\rho} - \partial_t \rho^* \mid_{\rho,t}) \ )$$
(7)

where the first term of the right hand side divergence is associated with 308 adiabatic advection, the second term with friction and the third one with 309 diapycnal mixing. For the last term, a correction is made to account for the 310 evolution of the reference profile  $\partial_t \rho^* \mid_{\rho,t} = \partial_t \rho^*(Z(\rho, t), t)$ . This evolution 311 is associated with restratification at global scale and has to be withdrawn 312 as it has no consequence on the generation of "dynamical" PV anomalies 313 (see Appendix B). Note that it has to be evaluated along the reference 314 profile following the density value of the physical domain (not the elevation). 315

Hereafter, PV will refer to the rescaled PV defined by Eq. 5 and whose evolution equation is Eq. 6 or 7.

For the upwelling simulation presented above, using the rescaled PV given by Eq. 5 ensures that the PV at rest is unchanged  $(PV_{rescaled}^{rest} = f)$ and that the isopycnic PV anomalies are representative of the geostrophic dynamics and in particular instabilities.

Finally, other forms are sometimes used for the right hand side of Eq. 6, but the present expression has strong similarities with the PV expression in Eq. 5, and is the preferred form for numerical calculations because all terms can be calculated using a single PV grid cell, which also simplifies coherency of PV budgets (see Morel et al., 2019, and Appendix C).

#### 327 3.3. Average PV field in a layer

Since (rescaled) PV represents quasigeostrophic PV at first order, a vertical average of PV in a layer bounded by two isopycnals is informative about dynamical fields. For example, an anticyclonic vortex is associated with a negative PV anomaly, localized in a core within some layer, and the PV budget within the layer is related to the vorticity and stretching fields (see for instance McWilliams and Flierl, 1979; Hoskins et al., 1985; Morel and McWilliams, 1997; Le Hénaff et al., 2012). When the upper bound of the layer is the sea surface, which is generally not an isopycnic surface, an additional term associated with density variations at the surface -outcroppinghas to be taken into account when evaluating the PV budget in relation with the dynamics. Indeed, density variation along the surface is equivalent to a Dirac delta sheet of PV that has to be taken into account (Bretherton, 1966; Schneider et al., 2003; Isern-Fontanet et al., 2006; Lapeyre et al., 2006). In this case, the correct calculation for the integrated PV is (Schneider et al., 2003; Morel et al., 2019; Ernst et al., 2023)

$$\overline{PV} = \frac{1}{h} \left( \int_{z=-h(\rho_{low})}^{z=0} PV \, dz - \left[ (\vec{\nabla} \times \vec{U} + \vec{f}) \, Z(\rho, t) \right]_{z=0} \right)$$
(8)

where  $h = h(\rho_{low})$  is the depth of the isopycnic level that defines the lower 328 boundary of the layer and  $Z(\rho, t)$  is the vertical level at density  $\rho$  of the 329 reference profile  $\rho^*(z, t)$ . The additional term is calculated from velocity 330 and density fields at the surface (z = 0). Note that for an upwelling, the 331 region where deep isopycnic levels outcrop is equivalent to a positive PV 332 anomaly  $(Z(\rho, t))$  corresponds to the depth of density  $\rho$  along the refer-333 ence profile and is always negative), which can potentially generate cyclonic 334 eddies (Bretherton, 1966; Legg and Marshall, 1993; Legg et al., 1996)<sup>6</sup>. 335

#### 336 4. Numerical results

#### 337 4.1. Reference experiment

For the reference experiment, the wind stress is  $\tau = 0.1 \ N/m^2$  and the 338 model is run for 25 days with hourly outputs, starting from rest. Figure 3 339 shows the evolution of the integrated PV anomaly (using Eq. 8 and a layer 340 bounded by the isopycnic level  $\rho = 1025 \ kg/m^3$  and the surface), surface 341 vorticity, a vertical section of PV anomaly and vorticity along a South-342 North transect. The PV anomaly is obtained from Eq. 5 and withdrawing 343 the reference PV (f). The vertical sections are taken along the dashed 344 line shown in the horizontal maps. It is a South-North section located at 345  $x = 205 \ km$ . Note that it crosses the core of a subsurface anticyclonic 346 vortex at time t = 21 days (Fig. 4), whose generation will be studied below. 347

<sup>&</sup>lt;sup>6</sup>Physically, if there is no PV anomaly inside the water column but isopycnals outcrop at the surface, internal layers must be stretched and cyclonic vorticity is then created.











During the early stage, up to day 15, the evolution remains zonal, no 348 instability is visible. From day 15 to 17, short scale instabilities with a 349 maximum length scale of 10 km develop, but remain trapped near the 350 coast. Then, from day 18 to 25, new instabilities develop with a domi-351 nant length scale starting at 20 km but evolving to about 40 km at day  $25^7$ . 352 The evolution is similar to that found in Morel et al. (2006), with initial, 353 short scale instabilities developing when the Richardson number becomes 354 smaller than 0.25, corresponding to Kelvin-Helmholtz like instabilities<sup>8</sup> and 355 larger scale eddies developing from day 18 corresponding to geostrophic 356 barotropic/baroclinic instabilities. At later stages, the merging of eddies 357 also favors the formation of larger scale vortices. 358

Initially, at days 1 and 4, the evolution of the vertical section of PV 359 anomaly and vorticity (columns 3 and 4) is limited to a region close to the 360 northern wall: although mixing modifies the stratification and Ertel PV ev-361 erywhere in the fluid, the rescaled PV mostly exhibits anomalies where it 362 is dynamically significant, i.e. the generated PV can generate eddies. In-363 deed, at a later stage, when eddies develop (days 19, 21 and 25) there is 364 a striking correspondence between the surface vorticity and the layer aver-365 aged PV. In particular, anticyclonic eddies are associated with negative PV 366 anomalies and cyclonic eddies with positive ones. Note that the positive 367 layer PV anomalies are associated with outcropping of isopycnic levels (red 368 areas associated with positive PV anomalies and black contours, associated 369

<sup>&</sup>lt;sup>7</sup>All length scales have been evaluated as the dominant wavelength of the x-axis Fourier transform of the surface PV in the upwelling area.

<sup>&</sup>lt;sup>8</sup>The initial growth of perturbations in KH instabilities is correctly reproduced in primitive equations, but their subsequent evolutions require non-hydrostatic dynamics.

with surface density variations, in the first column) and that the order of
magnitude of vorticity and PV are similar. Thus, as expected, the (rescaled)
PV anomaly can be integrated to evaluate the geostrophic dynamics.

