Chapter 1
Counter-gradient term applied to the turbulence parameterization in the BRAMS

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1.1 Introduction

The atmospheric dynamics is simulated by solving the Navier-Stokes equation, considering several physical phenomena. Some atmospheric processes are expressed by using parameterization: cloud formation, surface representation, turbulence, precipitation. The turbulence parameterization is closed under different orders. For zeroth order, the turbulent flux is represented by a function In the first closure order, Reynolds tensors are approximated as a product between an eddy diffusivity and the gradient of the main property. The second order closure is parameterized with the third order tensor expressed as a parameter multiplying the second order tensor.

On the top of the Planetary Boundary Layer (PBL), under convective regime, a counter-gradient flux is verified from observations. Indeed, turbulent flow is a part of physics strongly supported by experimental efforts. We are not going to explain details on the structure of the convective PBL. But, we note that only the second order closure is able to represent the latter flux. However, modifying the first order approach by adding a counter-gradient term, it is possible to represent such flow. The first studies for representing the latter issue were carried out by Deardorff [6, 7]. Here, the eddy diffusivity is formulated by Taylor's statistical theory of turbulence [10], and a new term is used – derived from the Large Eddy Simulation (LES) [5]. This new turbulence scheme is applied to BRAMS, a meso-scale meteorological model. The simulation is compared with experimental data from the Large Scale Biosphere-Atmosphere Experiment in Amazonia (LBA) experiment (`https://daac.ornl.gov/LBA/lba.shtml`).

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1.2 Turbulence model

The turbulent flux for a property $\bar{\varphi}$ can be represented by a first order closure:

$$\langle v_i' \varphi' \rangle = K_{\alpha\alpha} \frac{\partial \langle \varphi \rangle}{\partial x} \tag{1.1}$$

where v_i' is the wind velocity components, $K_{\alpha\alpha}$ is the eddy diffusivity, $\alpha = x, y, z$, and the operator $\langle \varphi \rangle$ denotes time average. From Taylor's statistical theory on turbulence [18, 19], the eddy diffusivity can be expressed as product between an average velocity and a characteristic length:

$$K_{\alpha\alpha} \sim \langle v_i(t) \rangle \langle x(t) \rangle \tag{1.2}$$

where the index-i indicates the wind components (u, v, w). The velocity is defined as $v(t) \equiv x(t)\, dt$. Substituting the velocity definition in the above equation and taking the average, the eddy diffusivity can be written as:

$$K_{\alpha\alpha} = \frac{d}{dt} \left[\langle x^2(t) \rangle \right] = 2 \langle v_i^2(t) \rangle \int_0^t \int_0^\tau \rho_{L_i}(\tau)\, dt' d\tau \tag{1.3}$$

where $v_i(t)$ is the i-th Lagrangian wind component of a *fluid particle*, and $x(t)$ is its displacement on the direction-i. The autocorrelation function is denoted by ρ_{L_i}, normalized by the Lagrangian velocity:

$$\rho_{L_i}(\tau) = \frac{\langle v_i(t+\tau) v_i(t) \rangle}{\langle v_i^2(t) \rangle} \ . \tag{1.4}$$

Eulerian formulation can be computed from Langrangian quantities by using Gifford-Hay and Pasquill's assumption, where Lagrangian and Eulerian autocorrelations (or spectral) functions are the same, but shifted by a constant β [8, 9]:

$$\rho_i(\tau) = \rho_{L_i}(\beta_i \tau) \ , \qquad \beta_i = \frac{\sigma_i}{U} \frac{\sqrt{\pi}}{4} \ , \qquad \sigma_i \equiv \sqrt{\langle v_i^2(t) \rangle} \ , \tag{1.5}$$

with U the wind intensity.

Applying Fourier transform to Eq. (1.3), and noting that $\rho_i(\tau)$ is an even function, Eulerian eddy diffusivity can be expressed by [8, 9, 4]

$$K_{\alpha\alpha} = \frac{\sigma_i^2 \beta_i}{2\pi} \int_0^\infty \left[\frac{F_i^E(n) \sin(2\pi n t / \beta_i)}{n} \right] dn \tag{1.6}$$

where $F_i^E(n) \equiv S_i^E(n) / \sigma_i^2$, being $S_i^E(n)$ the turbulent kinetic energy on direction i, and n is a frequency. For large diffusion time ($t \to \infty$), an asymptotic expression for the $K_{\alpha\alpha}$ can be derived [8, 9, 4] as

