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Eddy diffusivities for the convective boundary layer derived from LES spectral data

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ABSTRACT

Large Eddy Simulation (LES) spectral data and Taylor statistical diffusion theory are used to obtain Eddy diffusivities in a convective boundary layer. The derivation employs a fitting expression obtained from LES data for the vertical peak frequency. The vertical Eddy diffusivities are well behaved and show similar patterns and magnitudes as those derived from experimental spectral peak frequency data. In addition, this new vertical Eddy diffusivity was introduced into an advection diffusion equation which was solved by Generalized Integral Laplace Transform Technique (GILLT) method and validated with observed contaminant concentration data of the Copenhagen experiment. The results of this new approach are shown to agree with the measurements of Copenhagen.

Keywords: *Eddy diffusivities, Large Eddy Simulation, Taylor statistical diffusion theory, convective boundary layer*

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1. Introduction

Eddy diffusivities are fundamental parameters in contaminants Eulerian dispersion models. Such statistical quantities are utilized to describe the concentration fields originated from different types of pollutant sources.

A general formulation for Eddy diffusivities depending on height and source distance is expressed by (Batchelor, 1949; Degrazia et al., 2001):

$$K_\alpha = \frac{\sigma_i^2 \beta_i}{2\pi} \int_0^\infty F_i^E(n) \frac{\sin(2\pi t/\beta_i)}{n} dn \tag{1}$$

with a=x, y, z and i=u, v, w, where $F_i^E(n)$ is the Eulerian spectrum of turbulent energy normalized by the Eulerian velocity variance σ_i^2, β_i is defined as the ratio of the Lagrangian to the Eulerian integral timescales (Wandel and Kofoed–Hansen, 1962), n is the frequency, and t is the travel time. The presence of β_i in Equation (1) allows for description of K_α from a Lagrangian point of view. Therefore, Equation (1) represents a Lagrangian K_α in terms of the ratio of the Eulerian energy spectrum to the Eulerian velocity variance as kernel of a Fourier transform in frequency space.

The relation for Eulerian turbulent velocity spectrum in a convective planetary boundary layer (CBL) can be written as (Degrazia et al., 2000):

$$\frac{nS_i^E(n)}{w_*^2} = \frac{1.06 c_i f \psi^{2/3} (z/z_i)^{2/3}}{(f_m^*)_i^{5/3} \{1 + 1.5[f/(f_m^*)_i]\}^{5/3}} \tag{2}$$

where c_i=$a_i(0.50\pm0.05(2\pi k)^{2/3}$ and α_i=1,4/3, and 4/3 for u, v and w components (Champagne et al., 1977); k=0.4 is the von Karman constant, f=$nz/U(z)$ is the nondimensional frequency; z is the height above the ground; $U(z)$ is the horizontal mean wind speed at particular height; $(f_m^*)_i$ is the normalized frequency of the spectral peak; z_i is the top of the convective boundary layer height; w_* is the convective velocity scale and $\psi = \varepsilon z_i / w_*^3$ is the non–dimensional dissipation rate function, with ε being the mean dissipation of turbulent kinetic energy per unit time per unit mass of fluid.

The analytical integration of Equation (2) over whole frequency domain yields in a closed mathematical formulation expressed as:

$$\sigma_i^2 = 1.06 c_i \frac{\psi^{2/3}}{(f_m^*)_i^{2/3}} \left(\frac{z}{z_i}\right)^{2/3} w_*^2 \tag{3}$$

Equation (3) is used to normalize the turbulent spectrum yielding the following normalized Eulerian spectrum (Degrazia et al., 2000):

$$F_i^E(n) = \frac{z}{U(f_m^*)_i}\left[1 + 1.5\frac{f}{(f_m^*)_i}\right]^{-5/3} \tag{4}$$

Substituting Equations (3) and (4) into Equation (1), and assuming $\beta_i = 0.55U/\sigma_i$ the following formulation for K_α is obtained (Degrazia and Anfossi, 1998; Degrazia et al., 2001)

$$\frac{K_\alpha}{w_* z_i} = \frac{0.09c_i^{1/2}\psi^{1/3}(z/z_i)^{4/3}}{(f_m^*)_i^{4/3}} \times \int_0^\infty \frac{\sin\left[\frac{7.84c_i^{1/2}\psi^{1/3}(f_m^*)_i^{2/3}Xn'}{(z/z_i)^{2/3}}\right]}{(1+n')^{5/3}}\frac{dn'}{n'} \tag{5}$$

where $X = xw_*/Uz_i$ is the nondimensional distance defined by the ratio of travel time x/U and the convective timescale z_i/w_*.