As discussed above, outcropping is always associated with equivalent positive PV anomaly (Bretherton, 1966; Schneider et al., 2003). If cyclonic vorticity seems to be mostly associated with the outcropping of isopycnic surfaces, both positive and negative interior PV anomalies are generated, as shown in the vertical section of PV anomaly (third column). They are necessarily associated with non-conservative processes. Thus, we now analyze the importance of diabatic mixing and friction in modifying the interior PV.

#### 380 4.1.1. Eulerian analysis

The simplest diagnostics of PV production by mixing and friction are Eulerian maps of the terms in Eq. 7. As mentioned above, PV, friction and mixing tendency terms can be calculated coherently over a single numerical cell following Appendix C, but adiabatic Eulerian advection must be considered too.

Figure 5 shows snapshots of all terms appearing in the PV evolution 386 equation (Eq. 7). We focus on the initial stages of the PV evolution when 387 the dynamics remains 2D. The Eulerian PV time derivative at a given time 388 t is obtained from the difference between the PV fields at time t + 1h and 389 t-1h (using our hourly outputs). Other terms correspond to the tendency 390 terms on the right hand side of Eq. 7: Advection, Effect of friction and 391 diapycnal mixing. The good coherence between the sum of all terms (second 392 column) and the Eulerian time derivative of PV (first column) confirms the 393 accuracy of our computation. Note that for the present configuration high 394 frequency outputs are necessary to obtain this accuracy. Indeed, using lower 395

frequency outputs (daily or even 12-hourly) can lead to significant discrep-396 ancies, especially when the geostrophic instability develops, since smaller 397 scale structures appear and are rapidly advected, leading to rapid changes 398 in dynamical fields. Morel et al. (2006) have argued that the effect of the 399 wind stress associated with the friction tendency term (fourth row of Fig. 400 5) should produce negative PV anomalies (see also Thomas, 2005), as long 401 as the stratification remains 2D and with constant wind. From day 15 on, 402 the stratification becomes 3D, positive anomalies appear in the friction ten-403 dency term (see day 16, fourth row in Fig. 5), possibly generated by the 404 wind stress acting on 3D structures (see for instance Morel and Thomas, 405 2009, for the influence of the wind stress on vortices). Note that the lateral 406 friction could also play a role (even free slip boundary conditions can lead to 407 the generation of PV anomalies, see Morel and McWilliams, 2001) but since 408 horizontal viscosity is implicit, it is not calculated in the friction tendency 409 term and cannot be linked to the positive anomalies seen in Fig. 5. 410

From the impermeability theorem (Haynes and McIntyre, 1987, 1990), 411 one would expect mixing to produce negative PV anomalies in the upper 412 part of the mixed layer – where the fluid is homogenized – and positive ones 413 just below – where a pycnocline appears – (see also Morel and McWilliams, 414 2001). However, with the rescaled PV definition depending on time, this 415 principle is modified. Indeed, in Eq. 7 the time evolution of the reference 416 density (which represents the effect of mixing on a global scale) is discarded 417 from the local diabatic density change, since it does not affect the geostrophic 418 dynamics. Only the diapycnal flux anomaly with respect to the reference 419 density evolution has a dynamical effect and is considered here. 420

This explains the particularly striking fact that over most of the mixed layer, the mixing tendency term remains zero away from the boundary (see





Fig. 5 fifth column), even though mixing continuously modifies the den-423 sity profile throughout the basin, with a pycnocline that penetrates deeper 424 and deeper throughout the simulation. As discussed above, it is in fact the 425 modification of stratification and velocity in the upwelling area near the 426 coast that generates differential mixing and dynamically significant mixing 427 tendency terms. Since isopycnic levels bend upward, as long as the mix-428 ing homogenizes a roughly similar depth portion of the water column, we 429 can expect a similar behaviour as described above for the impermeability 430 theorem (the isopycnic levels being mixed in the upwelling region are ini-431 tially too deep to be affected by the mixing offshore, so the correction term 432 for these isopycnic levels is zero). This is indeed what is seen close to the 433 boundary in the upwelling area (fifth column in Fig. 5). However, the mix-434 ing associated with rapid offshore advection of denser water at the surface 435 (generating convective mixing) leads to a strong deepening of the mixed 436 layer in the upwelling area and the development of patterns that alter this 437 simple rule, with a complex structure of the mixing tendency term. 438

In fact, it is difficult to evaluate the importance of each process and ten-439 dency term on the global evolution of PV and the generation of eddies from 440 the Eulerian perspective. In particular, the advective term – which is not 441 associated with PV generation – is of paramount importance. In addition, 442 the tendency terms for mixing and friction often have similar magnitude 443 and extension but with opposite signs, so that the net effect is difficult to 444 evaluate. Note in particular the partial compensation between friction and 445 mixing terms at days 16, when submesoscale structures appear, a process 446 that has been observed and explained in Wenegrat et al. (2018). A better 447 approach is to consider Lagrangian diagnostics, and this is what is presented 448 in the next section. 449

Finally, Fig. 6 compares the previous results (upper panels) to Ertel 450 PV and the associated traditional frictional and mixing productions terms 451 at  $t = 1 \, day$  (lower panels). To obtain a scaling for Ertel PV that can be 452 compared to the rescaled PV, we have here used the rescaled form but with 453 the fixed reference profile given by the initial density profile. Indeed, since 454 the initial state has a linear stratification, the non-evolving rescaled PV and 455 tendency terms are proportional to Ertel PV calculations, and quantitatively 456 comparable to the (time evolving) rescaled one. This also allows to illustrate 457 the necessity to use a time evolving reference density profile. 458

As expected, the Ertel PV structure mostly represents the stratification. 459 In comparison with the rescaled PV, the mixing production term is primar-460 ily marked by the homogenization in the mixed layer and the deepening 461 of the pycnocline over the whole basin, which is not representative of the 462 geostrophic circulation developing in the upwelling area. On the other hand, 463 at this stage, the frictional term for both formulations are pretty close (see 464 Fig. 5). Thus, measuring the respective influence of mixing and friction on 465 the development of the geostrophic circulation using this traditional form of 466 PV can be biased. In the present case negative PV production by mixing 467 production would be over evaluated. 468

#### 469 4.1.2. Lagrangian Analysis

A Lagrangian approach is easier to interpret, since we can integrate the global effect for particles forming the core of eddies emerging from the instability of the upwelling current. However, it is numerically more demanding since it is combined with a tracking algorithm that has some positioning uncertainties associated with spatial and temporal resolution (again, the hourly output is a minimum to achieve good positioning in the rapidly



Figure 6: Upper panels : rescaled PV (left panel), frictional term (middle panel) and diapycnal mixing term (right panel) at  $t = 1 \, day$  (similar as in Fig. 3 and 5). Lower panels : Ertel PV (left panel), frictional term (middle panel) and diapycnal mixing term (right panel) at  $t = 1 \, day$ . Colorscales are given for PV and tendecy terms.

evolving dynamical structure of the upwelling). The coherence between the
PV evolution of a particle and its evaluation from the tendency terms (here
only friction and mixing) following the particle in Eq. 6 is thus even more
difficult to achieve.

