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

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

Reply to Reviewer #2

In this work, the authors incorporate new parameterizations of turbulent diffusivities developed for coastal profiles in Brazil into a pollutant diffusion model. The validation data came from an air pollution experiment developed in a coastal area of Denmark. Only unstable conditions are considered. The theme is original and suitable for the journal.

We thank the reviewer for useful comments and suggestions. Our responses to the comments are given below:

Major comments:

1. Although the original idea of the work is appropriate, the advantage of introducing these profiles in the proposed model is not demonstrated. The authors should first make a brief description of the original way in which there is solved the Eulerian pollutant diffusion equation in the model to understand the advantage of using the profiles developed in Brazil. In addition, the results obtained with the original model and those obtained with the modification of this work should be shown in Figure 1, to observe the improvements introduced.

2. On the other hand, in the introduction there is presented both methodological issues and information on the data used. These topics should be incorporated in the data and methodology section. The introduction should be enriched with a detail of the background that indicates the lack of information or of methodological development that leads to the aim of the work.

In the new version of the manuscript, we follow the reviewer suggestions. Our responses to the comments 1 e 2 are given below:

The Eulerian dispersion models solve the advection-diffusion equation and can employ distinct turbulent parameterizations using different numerical methods. Despite the limitation of the K-models they are used in different atmospheric conditions because the eddy diffusivities describe the turbulent transport in an Eulerian framework. In this case, almost all measurements are Eulerian in character. These Eulerian models generate results that agree with observational data as well as any more complex. The reliability of the K-models depends on the way the eddy diffusivities is determined based on the turbulent structure of the planetary boundary layer (Ulke, 2000).

It is important to note that the Eulerian model APUGRID is already a well developed Eulerian dispersion model (Rizza et al., 2003). In this model is enough to have turbulent parameterizations to obtain simulated contaminant concentrations. In our case, we use detailed turbulent data of coastal internal boundary layers and some equations (from Taylor Statistical diffusion Theory) to obtain quasi-experimental eddy diffusivities.

Therefore, the principal aim of this study is to not establish a comparison between the different eddy diffusivities parameterizations but, specifically to evaluate and test our quasi-experimental coastal eddy diffusivities with experimental concentrations results measured in a CIBL (Copenhagen diffusion experimental). Further, it is difficult to found in the literature coastal observed concentrations that allow the validation of our new coastal eddy diffusivities.

- For the new version of the manuscript we enrich the introduction with this definition of the CIBL:

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 (Ogawa and Ohara, 1985; Durand et al., 1988; Smedman and Högström, 1983; Shao et al. 1991). Wind-tunnel experiments and numerical simulations are found in Hara et al. (2009).

In the new version of the manuscript, two tables have been attached:

Table A1. Meteorological conditions during the Copenhagen dispersion experiments.

Exp.	U_{115m} (ms^{-1})	U_{10m}(ms^{-1})	u_*(ms^{-1})	L(m)	σ_w(ms^{-1})	h(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

Meteorological parameters for the Copenhagen runs are shown in Table A1, being $\mathbf{U_{115m}}$ the mean wind velocity measured at 115 m, $\mathbf{U_{10m}}$ the mean wind velocity measured at 10 m, $\mathbf{u_*}$ the friction velocity, **L** the Obukhov length, $\boldsymbol{\sigma_w}$ the vertical wind velocity variance and **h** the convective boundary layer dept.

Table A3 – Observed and estimated crosswind-integrated concentrations normalized by the emission rate ($\mathbf{C^y/Q}$) for Copenhagen experiment:

Exp.	**Sampler distance (m)**	**Q (gs^{-1})**	**$C^y/Q_{Observed}*10^4$ (sm^{-2})**	**$C^y/Q_{predicted}*10^4$ (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

In Table A3 the results of the predicted cross wind-integrated concentrations for the Copenhagen experiment obtained for the APUGRID model are compared with experimental data.

The aim should be written more clearly.

- For the new version of the manuscript we rewrote the aim more clearly:

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. Therefore, the study of Martins et al., (2018) uses these measurements and some few mathematical relations to determine turbulent dispersion parameters (Taylor Statistical diffusion Theory, Degrazia et al., 2000)

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 taken (accomplished) along the entire vertical extension occupied by the surface internal boundary layer. As a consequence, they can be called quasi-experimental eddy diffusivities. This work aims to obtain algebraic formulation from the fitting curves, that reproduce the observed vertical profile of these quasi-experimental convective 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 experiment.

3. It is not clear from the beginning of the methodological description that only unstable conditions will be considered. Authors should make it explicit.

In the new version of the manuscript, the stability conditions associated with the quasi-experimental eddy diffusivities have been included. Please see the answer above (1 e 2).