The generalized K_α [Equation (5)] describes the diffusion phenomenon in the near, intermediate and far fields of an elevated source. Furthermore, Equation (5) is dependent on *z* and as a consequence reports the inhomogeneous character of the turbulence in a convective boundary layer.

On the other hand, considering the asymptotic behavior of Equation (1) for large diffusion travel times the following formulation for the Eddy diffusivities can be derived (Degrazia et al., 2001):

$$K_a = 0.14\frac{\sigma_i z}{(f_m^*)_i} \tag{6}$$

At this point it is important to note that both Equations (5) and (6) are expressed in terms of the normalized frequency of the spectral peak. Therefore, $(f_m^*)_i$ is important for investigations of turbulent diffusion phenomenon in the CBL. Generally, algebraic relations for $(f_m^*)_i$ are obtained from fitting expressions to experimental atmospheric data. However, observational data of this frequency in all distinct levels of the CBL are very difficult to obtain. Hence, few observations extended to whole depth of CBL are available and for this motive Large Eddy Simulation (LES) methodology represents a very useful tool to provide expressions for $(f_m^*)_i$.

The purpose of the present investigation is to derive new formulations for the Eddy diffusivities in a convective boundary layer, obtained from spectral quantities determined from a LES model. An additional aim is to employ the new parameterization for the Eddy diffusivities in *a* Eulerian dispersion model to simulate atmospheric dispersion experiments that were accomplished in the Copenhagen region under moderately convective conditions (Gryning and Lyck, 1984).

2. Spectral Peak Frequency from Large Eddy Simulation

Large Eddy Simulation (LES) models represent a powerful computational methodology to describe the physical properties of the planetary boundary layer (Moeng, 1984). In LES, the energy–containing eddies of the turbulent field are explicitly resolved and the contribution of the smaller eddies (subfilter scales) is parameterized. Generally, the basic equations in the LES models are the incompressible Navier–Stokes equations. The resolved turbulent field parameters (velocity components, potential temperature and pressure) are calculated by the application of a low–pass spatial filter which presents a particular dimension, known as the turbulent resolution length scale. The LES technique allows the simulation of the large eddies with spatial scale within the inertial subrange of the turbulent kinetic energy spectrum (Moeng, 1984). In this context, information about the length scale of the energy–containing eddies, as well as the validity of the Kolmogorov inertial subrange relations can be investigated in details.

In this study, numerical simulations of the convective boundary layer were performed employing the LES code of Moeng (1984) with Sullivan et al. (1994) subfilter parameterization. The numerical experiments used in this study were accomplished with constant values of the kinematic turbulent heat flux and of the geostrophic wind. A (5x5x2) km^3 box domain with variable points in each direction was used in five simulations. All simulations have a dominant convective character but different combinations of the wind shear and buoyancy forces. This is obtained varying the resolutions of the geostrophic forcing and surface heat fluxes as indicated by Moeng and Sullivan (1994). The spatial spectra calculations of the wind components are obtained from series of LES runs described in Table 1. The spatial spectra were obtained according to Moeng and Wyngaard (1988), using a bidimensional Fast Fourier transform of the tridimensional fluctuations of the turbulent velocity components. Therefore, the spectral peak wavelenghts were estimated from these spatial spectra generated of the five LES numerical simulations. From the analysis the numerical data of the vertical peak wavelength, generated by the LES simulations, are fitted by the following algebraic relation:

$$(\lambda_m)_w = 1.3z_i[1 - \exp(-4.8\,z/z_i) - 0.005\exp(4.8\,z/z_i)] \tag{7}$$

Comparing the vertical profile provided by Equation (7) with observational measurements accomplished by Caughey and Palmer (1979) in the totality vertical of a CBL, yields a good agreement between LES and experimental data. This can be seen in Figure 1 which also presents the experimental fitting for $(\lambda_m)_w$ suggested by Caughey and Palmer (1979).

