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A quasi-experimental coastal region eddy diffusivity applied in the APUGRID model

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Abstract. In this study, Taylor statistical diffusion theory and sonic anemometer measurements collected at 11 levels on a 140-m high tower located at a coastal region in southeastern Brazil have been employed to obtain quasi-empirical convective eddy diffusivity parameterizations in a planetary boundary layer (PBL). The derived algebraic formulations expressing the eddy diffusivities were introduced into an Eulerian dispersion model and validated with Copenhagen tracer experiments. The employed Eulerian model is based on the numerical solution of the diffusion-advection equation by the Fractional Step/Locally One-Dimensional (LOD) methods. Moreover, the semi-Lagrangian cubic-spline technique and Crank-Nicholson implicit scheme are considered to solve the advection and diffusive terms. The numerical simulation results indicate that the new approach, based on these quasi-experimental eddy diffusivities, is able to reproduce the Copenhagen concentration data. Therefore, the new turbulent dispersion parameterization can be applied in air pollution models.

1 Introduction

Eulerian models are powerful tools to study and investigate the air pollution dispersion in the planetary boundary layer (PBL) (Hanna, 1982; Tirabassi, 2009; Zannetti, 2013). These models are based in the solution of the classical advection-diffusion equation, containing the turbulent eddy diffusivities, which provide the simulated contaminant concentration data (Batchelor, 1949; Pasquill and Smith, 1983).

$$\frac{\partial \overline{C}}{\partial t} + \overline{u}\frac{\partial \overline{C}}{\partial x} + \overline{v}\frac{\partial \overline{C}}{\partial y} + \overline{w}\frac{\partial \overline{C}}{\partial z} = -\frac{\partial \overline{u'C'}}{\partial x} - \frac{\partial \overline{v'C'}}{\partial y} - \frac{\partial \overline{w'C'}}{\partial z} + S \tag{1}$$

where C is the concentration and S a source term. These Eulerian models describe the concentration turbulent fluxes as the gradient of the mean concentration employing the eddy diffusivities (K-theory):

$$\overline{u'C'} = -K_x\frac{\partial \overline{C}}{\partial x} \qquad \overline{v'C'} = -K_y\frac{\partial \overline{C}}{\partial y} \qquad \overline{w'C'} = -K_z\frac{\partial \overline{C}}{\partial z} \tag{2}$$

where K_x, K_y, K_z are the eddy diffusivities in the x, y, z directions and $\overline{u}$, $\overline{v}$, $\overline{w}$ represent the longitudinal, lateral and vertical mean wind components, respectively. Thus, Eq. 1 can be written in the form:

$$\frac{\partial \overline{C}}{\partial t} + \overline{u}\frac{\partial \overline{C}}{\partial x} + \overline{v}\frac{\partial \overline{c}}{\partial y} + \overline{w}\frac{\partial \overline{C}}{\partial z} = \frac{\partial}{\partial x}\left(K_x \frac{\partial \overline{c}}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_y \frac{\partial \overline{c}}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_z \frac{\partial \overline{c}}{\partial z}\right) + S \tag{3}$$

From the numerical point of view, to solve the Eq. 3 it is required to provide the wind and turbulence physical description. For the turbulent diffusion it is needed to specify K_x, K_y and K_z. These turbulent parameters with dimensions of length times velocity, therefore describe the eddy ~~dimension~~ size and eddy velocity (Panofsky and Dutton, 1984).

Most of the eddy diffusivities employed in current operational dispersion models are based on PBL similarity theories (Leelőssy et al., 2014). However, a better description of the turbulent properties, associated with eddy diffusivities, is based on direct measurements of wind data with high vertical resolution (Martins et al., 2018).

