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Derivation of third–order vertical velocity turbulence moment in the convective boundary layer from large eddy simulation data: an application to the dispersion modeling

Silvana Maldaner [1], Gervasio Annes Degrazia [1], Umberto Rizza [2], Virnei Silva Moreira [3], Franciano Scremin Puhales [1], Otavio Costa Acevedo [1], Ivan Alves [1], Jonas da Costa Carvalho [4]

[1] *Departamento de Física, Universidade Federal de Santa Maria, 97110–900 Santa Maria, RS, Brazil*
[2] *ISAC–CNR, Istituto di Scienze dell'Atmosfera e del Clima, Dipartimento Terra e Ambiente, Consiglio Nazionale delle Ricerche, Lecce, Italy*
[3] *Departamento de Física, Universidade Federal do Pampa (UNIPAMPA), Itaqui, RS, Brazil*
[4] *Departamento de Meteorologia, Universidade Federal de Pelotas, RS, Brazil*

ABSTRACT

A new formulation for the vertical turbulent velocity third statistical moment in a convective boundary layer is proposed. The parameterization is based directly on the definition of this higher order moment, with velocity skewness and variance being calculated from large eddy simulation data. The formulation, included in a Lagrangian stochastic dispersion model, has been tested and compared with expressions for the third moment obtained from experimental data and reported in the literature, using concentration data from field experiments. The application of a statistical evaluation shows that the proposed parameterization has one of the best overall adjustments to the data.

Keywords: *Third moment of the vertical velocity, large eddy simulation, Lagrangian stochastic particle dispersion model*

Corresponding Author:
Gervasio Annes Degrazia
☎ : +55(55)-3220-8616
🖷 : +55(55)-3220-8616
✉ : gervasiodegrazia@gmail.com

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1. Introduction

The dispersion of pollutants by turbulent flows has a fundamental importance in a large number of environmental issues. Therefore, the investigation and employment of Lagrangian or Eulerian models for the analysis of environmental impact conditions is essential for air quality assessment in a wide range of temporal and spatial scales. In such models, the information regarding turbulence characteristics are commonly introduced through the statistical moments of the turbulent velocity probability distribution functions. Among these, the third–order statistical moment, usually referred as the skewness, and associated with the asymmetry of the distribution with respect to its mean, is one of the most important functions (Lamb, 1982; Moeng and Rotunno, 1990; Fedorovich et al., 1996; Arya, 1999; Anfossi and Physick, 2005; Degrazia et al., 2012). Particularly, in a convective boundary layer (CBL), with non–divergent horizontal flow, the vertical velocity has a zero mean value but a strongly negative mode (the most frequent value of the vertical velocity). This shows that within the CBL, the turbulent vertical velocity probability density function has a positive skewness. Physically, in a CBL, a positive vertical velocity skewness indicates that strong narrow updrafts are surrounded by larger areas of weaker downdraft (Moeng and Rotunno, 1990). As a consequence, large positive values of the vertical velocity are more frequent than the large negative values (Arya, 1999). The vertical velocity skewness is defined by the following expression:

$$S_w = \frac{\overline{w'^3}}{(\sigma_w^2)^{3/2}} \tag{1}$$

where $\overline{w'^3}$ is the third moment of the vertical velocity and σ_w^2 is the vertical velocity variance. Normally, one describes the dispersion of contaminants in a CBL employing the vertical profiles of the third moment of the turbulent vertical velocity in Lagrangian Stochastic Dispersion Models (Anfossi and Physick, 2005). A variety of profiles for the third moment, expressed in terms of a convective similarity theory, are obtained from field data (Lenschow et al., 1980; Luhar et al., 1996), water–tank data (Willis and Deardorff, 1974) and Lidar measurements (Lenschow et al., 2012). As examples of vertical profiles for $\overline{w'^3}$, obtained from observational data, we present below three fitting curves for the third moment of the vertical velocity in a CBL. Such profiles were suggested by De Baas and Troen (1989), Franzese et al. (1999) and Kastner–Klein et al. (2001), respectively. These formulations for the third moment of the vertical velocity are described in terms of a convective similarity theory and provided by the Equations (2), (3), and (4) by De Baas and Troen (1989), Franzese et al. (1999), and Kastner–Klein et al. (2001), respectively:

$$\frac{\overline{w'^3}}{w_*^3} = 1.4\left(\frac{z}{z_i}\right) exp\left(-2.5\frac{z}{z_i}\right) \quad (2)$$

$$\frac{\overline{w'^3}}{w_*^3} = 1.1\frac{z}{z_i}\left(1-\frac{z}{z_i}\right)^2 \quad (3)$$

$$\frac{\overline{w'^3}}{w_*^3} = 2\frac{z}{z_i}\left(1-\frac{z}{z_i}\right)^{1.2} \quad (4)$$

where, z_i is the top of the convective boundary layer height and w_* is the convective velocity scale. The purpose of the present study is therefore to obtain a new algebraic profile for the third moment of the vertical velocity in a CBL. This profile is obtained from a high resolution simulation employing a large eddy simulation (LES) model. An additional aim is to use a well known Lagrangian dispersion stochastic model and concentration data obtained from Prairie Grass classical short–range dispersion experiment in unstable conditions to compare this new vertical profile for $\overline{w'^3}$ with the profiles given by the Equations (2), (3) and (4).

2. Vertical Velocity Third Moment Algebraic Profile from LES Data

2.1. General concepts

Large eddy simulation (LES) is a numerical modeling technique whose concept is based on the idea that the most energetic turbulent eddies may be explicitly solved by the numerical grid chosen, while the smaller scales are parameterized based on the statistical turbulence theory. The idea behind such approach is that energy enters the turbulent field in large scales and is dissipated by molecular diffusion in very small ones, so that there is an intermediate range for which there is only an inertial decay of large eddies feeding the smaller ones in energy. Such range is, for these reasons, known as the inertial subrange. The energy of the inertial subrange eddies is known, since the classical analysis from Kolmogorov (1941) to obey a scaling law with respect to the eddy wavenumbers, and such relationship is used, in LES, to parameterize the unknown smaller scales. This is often regarded as a filtering approach, so that the parameterized scales are defined as subfilter processes. The LES simulation, employed in the present study, used a subfilter model based on the Taylor statistical diffusion theory. The turbulent subfilter viscosity derived from this model is described in terms of the inertial subrange velocity variance and time scale. This new subfilter viscosity contains a cutoff wavenumber (k_c), presenting an identical form (differing by a constant) to Kraichnan's eddy viscosity in spectral space (Lesieur and Metais, 1996) and to Heisenberg´s subfilter viscosity (Muschinski and Roth, 1993; Degrazia et al., 2007). Therefore, this viscosity is described by the following formulation (Degrazia et al., 2012):

$$v_t = 0.95\varepsilon^{1/3}k_c^{-4/3} \quad (5)$$

where $\mathcal{E}$ is the turbulent dissipation rate and k_c is the cutoff or limiting wave number for the inertial subrange. It is important to note that the subfilter viscosity, as given by Equation (5), establishes a sharp division between large and small wave number of a turbulent flow and, henceforth, such subfilter viscosities are in agreement with the sharp Fourier filtering operation, frequently employed in LES models (Armenio et al., 1999). Therefore, the Taylor subfilter turbulent viscosity [Equation (5)] has been used in the LES code of Moeng (1984) and Sullivan et al. (1994) to obtain the vertical velocity third moment profile in the CBL.

2.2. Simulation performed

In the LES simulation a variable vertical grid spacing was used Δ_z for $z < 0.1z_i$, as proposed by Degrazia et al. (2009). The numerical solutions presented in this study are obtained at grid points located in a (4, 4, 2) km box domain with 256 points in each direction (x, y, z). In the simulation we held the kinematic turbulent heat flux constant ($w\theta = 0.24$ m K/s), the geostrophic wind was set to U_g=10 m/s, the initial value for the CBL height was $z_i = 1\,000$ m and the initial surface potential temperature was set to $\theta = 300$ K. The performed numerical simulation has been intended to reproduce a CBL in a quasi–stationary (equilibrium) state. The vertical velocity fields obtained from the simulation are used to determine the third–order moment from Equation (1). A more detailed description of the LES simulation which generated the vertical velocity skewness and the velocity variance can be found in Rizza et al. (2006) and Degrazia et al. (2012).