Table 1. *Forcing parameters employed in the LES simulations. In this table, Ug, Vg are the geostrophic wind components and $\overline{w\theta}$ is the kinematic turbulent heat flux*

Turbulent Resolution Length Scale	$(Ug;Vg)$ (m s^{-1})	$\overline{w\theta}$ (m K s^{-1})
46.1	(5; 0)	0.20
46.1	(2; 0)	0.23
38.4	(2; 0)	0.23
38.4	(5; 0)	0.24
38.4	(1; 0)	0.24

Considering $(f_m)_w = z/(\lambda_m)_w$ yields the following relation for the vertical peak frequency obtained from LES spectral data:

$$(f_m)_w = 0.8\frac{z}{z_i}[1 - \exp(-4.8\,z/z_i) - 0.005\exp(4.8\,z/z_i)]^{-1} \tag{8}$$

3. Derivation of the Vertical Eddy Diffusivity

Formulations for the vertical Eddy diffusivity from LES spectral data can be obtained using Equations (5), (6) and (8). More specifically, the vertical Eddy diffusivity expressed in function of the adimensional height and the downwind distance X follows from Equations (5) and (8) employing c_w=0.36 yielding:

$$\frac{K_z}{w_* z_i} = 0.07\psi^{\frac{1}{3}}\left[1 - \exp\left(-4.8\frac{z}{z_i}\right) - 0.005\exp\left(4.8\frac{z}{z_i}\right)\right] \times \int_0^\infty \frac{\sin\left\{3.95\left[1 - \exp\left(-4.8\frac{z}{z_i}\right) - 0.005\exp\left(4.8\frac{z}{z_i}\right)\right]\psi^{1/3}Xn'\right\}}{(1+n')^{5/3}}\frac{dn'}{n'} \tag{9}$$

where the dissipation function derived by Hojstrup (1982) is given by:

$$\psi^{1/3} = \left[\left(1-\frac{z}{z_i}\right)^2\left(\frac{z_i}{-L}\frac{z}{z_i}\right)^{-2/3} + 0.75\right]^{1/2} \quad (10)$$

with L being the Obukhov length.

The asymptotic formulation (when $X\to\infty$), is obtained from Equation (6), as follows:

$$\frac{K_z}{w_* z_i} = 0.12\psi^{1/3}\left[1-\exp\left(-4.8\frac{z}{z_i}\right) - 0.005\exp\left(4.8\frac{z}{z_i}\right)\right]^{4/3} \quad (11)$$

Figure 2 presents the behavior of $K_z/w_* z_i$ as provided by Equation (9) for two different heights, z/z_i=0.1 and z/z_i=0.5. At each of those heights $K_z/w_* z_i$ is zero for X=0, increasing continually with the downwind distance X. For large distances, the rate of increase slows down, tending to an asymptotic limit, provided by Equation (11).

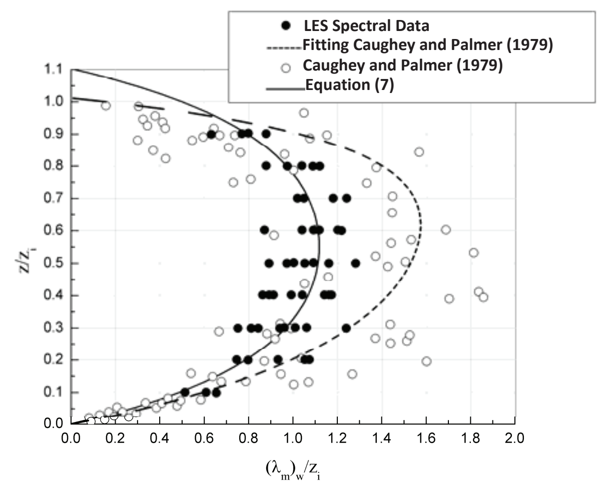

Figure 1. *The vertical profile of the normalized peak wavelength for the turbulent vertical velocity. The solid line represents the fitting from LES spectral data [Equation (7)]. The dashed line represents the experimental fitting obtained by Caughey and Palmer (1979). Open circles represent the observed data from Minnesota and Ashchurch experiments (Caughey and Palmer, 1979), while filled circles are the results obtained from LES spectral data.*

The behavior of the asymptotic vertical profile of $K_z/w_* z_i$ as given by Equation (11) is presented in Figure 3. Analyzing this profile it can be noted that this function represents a well behaved Eddy diffusivity characterized by maximum values occurring in middle region of the CBL and with small magnitudes at z=0 and z=z_i. Therefore, the vertical peak frequency obtained from LES spectral data correctly captures the physical structure of the eddies in a CBL, with large energy–containing eddies in the central regions of the CBL. On the other hand, the presence of the surface and the superior inversion (top of the CBL) prevent the development of large eddies in these interface regions, generating low values of $K_z/w_* z_i$ in the surface and entrainment layer of the CBL. These Eddy diffusivities present the same form and magnitudes as those obtained by Degrazia et al. (2001) employing observational data of the spectral peak frequency.