~~In the literature, different experimental K parameterizations have been proposed to be employed in the Eq. (3) to simulate the passive scalars dispersion in the PBL. Such parameterizations, frequently, are obtained from micrometeorological measurements in the P~~ ~~A better description of the turbulent properties, associated with eddy diffusivities, is based in turbulent wind data with high vertical resolution. In the present study we use eddy diffusivities that were derived from the observations of the turbulent wind components (u, v, w), in a convective PBL, at a coastal site.~~

The coastal internal boundary layers (CIBL) are generated by differences in surface temperature and aerodynamic roughness occurring between land and water atmospheric environments. Considering that a large number of power plants and industrial complexes and hence polluting installations are constructed in coastal regions it is necessary to obtain CIBL turbulent parameters that are employed in dispersion models to describe the coastal air pollution. The growing interest in the dispersion issues regarding pollutants emission in coastal areas demands the knowledge of the turbulent structure of the planetary boundary layer in this region. However, the characteristics of the turbulence in these boundary layers vary complexly in space and time due to the sudden changes in the surface characteristics, as heat flux and roughness, in the sea-land interface. In the occurrence of sea-breeze, the stably stratified air mass over the water reaches the coast and starts to be heated by the land surface. Thus, a convective boundary rises from the surface developing a Thermal Internal Boundary Layer (TIBL) that increases in height as it advances over the land. The TIBL is topped by a stably stratified inversion layer that affects the atmospheric diffusion in coastal regions. Therefore, to improve the response of the dispersion models is necessary to provide a truthful description of the turbulence through the TIBL. In this sense, several observational experiments are performed using airborne, tethered balloons and fixed mast measurements techniques (Smedman and Hoegstroem, 1983; Ogawa and Ohara, 1985; Durand et al., 1989; Shao et al., 1991). Wind-tunnel experiments and numerical simulations are found in Hara et al. (2009)

In this present study, we use eddy diffusivities that were derived from the observations of the turbulent wind components (u, v, w) in a convective CIBL to simulate the dispersion of contaminant released from an elevated continuous point source in a coastal region.

The turbulent observations were performed at a 140 m micrometeorological tower positioned 240 m north of a natural gas power plant and 4 km southwest of the ocean coastal environment in the city of Linhares (southeastern Brazil). The turbulent wind data were obtained from high frequency measurements (10 Hz) accomplished by tridimensional sonic anemometers at heights of 1, 2, 5, 9, 20, 37, 56, 75, 94, 113 and 132 m (Martins et al., 2018). Therefore, the study of Martins et al. (2018) employs these measurements, the turbulent energy spectra and some few mathematical relations to determine turbulent dispersion parameters (Taylor Statistical diffusion Theory, Degrazia et al. (2000, 2001)).

~~These turbulent wind data were obtained from high frequency measurements (10Hz) accomplished by tridimensional sonic anemometers at heights of 1, 2, 5, 9, 20, 37, 56, 75, 94, 113 and 132 m (Martins et al., 2018). The $K_{x,y,z}$ turbulent parameters were calculated from these turbulent wind data utilizing the Taylor statistical diffusion theory (Degrazia et al., 2000, 2001).~~

Differently, of previous studies in which the vertical profiles of turbulent parameters have been calculated using surface observations to throughout similarity-based relationship, our eddy diffusivities were locally calculated from the detailed measurements accomplished along the entire vertical extension occupied by the surface internal boundary layer. As a consequence, they can be called quasi-experimental eddy diffusivities. The aim of this work is to obtain algebraic formulation from the fitting curves, that reproduce the observed vertical profile of these quasi-experimental eddy diffusivities. As a test and to evaluate the quasi-experimental eddy diffusivities for a convective CIBL we substitute these turbulent diffusion parameters into Eq. 3 to simulate the contaminant concentration originated from an elevated continuous point source in a coastal environment. The simulated concentrations are compared to those measured in the Copenhagen diffusion experiments.