We first identify particles with negative PV anomalies in an anticyclonic 480 vortex whose center is located near  $x = 205 \ km, y = 235 \ km$  at day 21 (Fig. 481 4). 2000 particles were randomly seeded near this position, within a radius 482 of 10 km and with PV anomalies  $\delta PV < -10^{-5}s^{-1}$ . We backtracked them, 483 using time interpolated hourly velocity fields, to obtain their trajectories. 484 The tracking algorithm is the same as that used in Assene et al. (2020). 485 The position of the particles as well as the values of PV and the friction and 486 mixing tendency terms are calculated every  $600 \ s$ , interpolating the hourly 487 outputs. For each particle, we then integrate temporally the mixing and 488 friction tendency terms obtained from the record of the non-conservative 489 terms (right hand side of Eq. 6) to reconstruct a PV evolution from these 490 diagnostics and we compare it to the PV variations of the particle directly 491 diagnosed from the physical fields. The correspondence is generally good, 492 but given the complexity of the tendecy terms, the uncertainties associated 493 with the calculation of trajectories and the hourly sampling, there exist 494 some discrepancies. We then only keep the 1252 particles (representing 63%495 of the initial 2000 particles) for which the correlation between both PV 496 evolution estimates is greater than 0.9. Figure 7 shows their initial (day 1, 497 in red) and final (day 21, in blue) positions. All particles forming the core 498 of the anticyclonic eddy were initially deeper than their final depth. They 499 also originate from a coastal band that extends about  $350 \ km$  alongshore 500 (considering the periodicity of the domain) but only 25 km cross-shore, close 501 to the internal deformation radius. Figure 8 shows the PV evolution rate, 502



Figure 7: Initial ( $t = 1 \, day$ , in red) and final ( $t = 21 \, days$ , in blue) positions of selected particles constituting the anticyclonic eddy core. Panel (a) is an X/Y view, panel (b) is a side X/Z view and (c) a side Y/Z view.



Figure 8: PV evolution rate for a single particle (with maximum correlation between direct PV diagnostic and reconstructed from tendency terms). The blue dashed line corresponds to the calculation from the model PV (calculated using an interpolation of the model PV on the particle's trajectories) and the black plain line is the diagnostic associated with the sum of friction and mixing tendency terms (again interpolated on the particle's trajectories).

every  $600 \ s$ , calculated directly from physical fields and diagnosed from the 503 sum of the friction and tendency terms for a particle with a typical evolution: 504 the dashed blue curve is obtained from the PV record (calculating  $\frac{d}{dt}PV$ ) 505 and the plain black curve is the right hand side of Eq. 6, calculated from the 506 non-conservative terms, along the particle's trajectories. Note the good 507 agreement between the two estimates before the circulation becomes 3D and 508 exhibits small scale variability. This is generally the case for the retained 509 particles, however, some discrepancies can be seen on the evolution rates, in 510 particular, the model PV evolution rate exhibits abrupt changes that we do 511 not see in the diagnosed PV (using tendency terms). But the variations are 512 close enough to be exploited. 513



In Fig. 9 represents the latitudinal (upper panel) and vertical (middle



Figure 9: Latitudinal (upper panel) and vertical (middle panel) positions and PV evolution rate (lower panel) for the same particle as in Fig. 8. For the PV evolution rate, the green curve represents the friction tendency term and the red curve the mixing tendency term, the black plain line is the sum of both and is the same as in Fig. 8.



#### a) Effect of mixing : impermeability theorem

b) Effect of wind stress along isopycnal

Figure 10: a) Mixing produces negative PV anomalies in region where the stratification is reduced and positive ones in regions where stratification becomes stronger. b) The effect of friction on PV is associated with the curl of the stress, but calculated along an isopycnic surface. The wind stress generally diminishes in amplitude from the surface to the base of the mixed layer. Thus even an homogeneous wind can be associates with a curl, and PV production, along an isopycnal whose vertical position varies. c) In the upwelling case, mixing deepens the mixed layer and thus increases PV at its base and decreases it in the homogenized region. Isopycnic surfaces bend upward and are thus subject to an increasing along-wind stress generating negative curl and negative PV anomalies. In this case, a Lagrangian particle first moves along an isopycnic surface when it is below the mixed layer, and its properties are unchanged. Eventually, it enters the mixed layer where it is subject to friction, which modifies its PV and produces negative anomalies, and mixing, which changes both its density and PV. Mixing generates first positive and then negative anomalies as the particle moves upward.

panel) position of the particle and the lower panel shows the respective 515 contributions from friction (green) and mixing (red) to the global tendency 516 term (black plain line, already plotted in Fig. 8). The behaviour observed 517 here is the same for most particles: the particle first moves upward and 518 Northward – following an isopycnic surface – but is initially not subject 519 to diabatic forcings and the PV remains unchanged. PV is modified when 520 the particle enters the base of the mixed layer. As explained in Fig. 10, 521 it is first affected by mixing, producing positive anomalies (Fig. 10a and 522 c). Soon after, friction acts too with a negative production rate (Fig. 10b 523 and c). As the particle moves further upward into the mixed layer, it is 524 entrained by the surface Southward currents and the mixing PV production 525 strongly decreases (it can even become negative for some particle) but the 526 negative production by friction is maintained. The global (friction+mixing) 527 PV evolution thus evolves from positive to negative with longer and stronger 528 negative production, so that the final PV anomaly of the particle is generally 529 negative. After this strong modification episode when entering the mixed 530 layer, the particle is subject to a phase where mixing and friction production 531 equilibrate so that its PV value is maintained. After day 18, when the 532 instability develops and produces small scale variability, marked by higher 533 frequency changes in horizontal and vertical positions, PV evolves again but 534 the physics of this phase is more difficult to explain since there are strong 535 numerical uncertainties. 536