$$K_{\alpha\alpha} = \frac{\sigma_i^2 \beta_i F_i^E(0)}{4} \ . \tag{1.7}$$

An explicit formulation for eddy diffusivities $K_{\alpha\alpha}$ can be obtained by using empirical relations and Obukhov's similarity theory. A key issue is to derive an analytical formulation to the spectrum. Degrazia et al. [10] have derived a spectral formula for all atmospheric stability conditions:

$$nS_i^E(n) = \frac{1.06 c_i f\, \psi_\varepsilon^{2/3} (z/h)^{2/3} w_*^2}{[(f_m^*)_i^c]^{5/3} (1 + 1.5 [f/(f_m^*)_i^c])^{5/3}} + \frac{1.5 c_i f (\Phi_\varepsilon)^{2/3} u_*^2}{[(f_m^*)_i^{n+es}]^{5/3} \left(1 + 1.5 [f^{5/3}/(f_m^*)_i^{n+es}]\right)^{5/3}} \tag{1.8}$$

where c_i are empirical constants, z is the level over the surface, h is the planetary boundary layer height, w^* is the velocity scale for the convective condition, u^* is the friction velocity, $f = nU/z$ is the frequency in Hertz, U is the wind velocity, ψ_ε and Φ_ε are non-dimensional dissipation functions for convective and stable/neutral conditions, $(f_m^*)_i^c$ and $(f_m^*)_i^{n+es}$ are the maximum frequencies for a convective and stable/neutral conditions – respectively. The wind variances can be calculated by integrating the spectra over all frequencies: $\sigma_i^2 = \int_0^\infty S_i^E(n)\, dn$.

1.2.1 Counter-gradient model

As already mentioned, the first order closure is not able to represent a counter-gradient flux. Therefore, a new term must be added in the parameterization scheme for describing such flow:

$$\overline{u'_\alpha \varphi'} = -K_{\alpha\alpha} \left[\frac{\partial \langle \varphi \rangle}{\partial x_\alpha} - \gamma_\varphi \right] \tag{1.9}$$

being γ_φ the counter-gradient. From experiments, Deardorff had estimated $\gamma_\theta \approx 6.5 \times 10^{-6}\,\mathrm{C\,cm^{-1}}$ [6], and he did a new evaluation to $\gamma_\theta \approx 7 \times 10^{-6}\,\mathrm{K\,cm^{-1}}$ [6].

The counter-gradient term is only applied under convective condition, i.e., it is not used for neutral and stable boundary layers. The γ_φ is employed for heat and mass transport, but it is not used to the momentum due to the pressure effect. The planetary boundary layer stability can be calculated from the Monin-Obukhov's length L. In order to codify which parameterization should be applied for different stability conditions to the atmosphere, we adopted $|L| > 500$ to characterize the neutral boundary layer:

$$\begin{cases} -500 \le L < 0 : \text{Convective} \\ |L| > 500 : \text{Neutral} \\ 0 < L \le 500 : \text{Stable} \end{cases}$$

The Monin-Obukhov's length is expressed by

$$L = \frac{-u_*^3}{\kappa\left(g/\theta_{v_0}\right)\left(\overline{w'\theta_v'}\right)_0} \tag{1.10}$$

here κ is the von Kármán's constant, g is the gravity acceleration, θ_v virtual potential temperature, and $\left(\overline{w'\theta_v'}\right)_0$ is the heat flux from the surface. Cuijpers and Holtslag [5] have derived an expression to the counter-gradient from the LES results:

$$\gamma_\varphi = \beta_g \ell_w \frac{w_*^2}{\sigma_w}\frac{\varphi_*}{h}\ , \qquad \text{with:} \quad \varphi_* = \frac{1}{hw_*}\int_0^h \overline{w'\varphi'}\, dz\ . \tag{1.11}$$

where β_g is an experimental constant. The counter-gradient depends on the wind variance parameterization σ_w^2, the mixing length ℓ_w, and the quantity φ^*. The expressions for wind variance σ_i^2 and mixing length ($\ell_i = K_{\alpha\alpha}/\sigma_i$) are calculated from the Taylor's theory [4]:

$$\sigma_i^2 = \frac{0.98c_i}{(f_m)_i^{2/3}}\left(\frac{\psi_\varepsilon}{q_i}\right)^{2/3}\left(\frac{z}{h}\right)^{2/3} w_*^2 \tag{1.12}$$

$$\ell_w = 0.2h\left[1 - \exp\left(-4\frac{z}{h}\right) - 0.003\exp\left(8\frac{z}{h}\right)\right] \tag{1.13}$$

where $c_i = 0.3$ for u and 0.4 for (v,w), $f_m = 0.33$ is the frequency for the spectral peak, $q = (f_m)_i\,(f_m)_{n,i}^{-1}$ is a stability function. The dissipation function was derived by Campos Velho et al. [3]:

$$\psi_\varepsilon = 3\left(1-\frac{z}{h}\right)\left(\frac{z}{h}\right)\left[1 - \exp\left(4\frac{z}{h}\right) - 0.0003\exp\left(8\frac{z}{h}\right)\right]^{-1}\ . \tag{1.14}$$