~~From this analysis the vertical profiles of these quasi-empirical determined eddy diffusivities were obtained by Martins et al. (2018). The aim of this study is to obtain algebraic formulations, from the fitting curves, that reproduce the observed vertical profile of these quasi-experimental eddy diffusivities. An additional aim is to employ these algebraic formulations for the eddy diffusivities into Eq. 3 to simulate the contaminant concentration released from a continuous point source. The simulated concentrations are compared with those measured in the Copenhagen diffusion experiment. Therefore, the novelty in this work is to use coastal eddy diffusivities in a Eulerian numerical model, called APUGRID (Rizza et al., 2003; Rizza et al., 2006), to simulate the contaminant observed concentration.~~

From the point of view of originality and novelty the present development, from some asymptotic equations and detailed turbulent spectral observations of the surface coastal internal boundary layer, provides a general methodology for obtaining algebraic expressions that reliably represent the eddy diffusivities in the coastal internal boundary layer.

2 Eulerian grid-dispersion model

In this section to simulate the contaminant concentrations using Eq. 3, we present the Eulerian grid-dispersion model proposed by Rizza et al. (2003), so-called APUGRID. The APUGRID model employs a Fractional Step/Locally One-Dimensional (LOD) methods (Yanenko, 1971; McRae et al., 1982; Mařcuk, 1984) to solve the diffusion-advection equation. In the LOD numerical method, Eq. 3 is separated into time-dependent equations, each one locally one-dimensional (LOD)(Yanenko, 1971; Rizza et al., 2003; Yordanov et al., 2006). As a consequence:

$$\frac{\partial \overline{C}}{\partial t} = \Lambda_x \overline{C} + \Lambda_y \overline{C} + \Lambda_z \overline{C} \tag{4}$$

where $\Lambda_x = -\overline{u}\frac{\partial}{\partial x} + \frac{\partial}{\partial x}\left(K_x\frac{\partial}{\partial x}\right), \Lambda_y = -\overline{v}\frac{\partial}{\partial y} + \frac{\partial}{\partial y}\left(K_y\frac{\partial}{\partial y}\right)$ and $\Lambda_z = -\overline{w}\frac{\partial}{\partial z} + \frac{\partial}{\partial z}\left(K_z\frac{\partial}{\partial z}\right)$.

Employing Crank-Nicholson time integration (McRae et al., 1982; Yordanov et al., 2006; Rizza et al., 2010) we obtain that:

$$\overline{C}^{n+1} = \prod_{j=1}^{3}\left[I - \frac{\Delta t}{2}\right]^{-1}\left[I + \frac{\Delta t}{2}\Lambda_j\right]^{-1}\overline{C}^{n} \tag{5}$$

with I being the unity matrix and Δt the time step. The second order accuracy can be obtained following Rizza et al. (2010) by:

$$\overline{C}^{n} = \prod_{i=1}^{3}[A_i F D_i]\overline{C}^{n+1} \qquad \overline{C}^{n+1} = \prod_{i=1}^{3}[D_i A_i F]\overline{C}^{n} \tag{6}$$

In Eq. 6 $A_i = \overline{u_i}\frac{\partial}{\partial i}$, $D_i = \frac{\partial}{\partial i}\left(K_i\frac{\partial}{\partial i}\right)$ with $i = x, y, z$ and F representing the filter operation.

The advection terms were solved employing a quasi-Lagrangian cubic-spline technique (Long and Pepper, 1981), and the numerical model stability is carried out by Courant-Friedrichs-Lewy condition (cfl):

$$cfl = \bar{U}\frac{\Delta t}{\Delta x} \tag{7}$$

being $\bar{U}$ the mean wind speed, Δx the grid spacing with the stability condition $cfl \leqslant 1$ satisfied.

