https://doi.org/10.5194/angeo-2019-85
Preprint. Discussion started: 28 June 2019

Annales Geophysicae
Discussions
Open Access

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

Silvana Maldaner [1], Michel Stefanello [1], Luis Gustavo N. Martins [1], Gervásio Annes Degrazia [1], Umberto Rizza [2], Débora Regina Roberti [1], Franciano S. Puhales [1], and Otávio C. Acevedo [1]

[1]Universidade Federal de Santa Maria, Santa Maria, Brazil
[2]Institute of Atmospheric Sciences and Climate - National Research Council, Italy

Correspondence: Gervásio Annes Degrazia (gervasiodegrazia@gmail.com)

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).

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

These Eulerian models describe the concentration turbulent fluxes as the gradient of the mean concentration employing the eddy diffusivities (K-theory):

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

https://doi.org/10.5194/angeo-2019-85
Preprint. Discussion started: 28 June 2019

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 describe the eddy dimension and velocity (Panofsky, 1984). In the literature, different experimental K parameterizations have been proposed to be employed in the simulation of passive scalars in the PBL. Such parameterizations, frequently, are obtained from micrometeorological measurements in the PBL. Therefore, 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. 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). 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), to simulate the contaminant observed concentration.

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 numerical method is based on the solution of the diffusion-advection equation by the Fractional Step/Locally One-Dimensional (LOD) methods (Yanenko, 1971; McRae et al.; Mařcuk, 1984). 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 $\Lambda_z = -\overline{w}\frac{\partial}{\partial z} + \frac{\partial}{\partial z}\left(K_z \frac{\partial}{\partial z}\right)$.

https://doi.org/10.5194/angeo-2019-85
Preprint. Discussion started: 28 June 2019

Annales Geophysicae Discussions
Open Access
EGU

Employing Crank-Nicholson time integration (McRae et al.; Rizza et al., 2010; Yordanov et al., 2006) 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. 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 Jr and Pepper; Rizza et al., 2010) and the numerical model stability is carried out by Courant-Friedrichs-Lewy condition (cfl):

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

with $cfl \leqslant 1$.
In order to calculate the concentration advective transport by the mean wind speed, the logarithmic wind profile is used:

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

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 the Monin-Obukhov length
For $z > z_b$ the wind profile is

$$\overline{U}(z) = \overline{U}(z_b) \tag{10}$$

2.0.1 QUASI-EMPIRICAL EDDY DIFFUSIVITIES MODELS: EVALUATION IN APUGRID

The eddy diffusivities can be found by the following relationship:

$$K_i = \sigma_i^2 T_{Li} \tag{11}$$

https://doi.org/10.5194/angeo-2019-85
Preprint. Discussion started: 28 June 2019

Annales Geophysicae Discussions
Open Access

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:

$$\beta_i = \frac{T_{Li}}{T_{Ei}} = \frac{0.55\overline{U}}{\sigma_i} \tag{12}$$

where

$$T_{Ei} = \int_0^\infty \frac{1}{\sigma_i^2}\left[\overline{u'(t)+u'(t+\tau)}\right] d\tau. \tag{13}$$

Recently, (Martins et al., 2018) used Eqs. 11, 12 and 13 to derive experimental vertical profiles for K_x, K_y and K_z. From these set of eddy diffusivities vertical profiles we use the best fit curves approach to obtain the following simple algebraic formulations:

$$K_x(z) = 7.83\times10^1 - 6.42\times10^1 z \tag{14}$$

$$K_y(z) = 7.35\times10^1 log(z) + 4.25z - 3.73\times10^{-2}z^2 \tag{15}$$

$$K_z(z) = 8.34\times10^{-1}z \tag{16}$$

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).

In these experiments the contaminant was released at 115 m above the ground 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. Furthermore, Copenhagen data set provides wind and turbulence data at 10 and 115 m.

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 contaminate data in coastal regions.