Figure 11 shows the mean evolution calculated from the 1252 selected particles with high correlation. The mean PV anomaly gradually decreases (plain black and dashed blue curves) and the final value is strongly negative (the PV anomaly is  $\delta \overline{PV} \simeq -6.10^{-5}s^{-1}$ ). Note that after day 18, discrepancies appear between the model PV (blue dashed curve) and the

PV diagnosed from the tendency terms (black plain curve). As explained 542 above, the development of the instability generates small, rapidly evolving 543 eddies. Implicit diabatic terms, associated with imperfections of the numer-544 ical schemes at the grid scale and the limited (hourly) output frequency used 545 for our diagnostics, corrupt the PV budget. However, the development of the 546 PV structure responsible for the initial instability is correctly represented 547 before the emergence of small scale 3D structures, During this period, fric-548 tion produces negative PV anomalies (green curves in Fig. 11). Although 549 it produces both positive and negative anomalies, the effect of mixing is 550 to dampen the effect of friction by producing a net positive anomaly (red 551 curves) at a rate that is – on average – similar in amplitude in this refer-552 ence experiment. For particles entering the lateral boundary layer, lateral 553 friction can also affect the friction tendency term with an effect that can 554 be more difficult to predict as it depends on details of the velocity varia-555 tions near the wall and the horizontal viscosity scheme used in the model 556 (D'Asaro, 1988; Morel and McWilliams, 2001; Akuetevi and Wirth, 2015; 557 Morel et al., 2019), but the general negative friction tendency term observed 558 here is mostly associated with the effect of the wind stress and its redistribu-559 tion in the surface mixed layer. Testing with different anticyclonic vortices 560 or changing the selection criterion for retained particles does not change our 561 findings. 562

As can be seen from Fig. 4, cyclonic structures are constituted of smaller vortices and filaments and are not as well defined as anticyclonic vortices. It is also clear that the interior PV anomaly is mostly negative, although there are traces of positive PV anomalies on vertical sections (third column in Fig. 3). We selected areas with positive interior PV anomalies and performed a similar Lagrangian analysis (again backtracking 2000 particles from day



Figure 11: Mean PV evolution (upper panel) and evolution rate (lower panel) for all 1178 selected particles, constituting the anticyclonic eddy core (Fig. 7). For the upper panel, the blue dashed line corresponds to the PV anomaly of the model (calculated from the PV values of all selected particle at a given time from which we withdraw f), the green curve is obtained from the time integration of the friction tendency term and the red curve from the mixing tendency term, the black plain line is the sum of the integrated tendency terms and is to be compared to the blue dashed curve. The lower panel is similar but for the tendency terms (evolution rate).

21). We found that the positive interior PV anomaly of particles constitut-569 ing cyclonic eddies is determined during the last days of the evolution, i.e. 570 after day 18, when the instability starts to develop. The criterion for par-571 ticle selection had to be modified and the minimum correlation coefficient 572 between model and diagnosed PV evolution was lowered to 0.7 to keep a 573 few hundred particles. The mean PV anomaly of the particles constituting 574 cyclonic eddies at day 21 was  $\delta \overline{PV} \simeq +1.5.10^{-5} s^{-1}$ , much lower than for 575 anticyclonic structures (in absolute value). As mentioned above, the exten-576 sion of the eddies is also much smaller, but it is also constituted of different 577 subcores, i.e. disconnected parts associated with local maximum. In fact, 578 eddies associated with positive vorticity or average PV anomalies are domi-579 nated by the surface outcropping signature, under which the positive interior 580 PV anomaly eddies, generated during the development of the geostrophic 581 instability, align. As seen before, mixing creates the positive PV anomalies 582 at the base of the mixed layer, but during the late stage of the evolution, 583 friction can also produce positive PV. Indeed, we have seen (see Fig. 10) 584 that, during the upwelling development phase, the decrease of the stress 585 from the surface and the upward bending of isopycnals is associated with a 586 negative curl of stress along isopycnic levels, which explains the formation 587 of negative PV anomalies by friction. If the isopycnal bends downward, 588 which is the case when the instability develops and vortices emerge, the curl 589 becomes positive and positive PV anomalies is then produced by friction 590 (Morel et al., 2006). 591

#### 592 4.2. Sensitivity to wind stress

We now evaluate the sensitivity of the PV change to the wind stress. As noted above, although we have considered a constant wind, the stress <sup>595</sup> along isopycnic levels is locally modified in the upwelling region, since it
<sup>596</sup> depends on the isopycnal position, velocity shear and local vertical viscosity
<sup>597</sup> coefficient (Morel et al., 2006, 2019).

We lowered the wind intensity with W = 2 m/s corresponding to a 598 stress of  $\tau \simeq 0.006 \ N/m^2$ , 16 times smaller than before, and performed the 599 same analysis on PV evolution. Figure 12 is similar to Fig. 3 and shows 600 the evolution of vertically averaged upper-layer PV anomaly, surface vor-601 ticity, vertical section of PV anomaly, and vorticity along a South-North 602 transect at  $x = 205 \ km$ . Due to the lower forcing wind stress, mixing is 603 less intense and the layer affected by mixing and wind stress is shallower. 604 The upper layer over which PV is averaged is now bounded by the isopy-605 cnic level  $\rho = 1024.6 \ kg/m^3$  and the surface. The evolution is also slower 606 than before with some peculiarities. First, Kelvin-Helmholtz like instabili-607 ties start at day 22 with several sequences until about day 37 when longer 608 wavelength geostrophic instabilities develop, evolving into mesoscale struc-609 tures after about 70 days. The layer PV and the surface vorticity structures 610 are still strongly connected, but the patterns are different compared to the 611 reference experiment with smaller and weaker anticyclonic vortices. The 612 vertical sections of PV anomaly show little trace of positive PV anomalies 613 in the interior during most of the evolution, and it appears only at the stage 614 of fully developed turbulence (see the vertical section of PV at day 90, Fig. 615 12 last line, third row). Finally the isopycnic levels (black contours on the 616 vertical sections) are less steep in the upwelling region, indicating that the 617 fluid remains more stratified. 618