In order to calculate the concentration advective transport by the mean wind speed, we use the wind speed profile described by the following similarity law (Berkowicz et al., 1986) :

$$\bar{U}(z) = (u_*/\kappa)log(z/z_0) - \psi_m(z/L) + \psi_m(z_0/L) \tag{8}$$

Eq. 8 is valid for $z < z_b$, where $z_b = 0.1z_i$, where z_i is the convective boundary layer height, u_* is the friction velocity, κ is the von Kármán constant and z_0 is the surface roughness. ψ_m is a stability function defined as:

$$\psi_m = 2ln\left[\frac{1+A}{2}\right] + ln\left[\frac{1+A^2}{2}\right] - 2tan^{-1}(A) + \frac{\pi}{2} \tag{9}$$

with $A = (1-16z/L)^{1/4}$ and L being the Obukhov length. For $z > z_b$ the wind profile is the wind speed at $z = z_b$

2.0.1 QUASI-EMPIRICAL EDDY DIFFUSIVITIES MODELS: EVALUATION IN APUGRID

The eddy diffusivities can be found by the following relationship:

$$K_i = \sigma_i^2 T_{Li} \tag{10}$$

where σ_i^2 is the turbulent velocity variance quantifying the turbulence mixing degree and T_{Li} is the decorrelation local time scale that takes into account the characteristic time in which a fluid control volume maintains its motion in a particular direction (Hinze, 1975).

To obtain the Lagrangian K_i from the Eulerian measurements the relation between the Lagrangian T_{Li} and the Eulerian decorrelation T_{Ei} time scales are employed (Hanna, 1981; Degrazia and Anfossi, 1998):

$$\beta_i = \frac{T_{Li}}{T_{Ei}} = \frac{0.55\overline{U}}{\sigma_i} \tag{11}$$

where

$$T_{Ei} = \int_0^\infty \frac{1}{\sigma_i^2}\left[\overline{u_i' + u_i'(t+\tau)}\right] d\tau. \tag{12}$$

where $u_i{}'$ is the wind speed turbulent fluctuation and τ is the temporal lag. Recently, Martins et al. (2018) used Eqs. 10, 11 and 12 to derive experimental vertical profiles for K_x, K_y and K_z. To obtain such profiles, 1-h observation wind velocity time series intervals are tested for quality control requirements. Unstable conditions were considered as daytime time series which $-150 \leq$L< 0. From a total of four months of observations (August - November 2016), 343 1-h unstable intervals are retained. The variances and time scales profiles used to estimate the K_i vertical profiles are obtained averaging the whole 343 individuals profiles.

From these set of eddy diffusivities vertical profiles we use the best fit curves approach to obtain the following simple algebraic formulations:

$$K_x(z) = 7.83 \times 10^1 - 6.42 \times 10^1 z \tag{13}$$

$$K_y(z) = 7.35 \times 10^1 log(z) + 4.25z - 3.73 \times 10^{-2} z^2 \tag{14}$$

$$K_z(z) = 8.34 \times 10^{-1} z \tag{15}$$

In order to test these eddy diffusivities, we perform contaminant concentration simulations and compare the simulated data with the Copenhagen tracer dispersion experiments (Gryning and Lyck, 1984).

~~In these experiments the contaminant was released at 115 m above the ground~~

The tracer sulphur hexa fluoride (SF6) used in the Copenhagen dispersion experiments, was released at a height of 115 m from the TV tower in the Gladsaxe (Copenhagen) and the ground level contaminant concentrations were measured at 3 arcs located in the distance of 2000 to 6000 m from the elevated continuous point source.

The experiments site is limited by the Øresund coast, approximately 7 km east of the TV tower. Therefore, the turbulent effect acting on the tracer dispersion are characteristic of CIBL. The width of Øresund strait, the water portion separating Denmark and Sweden, is about 20 Km. On the western side of Øresund lies Copenhagen with its urban area. This area has high surface roughness due to the urban character. Thusly, a turbulent environment occurring in a region with relatively cold water and warm land surface. As a consequence, the turbulent structure acting on the tracer dispersion can be considered as one present in the coastal inner boundary layer.