Nor is variable C adequately described, since by its units (Fig. 1) I understand that it is a concentration per emission and surface area unit. Is that correct?

Yes, is correct, c^Y represents the ground-level cross wind integrated concentration normalized by the emission rate ($\bar{C}=\frac{c^y}{Q}$ (s m^{-2})).

It is also not known if the pollutant diffused is a gas (which?) or it is particulate matter.

In the new version of the manuscript we have been added the following paragraph:

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.

4. The authors should better describe how they chose the Copenhagen experiment cases for the model validation.

In the new version of the manuscript we have been added the following paragraphs:

The Copenhagen experimental site is limited by the Øresund coast, approximately 7 km east of the TV tower. Therefore, the turbulent effect acting on the tracer dispersion is an environment of the convective internal boundary layer (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, this represents 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.

Our quasi-experimental convective eddy diffusivities for a coastal site were derived from the turbulent observations originated by differences in surface temperature and aerodynamic roughness occurring between land and water atmospheric environments. The important characteristic here is the fact that there is a CIBL in the tropical region (Brazil) and also in mid-latitude (Copenhagen)

For example, did they consider ranges of Instabilities? It is measured by which variable? In addition, which were the atmospheric boundary layer characteristics in these cases? Were these characteristics decisive in the choice of cases?

Yes, the stability parameter used in our study was the Monin Obukhov length.

In the new version of the manuscript we have been added the following paragraph:

To derive our quasi-experimental convective eddy diffusivities profiles, 1-h observation wind velocity time series intervals are tested for quality control requirements. Unstable conditions were considered as daytime time series which $-150 \leq L < 0$, where *L* is Obukhov length. From a total of four months of observations (August–November 2016), 343 1-h unstable intervals are retained. The variances and time scale profiles used to estimate the K_i vertical profiles are obtained averaging the whole 343 individuals profiles.

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).

Even though the Linhares-ES CIBL data has been collected in the different latitude of the Copenhagen data the mean wind speed vertical profile as can be seen in Fig.1 also presents in high levels velocity magnitudes of the order of 10 m/s.

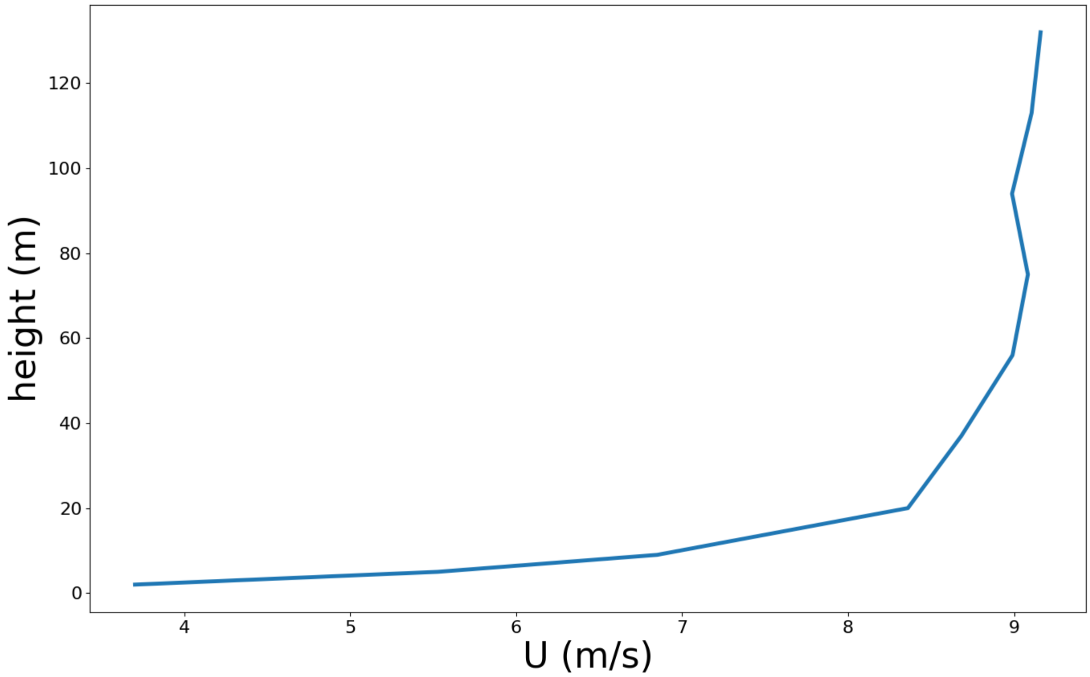

Fig.1: Mean wind speed vertical profile from CIBL Linhares-ES data.