The vertical profiles of Eddy diffusivity derived in the present study were all constructed from a fitting relation to LES simulation data. To emphasize the importance of the developed analysis, it is worth noting that observational data of spectral peak frequency covering all the heights of a CBL are very difficult to accomplish. As a consequence, very few of such observations are available and therefore LES simulations represent a relevant methodology to generate spectral peak frequencies. The present approach has, hence demonstrated that LES methodology is found to be suitable for derivation of Eddy diffusivities.

4. Evaluation of the New Eddy Diffusivities Employing an Analytical Air Pollution Model

4.1. Analytical air pollution model

The advection–diffusion equation, describing the turbulent dispersion of contaminants in the planetary boundary layer, can be expressed as:

$$\frac{\partial\bar{c}}{\partial t} + \bar{u}\frac{\partial\bar{c}}{\partial x} + \bar{v}\frac{\partial\bar{c}}{\partial y} + \bar{w}\frac{\partial\bar{c}}{\partial z} = -\frac{\partial\overline{u'c'}}{\partial x} - \frac{\partial\overline{v'c'}}{\partial y} - \frac{\partial\overline{w'c'}}{\partial z} \quad (12)$$

$\bar{c}$ is the average concentration of a contaminant, $\bar{u}$, $\bar{v}$ and $\bar{w}$ are the components of the wind velocity in x, y, z directions, respectively. The unknown statistics $\overline{u'c'}$, $\overline{v'c'}$ and $\overline{w'c'}$ are the contaminant turbulent fluxes and need to be parameterized. The method for closing the Equation (12) is to parameterize the contaminant turbulent fluxes in terms of the gradient of the mean concentrations employing K_α Eddy diffusivities, which are described by the physical characteristics and properties of the turbulent flow. This assumption can be mathematically formulated as (Pasquill and Smith, 1983):

$$\overline{u'c'} = -K_x\frac{\partial\bar{c}}{\partial x}\ ;\ \overline{v'c'} = -K_y\frac{\partial\bar{c}}{\partial y}\ ;\ \overline{w'c'} = -K_z\frac{\partial\bar{c}}{\partial z} \quad (13)$$

where K_x, K_y and K_z are the Eddy diffusivities along x, y, z directions respectively. Considering a Cartesian coordinate system in which the x direction coincides with that of the average wind and stationary conditions, the advection–diffusion equation [Equation (12)], employing Equation (13) is written as (Pasquill and Smith, 1983):

$$\bar{u}\frac{\partial\bar{c}}{\partial x} = \frac{\partial}{\partial x}\left(K_x\frac{\partial\bar{c}}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_y\frac{\partial\bar{c}}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_z\frac{\partial\bar{c}}{\partial z}\right) \quad (14)$$

The cross–wind integration of Equation (14), neglecting the diffusion in the x direction, yields:

$$\bar{u}\frac{\partial\overline{c_y}}{\partial x} = \frac{\partial}{\partial z}\left(K_z\frac{\partial\overline{c_y}}{\partial z}\right) \quad (15)$$

where $\overline{c_y}$ is the average cross–wind integrated concentration in the vertical region $0<z<z_i$ and for X>0, considering the following boundary conditions and emission rate Q:

$$k_z\frac{\partial\overline{c_y}}{\partial z} = 0\ at\ z = 0, z_i \text{ (zero concentration flux at the surface and CBL top)} \quad (16)$$

and

$$\bar{u}\bar{c}_Y(0,z) = Q\delta(z - H_s) \text{ (emission rate at source height } (H_s)\text{)} \quad (17)$$

In the present study, the solution for the problem defined by the Equations (15), (16) and (17) is obtained by the Generalized Integral Laplace Transform Technique (GILTT) method (Moreira et al., 2009; Buske et al., 2011). This general method to simulate pollutants dispersion in a planetary boundary layer is described in a detailed form in the following works (Moreira et al., 2009; Buske et al., 2011).