Different values are obtained in Eq. (1.11) if different turbulence model are used. Therefore, the constant β_g is a parameter to be calibrated according to the parameterization applied. Cuijpers and Holtslag [5] have used $\beta_g = 1.5$, and Roberti and co-authors [16] employed $\beta_g = 0.07$. The value $\beta_g = 0.02$ provides the better results for our approach using Taylor's theory [21].

1.3 Meso-scale atmospheric model: BRAMS

BRAMS is employed for CPTEC (Portuguese acronym for Center for Weather Forecasting and Climate Studies), a division of INPE (National Institute for Space Research, Brazil), as the operational system for numerical weather forecasting over South America. The prediction system deals with 5 km of horizontal resolution, executed on Cray XE6 massively parallel computer. Operational forecasting uses 9600 processing cores[1]. BRAMS can be also configured as the operational environmen-

[1] The Cray XE6 supercomputer installed CPTEC-INPE: 1280 processing nodes and 30,720 cores (2 processors per node and 12-cores for each processor).

tal prediction system – the old version of the environmental system was called as CCATT-BRAMS. The development for the BRAMS is a permanent feature [12].

The model is coded with finite differences, where type-C Arakawa grid is employed for solving the fully compressible non-hydrostatic equations. Other interesting feature is the multiple grid nesting scheme, allowing the model equations to be solved simultaneously on any number of two-way interacting computational meshes of increasing spatial resolution. In the type-C grid, the variables temperature (T), pressure (p), and density (ρ) are defined in the center of a computational cell, and the wind components (u, v, w) are described in center of the cell edge. BRAMS features include an ensemble version of a deep and shallow cumulus scheme based on the mass flux approach The surface model is the LEAF (Land Ecosystem Atmosphere Feedback model), representing the surface-atmosphere interaction.

1.4 Simulation with BRAMS on the Amazon Region

The counter-gradient parameterization presented was codified in the BRAMS version 3.2, the same version used in Barbosa's studies [1]. The simulation is compared with the measurements obtained in the LBA experiment.

The simulation domain embraces the North part of Brazil – see Figure 1.1. The LBA observations are collected inside of the red box (left), and the experimental sites are marked with the yellow points (right): Biological reserve Rebio Jaru, and Farm "Nossa senhora Aparecida" (Farm NSA), in the Rondonia state (Brazil).

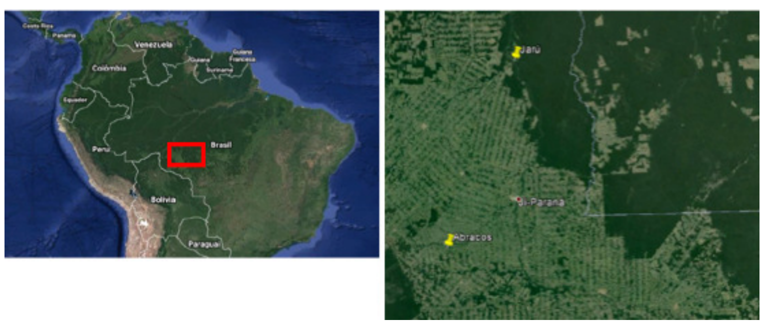

Fig. 1.1 Satellite images: the red box indicates the region of the measurements, and the yellow points indicate the location for the Rebio Jaru and Abracos LBA's stations.

Rebio Jaru (RJ): located at 100 km North to the Ji-Paraná city. This area is part of the rain forest. There is a tower 60 m high, installed at the end of the year 1998 placed at $10°04'42"$S and $61°56'01"$W.

Farm Nossa senhora Aparecida (RA) – site ABRACOS (Anglo Brazilian Amazonian Climate Observation Study): located at 50 km west direction from the Ji-

Paraná city. The site characterizes a deforestation area, and from 1991 it has a pasture covering the surface. The farm has a tower placed at 10°45"S and 62°22"W.

BRAMS was initiated with data from ECMWF re-analysis. The meteorological variables in the latter data set are: temperature, moisture, geopotential, zonal and meridional winds, with space resolution of 2.5×2.5 degrees. The LBA data are also merged to the re-analysis for providing initial and boundary conditions. The simulation covers the period without rainfall. The first day for the simulation started at 00UTC February 10th up to 12th, 1999, performing 48 hours of simulation.