Minor comments: 1.The years in citations and in the bibliography mentioned at lines 44,50, 55 and 86 are missing. In 26 the correct citation is Panofsky and Dutton (1984).

In the new version, we corrected the citations.

2. Describe what is S in Eq. 1.

In the new version, we described the variable: S represents a source term.

3. In line 43, APUGRID is a model or a numerical method?

Is a numerical dispersion model (Rizza et al., 2003; Yordanov, et al., 2006).

4. In Eq. 7, u is a mean or an instantaneous value?

In Eq. 7 u is the mean wind speed velocity. We corrected in the new version of the manuscript

5. In Eq. 8, which is the difference between u ÌˇE y U ÌˇE?

In the new version of the manuscript we correct to uniform the nomenclature: $\bar{u}$ represents the longitudinal wind velocity component, while $\bar{U}$ the mean wind speed velocity.

6. Add a citation for Eq. 12. 8.

In equation 7 we added the following reference:

DEGRAZIA, Gervasio; ANFOSSI, Domenico. Estimation of the Kolmogorov constant C0 from classical statistical diffusion theory. **Atmospheric Environment**, v. 32, n. 20, p. 3611-3614, 1998.

HANNA, Steven R. Lagrangian and Eulerian time-scale relations in the daytime boundary layer. **Journal of Applied Meteorology**, v. 20, n. 3, p. 242-249, 1981.

Variables units are missing in Table A1.

These "variables" represent statistical indices. In the new version of the manuscript, we explain these variables. Please see the answer to the next question.

In addition, variable COR is used in the table and R (line 99) is used in the text. Please, unify nomenclature. I suggest adding in the Table Caption the definition of the variables.

We agree with the reviewer. In the new version of the manuscript, we add the statistic indices defined in the following way:

NMSE (normalized mean square error) = $\frac{\overline{(c_o - c_p)^2}}{\overline{c_o c_p}}$

R (correlation coefficient) = $\frac{(c_o - \bar{c}_o)(c_p - \bar{c}_p)}{(\sigma_o \sigma_p)}$

FB (fractional bias) = $\frac{(\bar{c}_o - \bar{c}_p)}{0.5(\bar{c}_o + \bar{c}_p)}$

FS (fractional standard deviations) = $\frac{\sigma_o - \sigma_p}{0.5(\sigma_o + \sigma_p)}$

being c_p the predict concentration, c_o the observed concentration, σ_p the predict standard deviation, σ_o the observed standard deviation, and the overbar represent an averaged value.

REFERENCES:

OGAWA, Yasushi; OHARA, Toshima. The turbulent structure of the internal boundary layer near the shore. Boundary-Layer Meteorology, v. 31, n. 4, p. 369-384, 1985.

DURAND, Pierre; DRUILHET, Aime; BRIERE, Serge. A sea-land transition observed during the COAST experiment. Journal of the atmospheric sciences, v. 46, n. 1, p. 96-116, 1989.

GARRATT, J. et al. The atmospheric boundary layer. cambridge atmospheric and space science series. Cambridge University Press, Cambridge, v. 416, p. 444, 1992.

Goulart, A. G. O., Lazo, M. J., Suarez, J. M. S., & Moreira, D. M. (2017). Fractional derivative models for atmospheric dispersion of pollutants. *Physica A: Statistical Mechanics and its Applications*, *477*, 9-19.

HARA, Tomohiro et al. Wind-tunnel and numerical simulations of the coastal thermal internal boundary layer. Boundary-layer meteorology, v. 130, n. 3, p. 365-381, 2009.

Kaimal JC, Finnigan JJ. 1994. Atmospheric Boundary Layer Flows. Oxford University Press. 289 pp.

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, 2018.

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

SMEDMAN, Ann-Sofi; HOEGSTROEM, Ulf. Turbulent characteristics of a shallow convective internal boundary layer. Boundary-Layer Meteorology, v. 25, n. 3, p. 271-287, 1983.

SHAO, Yaping; HACKER, Jörg M.; SCHWERDTFEGER, Peter. The structure of turbulence in a coastal atmospheric boundary layer. Quarterly Journal of the Royal Meteorological Society, v. 117, n. 502, p. 1299-1324, 1991.

Ulke, A. G. (2000). New turbulent parameterization for a dispersion model in the atmospheric boundary layer. *Atmospheric Environment*, *34*(7), 1029-1042.

YORDANOV, D. et al. EVALUATION OF WIND AND TURBULENT PARAMETERISATIONS FOR SHORT RANGE AIR POLLUTION MODELING. Bulgarian Geophysical Journal, v. 32, p. 107-123, 2006.