In Fig. 14 we plot the PV tendency terms associated with friction and mixing and their sum. Before the development of the geostrophic instability, PV anomalies generated by mixing show a different pattern for this lower



Figure 12: Evolution (days 10, 20, 35 for the experiment with a wind stress reduced to  $\tau = 0.006 N/m^2$ . Each day corresponding to a row) of horizontal maps of surface layer average PV anomaly (first column), surface vorticity (second column) and vertical sections of PV anomaly (third column) and voticity (fourth column). The PV anomaly is obtained by withdrawing the reference PV, that is f. The vertical South-North sections are taken along the dashed line represented in the horizontal maps (at  $x = 205 \ km$ ). Note that it crosses the core of an anticyclonic subsurface vortex at day 46. In rows 1, 3 and 4, the solid black contours are associated with isopycnic levels.





stress simulation, with sometimes a layer of negative PV production below 622 the positive one (row 1 and 2 of MixFlux, third column), which is inverted 623 compared to Fig. 5. The influence of the correction term, associated with 624 the evolution of the reference profile, is more important here: the presence of 625 the upwelling close to the coast generates a stronger stratification that is not 626 compensated by the shear, and mixing diminishes in the upwelling region 627 in comparison to the rearranged profile. This shows that nonlinearities and 628 details of the evolution, associated with the mixing closure scheme, can 629 lead to strong differences for the -rescaled- PV production and subsequent 630 dynamics. 631

As for the reference experiment, 2000 particles were seeded into the anti-632 cyclonic structure observed in the vertical section at day 46, whose center is 633 located at  $x = 205 \ km$  and  $y = 242 \ km$ . These particles were backtracked 634 to their initial positions while computing their PV and the PV tendency 635 terms at their positions every  $600 \ s$ . Using a similar selection criterion as 636 for the reference experiment (correlation between the PV evolution and that 637 reconstructed from the tendency terms above 0.9) about 1100 particles were 638 retained. Figure 15 is similar to Fig. 11 and shows the evolution of the 639 mean PV anomaly from the model (blue dashed line), the integration of 640 the friction tendency term (green line), the mixing tendency term (red line) 641 and the sum of both tendency terms (black line). There are striking differ-642 ences with the reference experiment. First, both friction and mixing lead to 643 negative PV production on average, but mixing has a modest effect; most 644 of the variability is associated with friction, before the development of the 645 geostrophic instability and vortex formation. The rate of PV production is 646 also about 10 times weaker for friction or mixing. Another interesting as-647 pect is that the analysis of individual particles (not shown) shows that after 648



Figure 14: Evolution (days 10, 35, 46 and 90. Each day corresponding to a row) of vertical sections, taken along a South-North section located at  $x = 205 \ km$ , of the sum of diabatic tendency terms (first column), the frictional term (second column) and the diapycnal mixing term (third column) for the sensitivity test with a reduced wind stress ( $\tau = 0.006 \ N/m^2$ ). 41



Figure 15: Mean PV evolution (upper panel) and evolution rate (lower panel) of all 1083 selected particles forming the anticyclonic eddy core (Fig. 7) in the experiment with the wind stress reduced to  $\tau = 0.006 \ N/m^2$ . For the upper panel, the blue dashed line corresponds to the PV anomaly of the model (calculated from the PV values of all selected particles at a given time from which we remove f), the green curve is obtained from the time integration of the friction tendency term and the red curve from the mixing tendency term, the black solid line is the sum of the integrated tendency terms and is to be compared with the blue dashed curve. The lower panel is similar, but for the tendency terms (evolution rate).

day 40, small scale processes spoil the PV budget for individual particles,
but the mean evolution remains quite close to the estimated PV evolution
(black and blue dashed curves in the upper panel of Fig. 15), whereas in
the reference experiment, this leads to a bias.

#### **53** 5. Summary and Discussion

In the present paper, we advocate the use of a form of PV, rescaled by 654 the time-evolving Lorenz's rearranged density profile (Lorenz, 1955; Naka-655 mura, 1995; Winters and D'Asaro, 1996). The proposed PV is the only form 656 able to associate PV to the absolute vorticity for barotropic circulation. In 657 general circumstances, it is also a generalization of the QG PV and is easily 658 connected to the (cyclo)geostrophic circulation. We thus argue that this 659 form of PV provides an objective evaluation of the effect of mixing and fric-660 tion on the generation of PV. Its time evolution equation is derived and 661 it is shown that global changes in stratification must be removed from the 662 mixing production term, following isopycnal levels. The proposed form of 663 PV and its evolution equation are valid in general (realistic) circumstances 664 for the Navier-Stokes or Primitive equations. We believe this form has to be 665 chosen when interpreting PV evolution in terms of dynamics (that is when 666 using the inversion principle, relating PV to the circulation), especially to 667 evaluate the respective influence of mixing and friction. Equation 6 shows 668 that the objective rescaling of PV may lead to different interpretation de-669 pending on the characteristics of the water mass that is subject to diabatic 670 changes: wind stress effect is rescaled by  $Z(\rho)$  and mixing by  $\partial_{\rho} Z(\rho)$ . This 671 can lead to strong differences with respect to the traditional Ertel PV form, 672 for instance in region of ventilation, where a water mass is subject to heat 673

and momentum forcing at the surface before subducting and filling a deeplayer.

Note that the evolution equation 6 is valid for other choices of the refer-676 ence density profile, for instance using a "local" -but time evolving- reference 677 density profile chosen at a fixed position. In this case, the interpretation of 678 the PV evolution is different, relative to the PV and circulation fields at 679 the chosen location. In the numerical configuration tested here, a choice of 680 a reference profile chosen in the middle of the basin yielded similar results 681 (not shown). In previous studies (Delpech et al., 2020; Assene et al., 2020; 682 Aguedjou et al., 2021; Napolitano et al., 2022; Ernst et al., 2023) we chose a 683 profile in the area of interest and fixed in time, arguing that, since we con-684 centrated on the dynamics of deep layers, the reference stratification does 685 not evolve much. Thus simpler choices for the reference profile are possible, 686 but the ideal and rigorous choice remains Lorenz's rearranged profile. 687

The calculation of Lorenz's profile is generally straightforward and differ-688 ent methodologies have been proposed (Winters and D'Asaro, 1996; Tseng 689 and Ferziger, 2001; Tailleux, 2013b). However, specific configurations may 690 require adaptations, such as the periodic channel one used here. Other 691 possible difficulties may arise from realistic configurations over a restricted 692 region forced at its boundaries by fluxes from a larger domain. If the water 693 mass characteristics entering the region varies, the interpretation of the PV 694 evolution based on the rearranged profile in the region can be more difficult. 695 For instance, in the present configuration, we mimicked open boundaries by 696 restricting the calculation of the rearranged profile to the Northern half of 697 the basin. We found this can lead to some biases in PV production by mix-698 ing. Indeed, because de transverse circulation associated with the upwelling 699 development leads to light layers depletion and deep layers inflation, the 700

reference profile evolves even when there is no mixing. Interpretation of the
PV evolution must then be made with care.