BRAMS was configured with 194 and 100 mesh points for Longitude and Latitude, respectively. The horizontal resolution is 20 km over a stereograph polar grid, with center at Latitude 10S and Longitude 61W. For vertical direction, 40 mesh points were defined, with finer resolution close to the surface. Time discretization $\Delta t = 30$ seconds.

The boundary layer height h is determined by using different approaches depending on the stability condition. For neutral/stable conditions, the formulation presented by Zilitinkevich is applied [22]:

$$h = B_v u_*^{3/2} \tag{1.15}$$

where $B_v = 2.4 \times 10^3 \ \mathrm{m}^{-1/2}\,\mathrm{s}^{3/2}$. Under convective conditions, the approach suggested by Vogelezang and Holtslag [20] is employed:

$$Ri_g = \frac{(g/\theta_{v_s})\,(\theta_{v_h} - \theta_{v_s})\,(h - z_s)}{(u_h - u_s)^2 + (v_h - v_s)^2} \tag{1.16}$$

being $Ri_g = 0.4$ the critical Richardson number, and $z_s = 0.1h$ the reference value to express the values of the horizontal wind components and temperature.

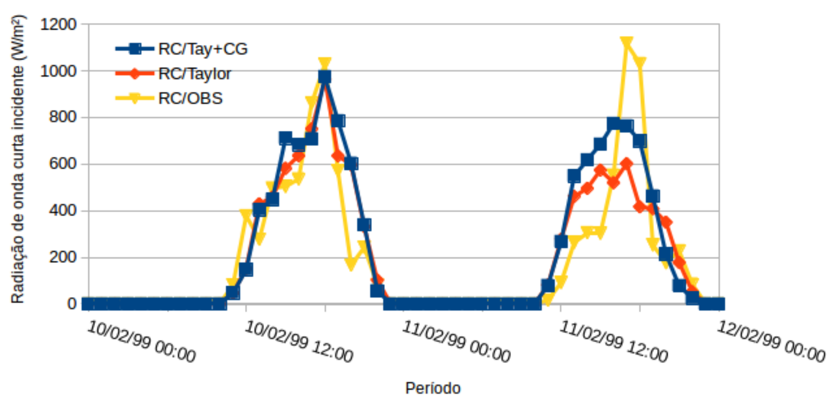

Fig. 1.2 Short wave radiation for Rebio Jaru station: Taylor's theory (Taylor), Taylor + Counter-Gradient (Taylor+CG), and observations.

Figure 1.2 shows the short wave radiation for the Taylor approach alone, the same simulation with counter-gradient term, and observations, considering two days of simulation for the Rebio Jaru experimental site. Figure 1.3 displays the vertical profiles for the potential temperature for different parameterizations for turbulence at the end of the simulation. The comparison with the observation shows similar results for all turbulent schemes.

Two snapshots for the wind field over the simulated region are shown in Figure 1.4. It is important to consider the wind influence, just to understand if the atmospheric dynamics response is due to the surface representation or an effect associated to the wind drag. During the day 10/Feb/1999 at 00 UTC (Fig. 4a), sites RJ and RA are under forest influence. For the day 11/Feb/1999 at 00 UTC (Fig. 4b), the sites have influence from the pasture covering.

1.5 Final Remarks

The paper describes a formulation for the counter-gradient term, where the Taylor's theory was applied. According with Figure 1.3, the simulation results were similar for all parameterizations used. However, the Smagorinsky's scheme requires the calculation of the vertical/horizontal deformation tensors for each grid point and the Brunt-Vaisäla frequency (depending on the temperature vertical gradient), and the Mellor-Yamada's method introduces more 12 new additional partial differential equations and parameterizations for the third order Reynolds tensors. Therefore, both latter approaches has a higher computational effort than Taylor's schemes.

With addition of the new term, the Taylor's parameterization can also simulate a counter-gradient flow, and the described parameterization is already codified to the BRAMS version 5.2 [12].

Considering the radiation for long (not shown) and short waves the counter-gradient approach had a slightly better representation [21]. But, more simulations are needed in order to have a definitive conclusion.