~~Furthermore, Copenhagen data set provides wind and turbulence data at 10 and 115 m.~~ Meteorological parameters for the Copenhagen runs are shown in Table A1, being $\bar{U}_{115m}$ and $\bar{U}_{10m}$ the mean wind velocity measured at 115 m and 10 m, respectively, σ_w the vertical wind velocity variance and z_i the convective boundary layer depth. Although some Copenhagen dispersion experiments occurred in conditions quasi-neutral the L parameter was negative. The presence of a slightly convective stratified boundary layer can be seen in u and v turbulent energy spectra (Kaimal et al., 1972; Martins et al., 2018). In this situation, it can be observed in spectral curves a structure that contains two peaks; one low-frequency peak and one high-frequency peak. This reflects the impact of the larger convective eddies on the turbulent structure (Garratt, 1992).

The choice of the Copenhagen experiment was motivated by the fact that the region in which the experiment occurred is located near the Øresund coast. Therefore, we expect that our eddy diffusivities obtained at a coastal site localized in south-eastern Brazil are adequate to reproduce contaminant data in coastal regions.

In Table A2, the predicted crosswind-integrated concentrations obtained from the APUGRID model are compared, with Copenhagen diffusion experiments, over the different distances of the release point source. The performance of the APUGRID model employing the quasi-experimental eddy diffusivities as given by Eqs. 13, 14 and 15 to simulate the Copenhagen observation data can also be evaluated by analyzing the results shown in Table A3 and Figure A1.

Table A3 exhibits Hanna's statistical indices, which are commonly used to calibrate air pollution dispersion models. Such indices are defined as:

$$\text{normalized mean square error (NMSE)} = \frac{\overline{(C_o - C_p)^2}}{\overline{C_o C_p}} \tag{16}$$

$$\text{correlation coefficient (R)} = \frac{\left(C_o - \bar{C_o}\right)\left(C_p - \bar{C_p}\right)}{\sigma_o \sigma_p} \tag{17}$$

$$\text{fractional bias (FB)} = \frac{\left(\bar{C_o} - \bar{C_p}\right)}{0.5\left(\bar{C_o} + \bar{C_p}\right)} \tag{18}$$

$$\text{fractional standard deviations (FS)} = \frac{\sigma_o - \sigma_p}{0.5\left(\sigma_o \sigma_p\right)} \tag{19}$$

where C_p is the predict concentration, C_o is the observed concentration, σ_p is the predict standard deviation, σ_o is the observed standard deviation, and the overbar represents an averaged value.

The observed and predicted scatter diagram of concentrations in Fig. A1 demonstrates that the simulated concentration reproduces fairly well the measured concentration data. Furthermore, the statistical analysis of the results (Table A3) shows a good agreement between the results of the proposed approach with the experimental ones. The indices are found within an acceptable interval with NMSE (normalized mean square error), FB (fractional bias) and FS (fractional standard deviation) close to zero and R (correlation coefficient) near to one.

Thus, the present development based on an analysis of high resolution turbulence data from an elevated micrometeorological tower provides suitable eddy diffusivities that describe the turbulent transport patterns in a CIBL.

3 Conclusions

The Eulerian operational air dispersion models that simulate contaminant observed concentration data need to incorporate into their formulation the characteristics of the PBL turbulent diffusion process. To accomplish this parameterization they use turbulent transport terms known as eddy diffusivities. These turbulent parameters represent approximate quantities which intend to reproduce the complex natural dispersive effects. In this study, algebraic expressions for quasi-experimental convective eddy diffusivities for a coastal site are derived. The derivation employed the Taylor statistical diffusion theory and sonic anemometer observations with high vertical resolution in a CIBL.

The complexity of the subject does not allow a direct confrontation between experiment and model. However utilizing the APUGRID Eulerian dispersion model and a concentration data set of dispersion experiments performed in a CIBL, the derived eddy diffusivities have been tested and validated. The comparison results show that there is a fairly well agreement between simulated and measured concentrations. As a consequence, the results provided in this investigation are encouraging. Thus, the new eddy diffusivities for a coastal site may be suitable for applications in regulatory air pollution modeling.