We then numerically evaluate the use of this PV formulation using a 703 simplified configuration of an upwelling developing in a periodic channel. In 704 the reference upwelling simulation, with a strong mean wind, both diapycnal 705 mixing and friction influence the PV evolution of particles. Outcropping of 706 isopycnals at the surface provides the main reservoir for cyclonic eddy gen-707 eration (Bretherton, 1966; Morel et al., 2006). Interior diabatic effects asso-708 ciated with friction or mixing also create positive PV anomaly eddies, but 709 the latter are generated after the onset of the instability and remain weak. 710 They play little role in the early stages of the instability. On the contrary, 711 anticyclonic vortices are associated with the generation of interior negative 712 PV anomalies, which require non-conservative effects. Prior to the onset 713 of the geostrophic instability, the friction associated with the wind stress 714 generates negative PV anomalies and the interior PV is predominantly neg-715 ative. Mixing generates both positive and negative PV anomalies, with a net 716 effect toward positive, only partially compensating the negative generation 717 by friction. This explains the initial PV structure of the upwelling and its 718 destabilization at geostrophic scales. 719

As the instability develops, the stratification and velocity fields become complex and modulate the effect of mixing and friction at small scales, leading to strong changes in the PV structure. At this stage, implicit dissipation associated with numerical schemes becomes influential and spoils the PV budget when using the explicit friction and mixing terms.

For a lower intensity of the wind stress, the effect of friction remains similar with a negative production, but at a lower rate. On the other hand, the effect of mixing is strongly modified: higher stratification associated with the upwelling development under a weaker wind leads to less intense mixing in the upwelling region than in the open ocean and a net negative production rate for the rescaled PV. The global PV production due to mixing is an order of magnitude smaller than that due to friction. This shows the sensitivity of PV modification by non-conservative processes and their parameterizations. A downwelling develops along the southern boundary and PV is also

modified in this area, but the current remains stable in our configuration, 734 so we did not focus on this area. In more realistic configurations, capes or 735 topographic variations along the coast may generate localized eddies that are 736 necessarily associated with the generation of PV anomalies. It is interesting 737 to evaluate the influence of non-conservative processes in such a situation. 738 Discrepancies between the characteristics of such eddies in models and in 739 nature could well be associated with erroneous PV production associated 740 with closure schemes. 741

More generally, the present study emphasizes that parameterizations 742 play an important role in the determination of PV, the subsequent charac-743 teristics of the eddies and the structuring of the large scale circulation (which 744 is partly determined by the redistribution of PV by the eddies). Testing dif-745 ferent closure schemes, or parameters within a closure scheme, from the 746 perspective of PV is therefore very informative. For example, recent stud-747 ies have shown that accounting for the modulation of the wind stress by 748 the surface ocean current feedback to the atmosphere drastically improves 749 the surface eddy properties (Renault et al., 2016b, 2020). In upwelling sys-750 tems, the wind drop-off near the coast (Capet et al., 2004; Renault et al., 751 2016a) or wind acceleration near capes modulates the surface stress, which, 752 combined with the vertical redistribution of momentum by the turbulent 753 fluxes, can lead to more complex effects of the wind stress (Kessouri et al., 754

<sup>755</sup> 2022). It is also possible to refine the analysis and to distinguish specific <sup>756</sup> non-conservative effects on PV evolution (e.g. separating vertical momen-<sup>757</sup> tum fluxes from horizontal ones, or separating different diapycnal mixing <sup>758</sup> processes). All of these mechanisms, and many more, could benefit from an <sup>759</sup> analysis of PV generation associated with friction, mixing and their depen-<sup>760</sup> dence on parameterization choices. The tools we have presented here can <sup>761</sup> be very helpful for this perspective.

We have seen that when the dynamics becomes fully turbulent, there 762 are discrepancies between the PV evolution and its reconstruction from the 763 tendency terms. Temporal sub-sampling is one issue. It can be addressed by 764 on-line Lagrangian diagnostics of PV, but the strategy for the initial particle 765 positioning may be difficult, and backtracking of particles remains necessary 766 to analyze the generation of PV for a particular region or eddy. We have also 767 cited the imperfections of numerical schemes, which lead to non-conservative 768 terms that can affect the PV evolution at the grid scale, when the dynamics 769 generates small scale structures (filaments or other submesoscale eddies). 770 If these uncertainties seem to cancel out when averaging many particles in 771 the moderate wind experiment, we have seen that there is a bias possibly 772 associated with this effect in the strong wind -reference- experiment. This 773 can be problematic in achieving correct properties for eddies in numerical 774 models, but again, the tools we have proposed can help to identify numerical 775 effects and test the influence of improved numerical schemes. 776

Finally, Lorenz's profile corresponds to the minimum energy state which is linked to the available potential energy (APE). In some previous studies, we discussed a link between the PV structure of vortices or jets and their energy (Morel and McWilliams, 2001; Morel et al., 2019). The fact that, to get a rescaled PV related to the circulation, Lorenz's rearranged profile

is the ideal choice is thus probably not chance. The relationship between 782 rescaled PV and APE in general is thus worth investigating and some studies 783 dedicated to APE can be of great interest to substantiate the definition of the 784 ideal PV form and also possibly to identify other sources of PV modification. 785 For instance, Scotti and Passaggia (2019) have shown that the choice of 786 the Lorenz's rearranged profile to define APE can be justified because in 787 this case the effective energy does not depend on the time evolution of the 788 restratified flow, and argument that has strong similarities with the one used 789 here for the necessity of taking into account time evolution of the reference 790 profile for the rescaled PV. Finally, depending on the form of the equation 791 of state, the calculation of the Lorenz's profile is not straightforward, and 792 thermobaric effects can also make PV analysis more complicated (Straub, 793 1999). Recent studies in this field (Tailleux, 2013a,b; Saenz et al., 2015; 794 Tailleux, 2018) offer an interesting perspective for the use of PV analysis in 795 realistic configurations and are worth pursuing. 796