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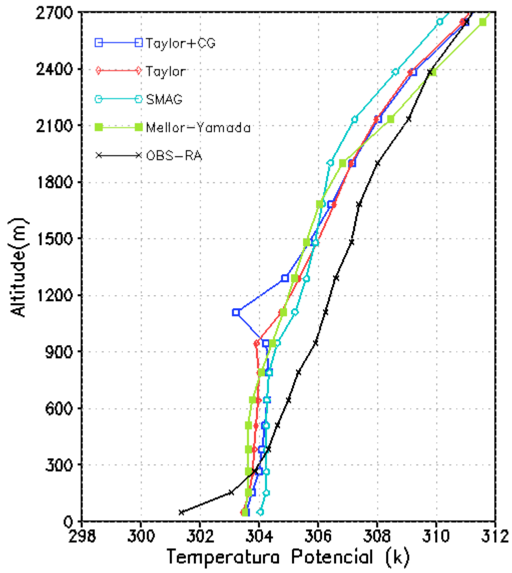
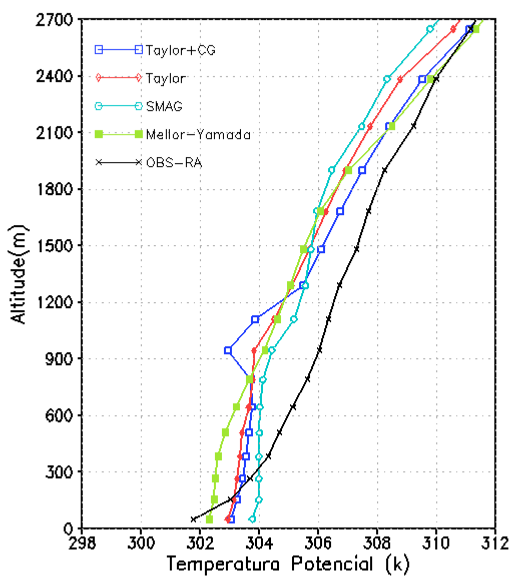
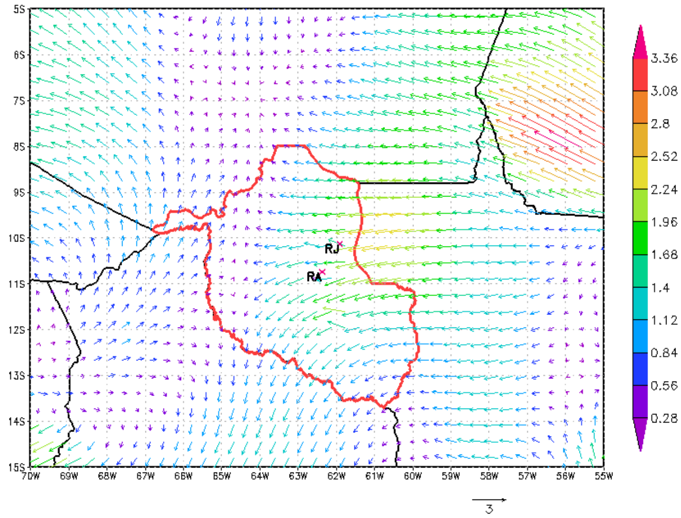


(a)

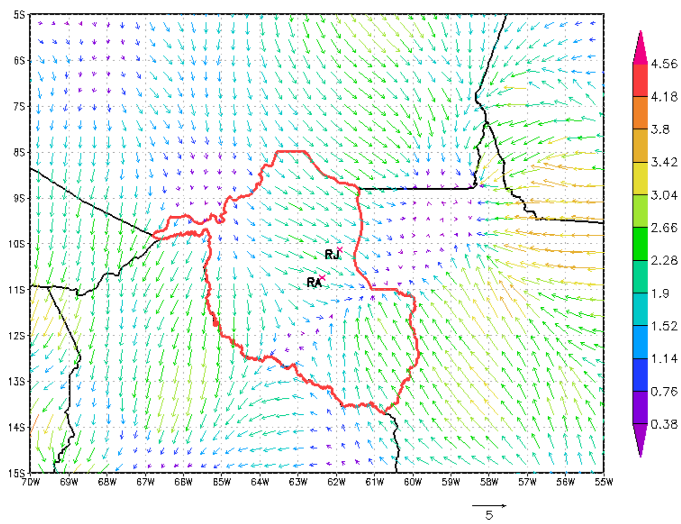


(b)

Fig. 1.3 Vertical potential temperature profiles for Taylor's theory (Taylor), Taylor + Counter-Gradient (Taylor+CG), Smagorinsky (SMAG), Mellor-Yamada, radiosonde data (OBS), day 12/Feb/1999 at 00UTC: (a) ABRACOS, (b) Rebio Jaru.



(a)



(b)

Fig. 1.4 Wind field from the BRAMS (Taylor+CG): (a) day 10/Feb/1999 at 00 UTC, (b) day 11/Feb/1999 at 00 UTC.

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