The vertical velocity third moment data derived from LES simulation are represented by the filled circles in Figure 1. In this figure we compare the LES third moment profile (filled circles) with experimental data obtained from observations accomplished in different experiments: (Lenschow et al., 1980) AMTEX – triangles; (Willis and Deardorff, 1974) – filled squares; (Luhar et al., 1996) – open circles; (Lenschow et al., 2012) – open diamond and averaged data from the most convective cases of Lenschow et al. (2012) – open squares. It can be seen that there is a fairly good agreement between LES data and observations in the CBL. Particularly, over the lower portion of the CBL, a vertical region in which LES models provide a poorer description of the flow, there is a good agreement between LES and observational data. The continuous line in Figure 1 is a fitting from LES data, and is described by the following polynomial equation:

$$\frac{\overline{w'^3}}{w_*^3} = 1.09\frac{z}{z_i}\left(1-\frac{z}{z_i}\right)^{1.02} \quad (6)$$

Furthermore, in Figure 1 are represented the vertical profiles for $\overline{w^3}$ given by the Equations (2)–dotted line, (3)–dashed dotted line and (4)–dashed line. It can be seen that only the Equation (4) exhibits different behavior of the experimental data.

3. Employment of the Vertical Velocity Third Moment Parameterizations in a Dispersion Model

It is the aim of this Section to use a Lagrangian stochastic dispersion model and observational concentration data to test our parameterization for the third moment of the vertical velocity derived from LES data [Equation (6)]. To accomplish this procedure we simulate the classical Prairie Grass dispersion experiment using the Equations (2), (3), (4), (6) into the well–known Lagrangian Stochastic Dispersion Model – LAMBDA (Ferrero et al., 1995). The Prairie Grass experiment was performed in O'Neill, Nebraska, in 1956 and it is described in detail by Barad (1958). The contaminant (SO_2) was emitted without buoyancy at a height of 0.5 m and it was measured by samplers at a height of 1.5 m at five downwind distances (50, 100, 200, 400, 800 m) (Carvalho et al., 2002). The Prairie Grass site was flat with a surface roughness length of 0.6 cm (Carvalho et al., 2002; Moreira et al., 2011). From Prairie Grass runs we select the most convective cases. Ferrero and Anfossi (1998a) and Ferrero and Anfossi (1998b) provide a detailed presentation and discussion of LAMBDA dispersion model. The current version of the LAMBDA dispersion model is based on the generalized Langevin equation, whose coefficients are obtained by solving the Fokker–Planck equation, and satisfies the well–mixed condition (Thomson, 1987). It can use, as input, higher–order moments of the atmospheric probability density function (PDF) of wind velocity. In this study the fourth order moment was parameterized according to Ferrero and Anfossi (1998a) and Ferrero and Anfosi (1998b) ($\overline{w^4} = 3.5\left(\sigma_w^2\right)^2$). In present application, LAMBDA uses a Gaussian PDF on the horizontal plane and a Gram–Charlier PDF, truncated to the fourth order, in vertical. All the available data (see Table 1) were used to create an input file for the simulations. The profiles of wind velocity standard deviations and the Lagrangian time scales were obtained from the turbulence spectra and were calculated from the turbulence parameterization derived by Degrazia et al. (2000). Wind speed profiles were parameterized following the similarity theory of Monin–Obukhov and OML model (Berkowicz et al., 1986):

$$U(z) = \frac{u_*}{k}\left[\ln\left[\frac{z}{z_0}\right] - \Psi_m\left[\frac{z}{L}\right] + \Psi_m\left[\frac{z_0}{L}\right]\right] \quad \text{if } z < z_b \tag{7}$$

$$U(z) = U(z_b) \quad \text{if } z > z_b \tag{8}$$

where, $z_b = min\left||L|, 0.1h\right|$, k = 0.4 is the Von Karman constant, u_* is the friction velocity, Z_0 is the roughness length, L is the Monin–Obukhov length and Ψ_m is a stability function given by (Paulson, 1970):