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### Appendix A. Numerical calculation of the reference density profile

Calculating Lorenz's rearranged density profile can be efficiently done 806 by computing the pdf of the density field (Tseng and Ferziger, 2001) or 807 other methods proposed in the litterature (see for instance Tailleux, 2013b). 808 The pdf of density is easily calculated by defining fixed density classes and 809 using the density values in existing numerical cells of the configuration. The 810 obtained distribution should not suffer from biases when sigma levels and 811 density fields vary over the domain because of a varying bottom topography 812 and/or a complex -realistic- circulation is considered. 813

However, in the present configuration, we start from rest, with flat isopy-814 cnal over a flat topography. Discarding mixing, so that the initial linear ref-815 erence profile should be maintained, the stratification evolution consists in 816 bending isopycnals in narrow regions near the domain boundaries. In such 817 a circumstance, the density pdf might be strongly biased, with large classes 818 associated with density values over the middle of the domain and that are 819 almost unchanged with respect to the initial state, and small classes asso-820 ciated with the slight variation near the boundaries. Such a pdf results in 821 staircase like stratification instead of the linear one, which is very problem-822 atic for the evaluation of the rescaled PV. To avoid this problem, the existing 823 methodologies to calculate the rearranged profile was adapted as follows: 824

- 1. Define the variation of volume and surface with depth, from the surface to the bottom of the domain, as a function of the vertical position z, with high enough discretization ( $\Delta z \simeq 0.1 m$ ). For our flat bottom configuration, this is trivial.
- 829
  - 2. Define intervals of density (density classes) covering the whole range

of densities present in the domain. The density range of each interval should be very small because we want to represent very small variations in the mixed layer. Here, to achieve good comparisons between direct calculation of the PV evolution rates and the one reconstructed from the tendency terms, we had to chose  $\Delta \rho = 10^{-5} kg/m^{-3}$ .

3. Calculate the density pdf: affect each density cell of the 3D domain to 835 a density class and affect its volume to the class. This is the stage when 836 adaptations are necessary to avoid biases for the present configuration. 837 For each horizontal position, we interpolate the density profile on a 838 virtual vertical grid with higher resolution. This allows to refine the 839 pdf but is more computationally demanding. To achieve good results, 840 the vertical step we had to choose for the present configuration is 841  $\Delta z = 0.1 \ m.$ 842

# 4. Calculate the net volume and mean density of each class and construct the initial rearranged 1D density profile filling the ocean from top and using the 1D volume and surface vectors determined at stage 1.

5. Interpolate the obtained profile using a regular density spacing (again a density step  $\Delta \rho = 10^{-5} kg/m^{-3}$  is necessary here) to define the rescaling function at time  $t Z(\rho, t)$ .

#### <sup>849</sup> Appendix B. Generalized PV evolution equation

The traditional Ertel PV is defined as

$$PV_{Ertel} = -(\vec{\nabla} \times \vec{U} + \vec{f}).\vec{\nabla}\rho \tag{B.1}$$

where  $\vec{U}$  is the velocity field,  $\vec{f}$  is the Earth rotation vector, whose projection on the local vertical axis defines the Coriolis parameter f, and  $\rho$  is the potential density. As already mentioned by Ertel (1942) (see also Muller, 2006; Morel et al., 2019), other forms for the potential vorticity are possible, with the same adiabatic conservation properties, obtained with

$$PV_{rescaled} = (\vec{\nabla} \times \vec{U} + \vec{f}) \cdot \vec{\nabla} Z(\rho)$$
$$= \vec{\nabla} \cdot ((\vec{\nabla} \times \vec{U} + \vec{f}) Z(\rho))$$
(B.2)

where  $Z(\rho)$  can be any function of potential density alone.

For geophysical flows, isopycnic variations of PV can be inverted to de-851 termine the geostrophic currents and associated stratification (Hoskins et al., 852 1985). But the Ertel PV is not the best PV expression to do so, in partic-853 ular, for small geostrophic perturbations relative to a state at rest, quasi-854 geostrophic PV (Pedlosky, 1987; Muller, 2006; Cushman-Roisin and Beck-855 ers, 2011) should be recovered. Indeed the quasigeostrophic PV is given 856 by the sum of the Coriolis parameter and the 3D Laplacian of the pres-857 sure variations associated with the small perturbation, from which both the 858 geostrophic current and stratification can be obtained. With this straight-859 forward link between PV and dynamical fields, the quasigeostrophic physics, 860 associated with conservation and inversion of quasigeostrophic PV, provides 861 important insights and is a fundamental approach for the understanding of 862 the ocean dynamics from mesoscale to large scale (Pedlosky, 1987; Cushman-863 Roisin and Beckers, 2011). It is also at the base of the "PV thinking" ap-864 proach (see in particular Hoskins et al., 1985, among many other) based on 865 the analysis of the evolution of the PV field. 866

As discussed in the introduction, to overcome some problems associated with  $PV_{Ertel}$  and simplify its interpretation, Morel et al. (2019) proposed  $Z(\rho^*) = z$  (where z is the vertical coordinate oriented upward), a rescaling function defined using a reference density profile  $\rho^*(z)$  representing the

stratification at rest (see also Delpech et al., 2020; Assene et al., 2020). It 871 is rigorously obtained using Lorenz (1955) diabatic rearrangement, where 872 each fluid particle is classified according to its potential density and the do-873 main is gradually uniformly filled following this stable rearrangement (see 874 also Nakamura, 1995; Winters and D'Asaro, 1996). For such a choice, the 875 rescaled PV at rest is  $PV_{rescaled}^{rest} = f$ . The calculation of the reference profile 876 can be cumbersome, and in general taking into account a profile which is 877 typical of the stratification of the studied region can be taken as a reference 878 to rescale the PV. 879

In the present paper, to study the vortical dynamics of the upper layer in a context of rapid diabatic evolution associated with wind stress and mixing, the evolution of the reference stratification has to be taken into account.