The performance of the APUGRID model employing the quasi-experimental eddy diffusivities as given by Eqs. 14, 15 and 16 to simulate the Copenhagen observation data can be evaluated by analyzing the results shown in Table 1 and Figure 1. Table 1 exhibits Hanna's statistical indices, which are commonly used to calibrate air pollution dispersion models

https://doi.org/10.5194/angeo-2019-85
Preprint. Discussion started: 28 June 2019

The values of these indices and the observed and predicted scatter diagram of concentrations, in Fig. 1 demonstrate that the simulated concentration reproduces fairly well the measured concentration data. The magnitudes of the concentration evaluated statistical parameters (Table 1) 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.

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 convective planetary boundary layer.

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 convective PBL, the newly 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 1. Statistic evaluation of the APUGRID model employing the quasi-experimental eddy diffusivities

NMSE	COR	FB	FS
0.10	0.82	-0.07	-0.006

Acknowledgements. This study has been developed within the context of a research and development project regulated by the Brazilian National Agency for Electric Energy and sponsored by the companies Linhares Geração S.A. and Termelétrica Viana S.A. The study also has been partially supported by Brazilian funding agencies CNPq ,CAPES and FAPERGS.

https://doi.org/10.5194/angeo-2019-85
Preprint. Discussion started: 28 June 2019

Annales Geophysicae
Discussions
Open Access

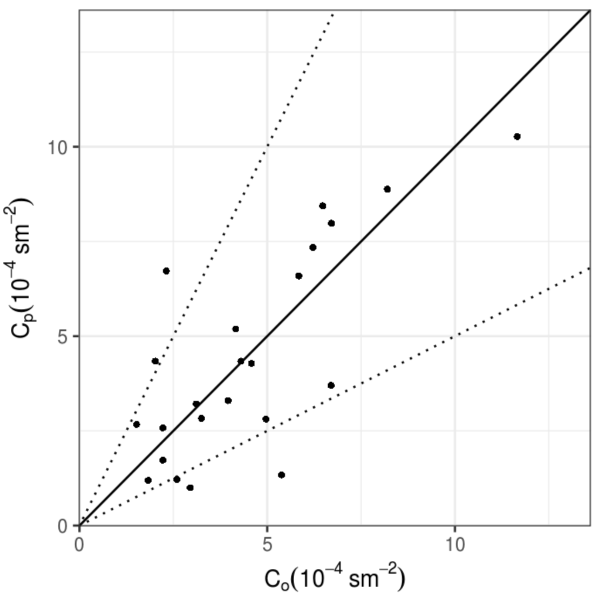

Figure 1. Scatter diagram between Copenhagen observed (Co) and predict (Cp) ground-level cross wind integrated concentration.

References

Batchelor, G. K.: Diffusion in a field of homogeneous turbulence. I. Eulerian analysis, Australian Journal of Chemistry, 2, 437–450, https://doi.org/https://doi.org/10.1071/CH9490437, http://www.publish.csiro.au/ch/CH9490437, 1949.

Degrazia, G., Anfossi, D., Carvalho, J., Mangia, C., Tirabassi, T., and Velho, H. C.: Turbulence parameterisation for PBL dispersion models in all stability conditions, Atmospheric environment, 34, 3575–3583, https://doi.org/https://doi.org/10.1016/S1352-2310(00)00116-3, https://www.sciencedirect.com/science/article/pii/S1352231000001163, 2000.

Degrazia, G. A., Moreira, D. M., and Vilhena, M. T.: Derivation of an eddy diffusivity depending on source distance for vertically inhomogeneous turbulence in a convective boundary layer, Journal of Applied Meteorology, 40, 1233–1240, https://doi.org/https://doi.org/10.1175/1520-0450(2001)040<1233:DOAEDD>2.0.CO;2, https://journals.ametsoc.org/doi/full/10.1175/1520-0450%282001%29040%3C1233%3ADOAEDD%3E2.0.CO%3B2, 2001.