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

and

$$A = \left[1 - 16\frac{z}{L}\right]^{1/4} \tag{10}$$

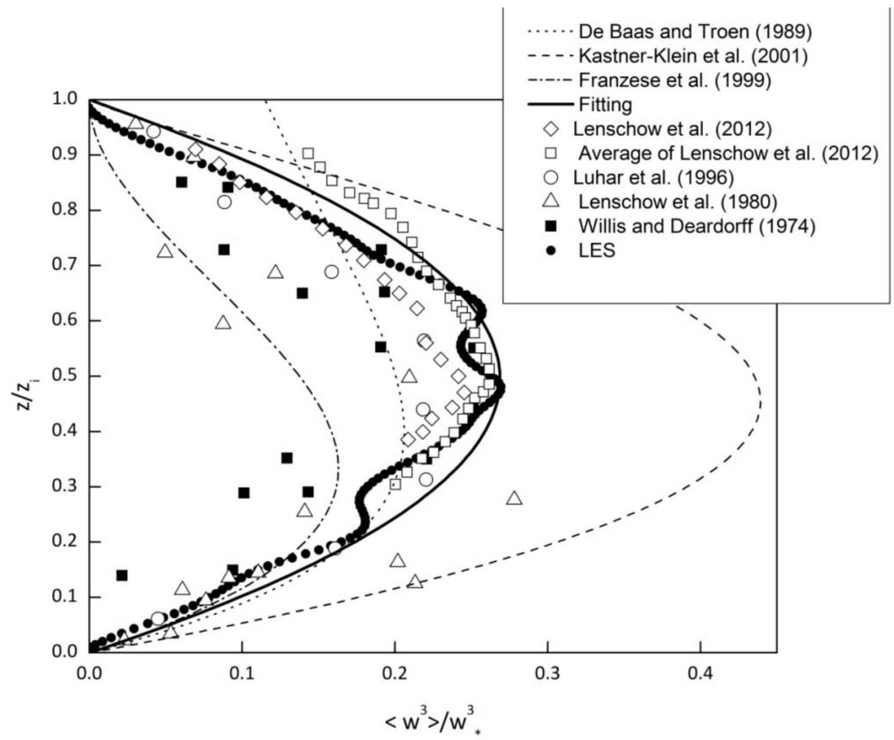

***Figure 1**. Normalized third moment of the vertical velocity $(< w^3 >= \overline{w^3})$. The following data are shown: LES simulation (filled circles), a fitting from LES data - Equation (6) (continuous line), the vertical profiles for $\overline{w^3}$ given by the Equations (2)-dotted line, (3)-dashed dotted line and (4)-dashed line and experimental data obtained from observations accomplished in different experiments (filled squares - Willis and Deardorff (1974); (triangles- Lenschow et al. (1980); open circles- Luhar et al. (1996); open diamond – Lenschow et al. (2012) and averaged data of Lenschow et al. (2012) - open squares).*

***Table 1**. Meteorological parameters and ground-level cross-wind-integrated concentrations measured during the Prairie Grass experiment C_{obs} and simulated concentrations C_{sim} with the LAMBDA model*