We thus define a general rescaled PV field as

$$PV_{rescaled} = \vec{\nabla}.( (\vec{\nabla} \times \vec{U} + \vec{f}) Z(\rho, t) )$$
(B.3)

where  $Z(\rho, t)$  is now a function of both potential density and time and associated with a reference profile  $\rho^*(z, t)$  that is time dependent. At any time,  $Z(\rho^*(z, t), t) = z$ , so that the rescaled PV at rest is still given by the Coriolis parameter  $PV_{rescaled}^{rest} = f$ .

The evolution equation for  $PV_{rescaled}$  is obtained from Eq. 1 and, following Muller (2006), we get (see also Morel et al., 2019, for the specific divergence form we chose here)

$$\frac{d}{dt}PV_{rescaled} = \vec{\nabla}.( (\vec{\nabla} \times \vec{F}) \ Z(\rho, \ t) + (\vec{\nabla} \times \vec{U} + \vec{f}) \ \frac{d}{dt}[Z(\rho, \ t)] ) \quad (B.4)$$

The last term can be rewritten using

$$\frac{d}{dt}Z(\rho, t) = \partial_{\rho}Z(\rho, t) \dot{\rho} + \partial_{t}Z(\rho, t)$$
(B.5)

We now take into account the specific form chosen for the function  $Z(\rho, t)$ , which verifies  $Z(\rho^*(z, t), t) = z$ . Differentiating the latter with respect to time yields

$$\partial_{\rho} Z(\rho^*(z, t), t) \ \partial_t \rho^*(z, t) + \partial_t Z(\rho^*(z, t), t) = 0$$
(B.6)

or equivalently

$$\partial_t Z(\rho^*, t) = -\partial_\rho Z(\rho^*, t) \ \partial_t \rho^*$$
 (B.7)

from which we get

$$\partial_t Z(\rho, t) = -\partial_\rho Z(\rho, t) \ \partial_t \rho^*(Z(\rho, t), t)$$
(B.8)

Using Eq. B.8 into B.5 and finally replacing terms in B.4 we get

$$\frac{d}{dt}PV_{rescaled} = \vec{\nabla}.(\ (\vec{\nabla} \times \vec{F})\ Z(\rho,\ t) + (\vec{\nabla} \times \vec{U} + \vec{f})\ \partial_{\rho}Z(\rho,\ t)\ (\dot{\rho} - \partial_{t}\rho^{*}(Z(\rho,\ t),\ t)\ ) \quad (B.9)$$

or in Eulerian form

$$\partial_t \ PV_{rescaled} = \vec{\nabla}.(\ \vec{U} \ PV_{rescaled} + (\vec{\nabla} \times \vec{F}) \ Z(\rho, \ t) + (\vec{\nabla} \times \vec{U} + \vec{f}) \ \partial_\rho Z(\rho, \ t) \ (\dot{\rho} - \partial_t \rho^* \mid_{\rho,t}) \ )$$
(B.10)

where the first term of the right hand side divergence is associated with adiabatic advection, the second term with friction and the third one with diapycnal mixing. For the latter term, a correction is made for the generalized rescaled PV we propose here : the diabatic mixing term has to be corrected and the evolution of the reference profile  $\partial_t \rho^* |_{\rho,t} = \partial_t \rho^*(Z(\rho, t), t)$ has to be withdrawn as it has no consequence on the generation of "dynamical" PV anomalies. Note it has to be evaluated using the reference profile time evolution at a vertical level corresponding to the density value in the physical domain (not the elevation).

#### <sup>896</sup> Appendix C. Calculation of PV and tendency terms

Morel et al. (2019) showed that the divergence form of PV (Eq. 5) 897 preserves budgets and drastically simplifies the numerical calculation of PV, 898 which can be expressed with a compact scheme, i.e. using a single PV 899 grid cell on a 3D Arakawa C-grid (see Fig. C.16 and Arakawa and Lamb, 900 1977). As mentioned above, if we note the similarity between the divergence 901 expression of PV (Eq. 5) and the diabatic PV tendency terms of its evolution 902 equation (Eq. 6), we can see that the same scheme can be used to calculate 903 the friction and mixing tendency terms. 904

Indeed, all terms can be written as

$$Div^{PV} = \vec{\nabla}.(\ \vec{\nabla} \times \vec{F}^{vel} \ Z^{\rho} \) \tag{C.1}$$

where  $Div^{PV}$  is the divergence calculated at PV points of the staggered C-grid (see Fig. C.16),  $Z^{\rho}$  is a function of density calculated at density points and  $\vec{\nabla} \times \vec{F}^{vel}$  is the curl of a 3D vector  $\vec{F}^{vel} = (F^U, F^V, F^W)$  whose components are located at (U, V, W) points.

Integrating Eq. C.1 over the PV cell, whose corners are located at density points (see Fig. C.16), we get

$$\delta V^{PV} \ Div^{PV} = \bigoplus_{S} Z^{\rho} \ \vec{\nabla} \times \vec{F}^{vel}.d\vec{S}$$
(C.2)

where  $\delta V^{PV}$  is the volume of the PV cell and the right hand side integral is the flux of  $Z^{\rho} \vec{\nabla} \times \vec{F}^{vel}$  though all sides of the cell. Using the Stokes circulation theorem, the calculation of the latter term is simplified for the



Figure C.16: Elementary cell, for a 3D C-grid, used for the calculation of PV and the tendency terms. We consider Cartesian coordinates (x, y, z) associated with indices (i, j, k). Note that the calculation of the flux through each side of the cell is simplified for the C-grid because we can use the Stokes circulation theorem.

C-grid where velocity points are located at the center of edges parallel to the velocity component (see Fig. C.16). For instance, the flux through the side given in Fig. C.16 (right panel) is

$$\left[ \oint_{S} Z^{\rho} \, \vec{\nabla} \times \vec{F}^{vel}.d\vec{S} \right]_{i,j,k}^{x} = \overline{Z^{\rho}}_{i,j,k}^{x} . \left( F_{i,j-1,k}^{W}.\delta z - F_{i,j,k}^{W}.\delta z + F_{i,j,k}^{V}.\delta y - F_{i,j,k-1}^{V}.\delta y \right)$$
(C.3)

with

$$\overline{Z^{\rho}}_{i,j,k}^{x} = \frac{Z^{\rho}_{i,j,k} + Z^{\rho}_{i,j,k-1} + Z^{\rho}_{i,j-1,k} + Z^{\rho}_{i,j-1,k-1}}{4}$$
(C.4)

<sup>909</sup> and so on for the fluxes through other sides.

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