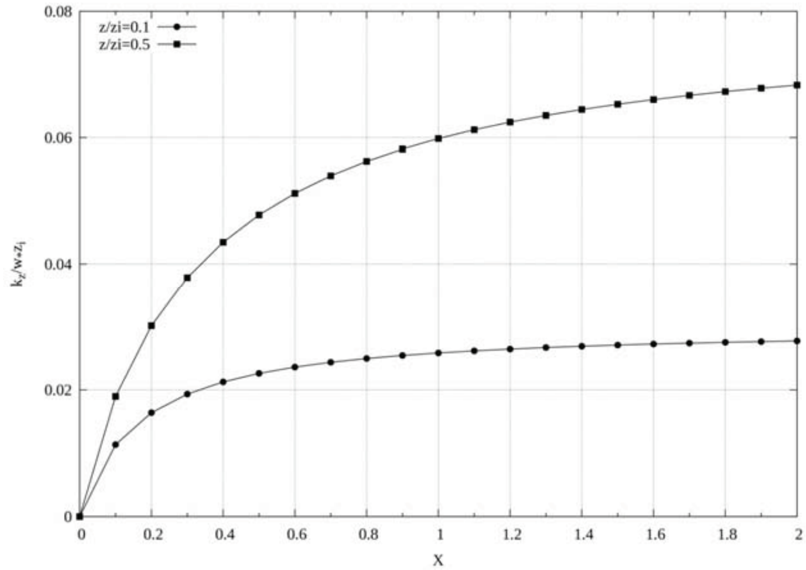

Figure 2. *Vertical Eddy diffusivity for two different heights (z/z_i=0.1 and z/z_i=0.5) as given by Equation (9).*

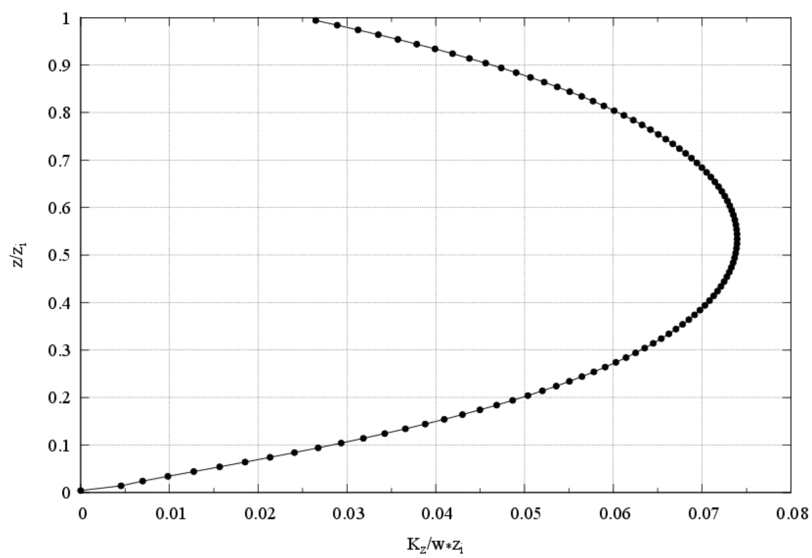

Figure 3. *Asymptotic vertical profile for the Eddy diffusivity [Equation (11)].*

4.2. Comparison with Copenhagen concentration observed data

In this section, the vertical Eddy diffusivity derived from LES spectral data [Equation (9)] is introduced in Equation (15) and solved with the GILTT method with the aim of evaluating the performance of this new parameterization in reproducing the observed ground–level concentrations. To accomplish this task, observed concentration data from the Copenhagen dispersion experiment were simulated. The Copenhagen experiment was carried out in northern part of Copenhagen. The pollutant (SF_6) was released without buoyancy from a tower of 115 m and measured at ground–level at a maximum of three crosswind arcs (Gryning and Lyck, 1984; Degrazia, 2001; Carvalho et al., 2002). The wind speed profile employed in the simulations is expressed by a power law provided by the following relation (Alves et al., 2012):

$$\frac{\overline{u_z}}{\overline{u_1}} = \left(\frac{z}{z_1}\right)^n \tag{18}$$

where $\overline{u_1}$ and $\overline{u_z}$ are the mean horizontal wind speeds at heights z and z_1, while n is an exponent that is related to the intensity of turbulence. For convective conditions n=0.1 (Irvin, 1979). Table 2 shows the micrometeorological parameters that were observed during Copenhagen experiment and a comparison between observed and simulated values of ground–level crosswind integrated concentration $\left(\overline{c_y}(x,0)/Q\right)$.