Table A1. Meteorological conditions during the Copenhagen dispersion experiments.

Exp.	$\bar{U}_{115m}(ms^{-1})$	$\bar{U}_{10m}(ms^{-1})$	$u_*(ms^{-1})$	$L(m)$	$\sigma_w(ms^{-1})$	$z_i(m)$
1	3.4	2.1	0.37	-46	0.83	1980
2	10.6	4.9	0.74	-384	1.07	1920
3	5.0	2.4	0.39	-108	0.68	1120
4	4.6	2.5	0.39	-173	0.47	390
5	6.7	3.1	0.46	-577	0.71	820
6	13.0	7.2	1.07	-569	1.33	1300
7	7.6	4.1	0.65	-136	0.87	1850
8	9.4	4.2	0.70	-72	0.72	810
9	10.5	5.1	0.77	-382	0.98	2090

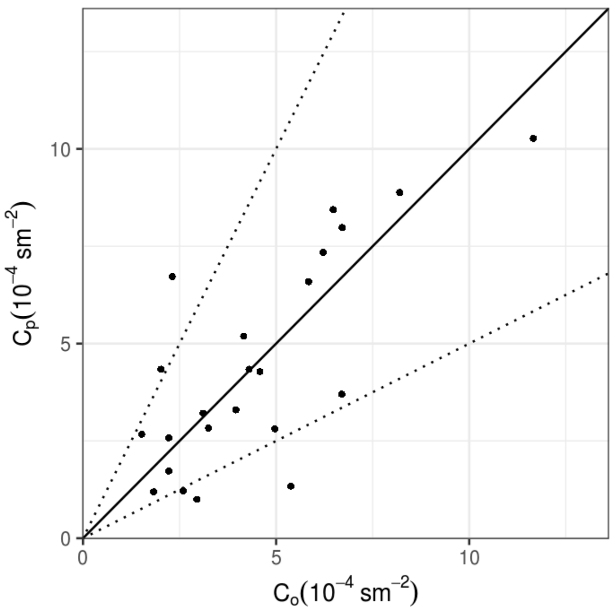

Figure A1. Scatter diagram between Copenhagen observed (C_o/Q) and predict (C_p/Q) ground-level cross wind integrated concentration normalized by the emission rate.

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Table A2. Observed C_o and predicted C_p crosswind-integrated concentrations normalized by the emission rate (Q) for Copenhagen experiments.

Exp.	Sampler distance (m)	Q (gs^{-1})	C_o/Q $(10^4 sm^{-2})$	C_p/Q $(10^4 sm^{-2})$
1	1900	3.2	6.48	8.44
1	3700	3.2	2.31	6.72
2	2100	3.2	5.38	1.34
2	4200	3.2	2.95	1.00
3	1900	3.2	8.20	8.88
3	3700	3.2	6.22	7.34
3	5400	3.2	4.30	4.34
4	4000	2.3	11.66	10.27
5	2100	3.2	6.71	7.98
5	4200	3.2	5.84	6.59
5	6100	3.2	4.96	2.81
6	2000	3.1	3.96	3.30
6	4200	3.1	2.22	2.58
6	5900	3.1	1.83	1.19
7	2000	2.4	6.70	3.70
7	4100	2.4	3.25	2.83
7	5300	2.4	2.22	1.73
8	1900	3.0	4.16	5.19
8	3600	3.0	2.02	4.34
8	5300	3.0	1.52	2.67
9	2100	3.3	4.58	4.28
9	4200	3.3	3.11	3.21
9	6000	3.3	2.59	1.22

Table A3. Statistic evaluation of the APUGRID model employing the quasi-experimental eddy diffusivities.

NMSE	R	FB	FS
0.10	0.82	-0.07	-0.006

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