Gryning, S.-E. and Lyck, E.: Atmospheric dispersion from elevated sources in an urban area: comparison between tracer experiments and model calculations, Journal of Climate and Applied Meteorology, 23, 651–660, https://journals.ametsoc.org/doi/abs/10.1175/1520-0450(1984)023%3C0651:ADFESI%3E2.0.CO%3B2.

Hanna, S. R.; BRIGGS, G. A. H. J. R. P.: Handbook on atmospheric diffusion, 1982.

Hinze, J.: Turbulence, vol. 218, McGrawHill, New York, 1975.

Long Jr, P. and Pepper, D.: An examination of some simple numerical schemes for calculating scalar advection, Journal of Applied Meteorology, 20, 146–156, https://journals.ametsoc.org/doi/abs/10.1175/1520-0450(1981)020%3C0146:AEOSSN%3E2.0.CO;2.

Mařcuk, G. I.: Metodi del calcolo numerico, Editori riuniti, Roma, 1984.

https://doi.org/10.5194/angeo-2019-85
Preprint. Discussion started: 28 June 2019

Martins, L. G. N., Degrazia, G. A., Acevedo, O. C., Puhales, F. S., de Oliveira, P. E., Teichrieb, C. A., and da Silva, S. M.: Quasi-Experimental Determination of Turbulent Dispersion Parameters for Different Stability Conditions from a Tall Micrometeorological Tower, Journal of Applied Meteorology and Climatology, 57, 1729–1745, https://doi.org/https://doi.org/10.1175/JAMC-D-17-0269.1, https://journals.ametsoc.org/doi/abs/10.1175/JAMC-D-17-0269.1, 2018.

McRae, G. J., Goodin, W. R., and Seinfeld, J. H.: Numerical solution of the atmospheric diffusion equation for chemically reacting flows, Journal of Computational Physics, 45, 1–42, https://www.sciencedirect.com/science/article/pii/0021999182901012.

Panofsky, H. A.; Dutton, J.: Atmospheric Turbulence: Models and Methods for Engineering Applications, John Wiley Sons, New York, 1984.

Pasquill, F. and Smith, F.: Atmospheric diffusion, John Wiley and Sons, New York, NY 10016, USA, 3 edn., 1983.

Rizza, U., Gioia, G., Mangia, C., and Marra, G. P.: Development of a grid-dispersion model in a large-eddy-simulation generated planetary boundary layer, IL NUOVO CIMENTO, 26, 297–309, https://www.researchgate.net/profile/Umberto_Rizza/publication/260456245_Development_of_a_grid-dispersion_model_in_a_large-eddy-simulation--generated_planetary_boundary_layer/links/02e7e53730d031c5a4000000.pdf, 2003.

Rizza, U., Gioia, G., Lacorata, G., Mangia, C., and Marra, G. P.: Atmospheric Dispersion with a Large-Eddy Simulation:Eulerian and Lagrangian Perspectives, in: Air Pollution and turbulence modelling and aplications, edited by Moreira, D. and Vilhena, M., pp. 237–268, CRC Press, 2010.

Tirabassi, T.: Mathematical Air Pollution Models: Eulerian Modelss, in: Air pollution and turbulence: modeling and applications, edited by Moreira, D, . V. M., pp. 131– 156, CRC Press, 2009.

Yanenko, N. N.: The method of fractional steps, Springer, 1971.

Yordanov, D., Kolarova, M., Rizza, U., Mangia, C., Tirabassi, T., and Syrakov, D.: EVALUATION OF WIND AND TURBULENT PARAMETERISATIONS FOR SHORT RANGE AIR POLLUTION MODELING, Bulgarian Geophysical Journal, 32, 107–123, http://www.niggg.bas.bg/wp-content/uploads/2012/01/BGJ/2006/8_statia.pdf, 2006.

Zannetti, P.: Air pollution modeling: theories, computational methods and available software, Springer Science & Business Media, 2013.