The performance of the GILTT method employing the vertical Eddy diffusivity obtained from LES spectral data given by Equation (9) is shown in Table 3 and Figure 4. Table 3 exhibits the statistical analysis that allows comparison of observed and simulated magnitudes of the ground–level crosswind integrated concentration $(\overline{c_y}(x,0)/Q)$. The statistical indices to evaluate the performance of the new vertical Eddy diffusivity were proposed by Hanna (1989). The NMSE is the normalized mean square error, FA2 is Factor 2, COR is the correlation coefficient, FB is the fractional bias and FS is the fractional standard deviations. The meaning of these indices is discussed and explained in a detailed form in Moreira et al. (2011) and Maldaner et al. (2013). The statistical indices NMSE, FB and FS represent good results when they approach zero, whereas COR and FA2 are optimized at the value 1. Therefore, analyzing the magnitude of the statistical indices in Table 3 and observing the scatter diagram in Figure 4, it is possible to conclude that the advection–diffusion equation [Equation (15), solved by GILTT method], employing the vertical Eddy diffusivity obtained from LES spectral data, reproduces very well the observed crosswind integrated concentration from the Copenhagen experiment.

5. Conclusions

An embracing approach to derive Eddy diffusivity in a CBL is suggested. This approach is based upon Taylor statistical diffusion theory and fitting expressions for the vertical peak frequency calculated from LES spectral data. These Eddy diffusivities can be applied to parameterize turbulent dispersion in the near, the intermediate and far field of an elevated continuous point source. Furthermore, its asymptotic limit valid for large travel times, describes the dispersion of area sources.

The peak frequency of the turbulent vertical velocity spectrum is a relevant quantity of great application in turbulent transport problems. Its magnitude informs the length and time scale of energy–containing eddies. Generally, formulations for this particular frequency are derived from experimental data observed directly in the CBL. However, these observations are expensive and very difficult to be performed. Equation (7), derived from LES simulation data, shows a good agreement with measurements accomplished in a well developed CBL. Furthermore, turbulent parameters generated by the LES approach provide more detail (better spatial representation) and do not depend on quite difficult observations, which are also somewhat uncertain.

The present analysis allows obtaining a vertical Eddy diffusivity described in terms of the source distance for an inhomogeneous turbulent field associated to a CBL. In this case, K_z is dependent on the non–dimensional distance X, on the stability parameter z_i/L and of the adimensional height z/z_i. Differently, the K_z asymptotic is dependent only on the stability parameter z_i/L and the height z/z_i. Therefore, Equations (9) and (11) that describe the vertical Eddy diffusivities from LES data, are well defined functions and are described in the form of a similarity profile employing the convective velocity scale and the inversion height. To test the new vertical Eddy diffusivity [Equation (9)] in a Eulerian dispersion model, we employ Equation (9) in the advection–diffusion Equation (15) to simulate the Copenhagen observed ground–level crosswind integrated concentrations. The results show that there is a good agreement between simulated and observed concentrations. Therefore, the new Eddy diffusivity generated by LES spectral data, expressed by Equation (9), depending on source distance and describing an inhomogeneous turbulence, can be applied in regulatory air pollution modeling.

Table 2. *Micrometeorological parameters and observed and simulated ground–level cross–wind integrated concentrations at different distances from the source. In this table, L is the Monin–Obukhov length, w_* is the convective velocity scale, u_* is the friction velocity, z_i is the top of the convective boundary layer height, X is the nondimensional distance, U10 m is the mean wind speed at 10 m height, U115 m is the mean wind speed at 115 m height, Q is the emission rate and $(c_y(x,0)/Q)$ is the ground–level cross–wind integrated concentrations*

Run	Sampler Distance (m)	X	L (m)	w_* (m s^{-1})	u_* (m s^{-1})	z_i (m)	U10 m (m s^{-1})	U115 m (m s^{-1})	Q (g s^{-1})	$[c_y(x,0)/Q]$ Observed 10^{-4} s m^{-2}	$[c_y(x,0)/Q]$ Predicted 10^{-4} s m^{-2}
1	1 900	0.496	–37	1.8	0.36	1 980	2.1	3.4	3.2	6.48	6.40
1	3 700	0.967	–37	1.8	0.36	1 980	2.1	3.4	3.2	2.31	4.09
2	2 100	0.177	–292	1.8	0.73	1 920	4.9	10.6	3.2	5.38	3.53
2	4 200	0.355	–292	1.8	0.73	1 920	4.9	10.6	3.2	2.95	2.33
3	1 900	0.390	–71	1.3	0.38	1 120	2.3	5.0	3.2	8.20	7.93
3	3 700	0.760	–71	1.3	0.38	1 120	2.3	5.0	3.2	6.22	5.28
3	5 400	1.110	–71	1.3	0.38	1 120	2.3	5.0	3.2	4.30	4.17
4	4 000	1.540	–133	0.7	0.38	390	2.5	4.6	2.3	11.66	8.67
5	2 100	0.270	–444	0.7	0.45	820	3.1	6.7	3.2	6.72	7.63
5	4 200	0.530	–444	0.7	0.45	820	3.1	6.7	3.2	5.84	5.48
5	6 100	0.780	–444	0.7	0.45	820	3.1	6.7	3.2	4.97	4.86
6	2 000	0.220	–432	2	1.05	1 300	7.2	13.2	3.1	3.96	2.95
6	4 200	0.470	–432	2	1.05	1 300	7.2	13.2	3.1	2.22	2.03
6	5 900	0.660	–432	2	1.05	1 300	7.2	13.2	3.1	1.83	1.57
7	2 000	0.300	–104	2.2	0.64	1 850	4.1	7.6	2.4	6.70	3.95
7	4 100	0.620	–104	2.2	0.64	1 850	4.1	7.6	2.4	3.25	2.50
7	5 300	0.790	–104	2.2	0.64	1 850	4.1	7.6	2.4	2.23	2.11
8	1 900	0.530	–56	2.2	0.69	810	4.2	9.4	3.0	4.16	5.01
8	3 600	1.010	–56	2.2	0.69	810	4.2	9.4	3.0	2.02	3.44
8	5 300	1.480	–56	2.2	0.69	810	4.2	9.4	3.0	1.52	2.72
9	2 100	0.180	–289	1.9	0.75	2 090	5.1	10.5	3.3	4.58	3.31
9	4 200	0.350	–289	1.9	0.75	2 090	5.1	10.5	3.3	3.11	2.20
9	6 000	0.520	–289	1.9	0.75	2 090	5.1	10.5	3.3	2.59	1.75

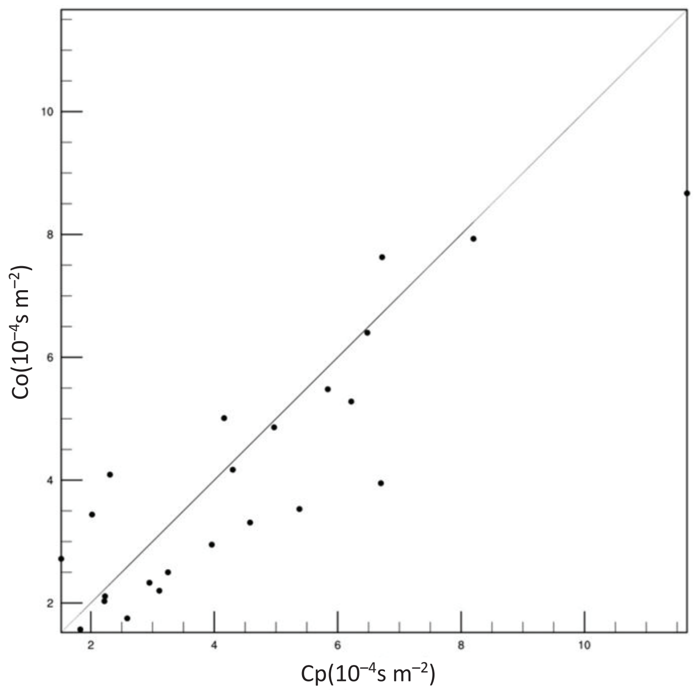

Figure 4. *Scatter diagram between observed (Co) and predicted (Cp) ground–level cross–wind integrated concentrations* $(\overline{c_y}(x,0)/Q)$.

Table 3. *Statistical indices assessing the model performance. In this table, NMSE is the normalized mean square error, COR is the correlation coefficient, FA2 is Factor 2, FB is the fractional bias and FS is the fractional standard deviations*

NMSE	COR	FA2	FB	FS
0.08	0.88	1	0.09	0.17

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