Run	L (m)	Z_i (m)	W (m/s)	U (m/s)	Q (g/s)	Cy	50 m	100 m	200 m	400 m	800 m
1	-9	260	0.84	3.2	82	C_{obs}	7.00	2.30	0.51	0.16	0.062
						C_{sim}	6.88	2.44	1.28	0.67	0.40
7	10	1 340	2.27	5.1	90	C_{obs}	4.00	2.20	1.00	0.40	0.18
						C_{sim}	4.52	2.16	1.02	0.37	0.21
8	18	1 380	1.87	5.4	91	C_{obs}	5.10	2.60	1.10	0.39	0.14
						C_{sim}	5.54	2.55	0.92	0.44	0.24
10	11	950	2.01	5.4	92	C_{obs}	4.50	1.80	0.71	0.20	0.032
						C_{sim}	4.56	1.69	0.77	0.40	0.24
15	8	80	0.70	3.8	96	C_{obs}	7.10	3.40	1.35	0.37	0.11
						C_{sim}	7.16	3.39	1.43	0.40	0.21
16	5	1 060	2.03	3.6	93	C_{obs}	5.00	1.80	0.48	0.10	0.017
						C_{sim}	5.36	1.53	0.36	0.28	0.18
25	6	650	1.35	3.2	104	C_{obs}	7.90	2.70	0.75	0.30	0.063
						C_{sim}	7.30	2.95	0.56	0.43	0.31

In the Lagrangian Diffusion model, the horizontal domain was determined according to sampler distances and the vertical domain was equal to the observed mixing height. The time step was maintained constant and it was obtained according to the value of the Lagrangian decorrelation time scale ($\Delta t = \tau_{Li}/c$), where τ_{Li} must be the smaller value among $\tau_{Lu}, \tau_{Lv}, \tau_{Lw}$. The constant c is an empirical coefficient set equal to 10, a choice that guarantees that the model time step is on the same order as the inertial sub–range timescales (Rodean, 1996). One hundred particles were released in each time step during 1 000 time steps. The Lagrangian simulations were performed according to Carvalho et al. (2002) and Moreira et al. (2011). LAMBDA simulations results employing the third moment of the vertical velocity obtained from LES data are presented in Table 1. Table 1 shows the meteorological parameters and ground–level cross–wind–integrated concentration measured during the Prairie Grass experiment (Barad, 1958; Carvalho et al., 2002). In Table 1, Run represents the experiment, L is the Monin–Obukhov length, z_i is the convective PBL height, U is the wind speed at 10 m, Q is the emission rate, Cy is the ground–level cross–wind integrated concentration, c_{obs} is the observed concentration and c_{sim} is the simulated concentration. It is important to note that the employment of the Equation (6) in the LAMBDA model allowed a good characterization of the pollutants dispersion phenomenon in regions near and far from the source (400 m). The model performances using the third moments given by the Equations (2), (3), (4), (6) are shown in Figures 2, 3, 4, 5 and Table 2. Figures 2–5 show the scatter diagrams between observed and predicted cross–wind concentrations. Altogether, the results given by simulations are quite satisfactory for all parameterizations representing the dispersion effects caused by the third moment of the vertical velocity. The results of Figure 5 are particularly good for the highest concentrations and this is always a favorable result for a dispersion model. This is also confirmed by the statistical indices contained in Table 2. Table 2 exhibits the results of the statistical analysis made with observed and predicted values of the ground–level cross–wind integrated concentration. Additionally, Table 2 presents a comparison between the vertical velocity third moment derived from LES data [present parameterization, Equation (6)] with those formulations found in literature and derived from observational data [Equations (2), (3), (4)]. The statistical indices in Table 2 are suggested by Hanna (1989):

Normalized Mean Error (*NMSE*):

$$NMSE = \overline{(C_o - C_p)^2} / \overline{C_o C_p} \tag{11}$$

Fractional Bias (*FB*):

$$FB = (\overline{C_o} - \overline{C_p})/0.5(\overline{C_o} + \overline{C_p}) \tag{12}$$

Fractional Standard Deviation (*FS*):

$$FS = 2(\sigma_o - \sigma_p)/(\sigma_o + \sigma_p) \tag{13}$$

Correlation Coefficient (*R*):

$$R = \overline{(C_o - \overline{C_o})(C_p - \overline{C_p})} / \sigma_o \sigma_p \tag{14}$$

Factor 2 (*FA*2):

$$FA2 = 0.5 \leq C_o/C_p \leq 2 \tag{15}$$

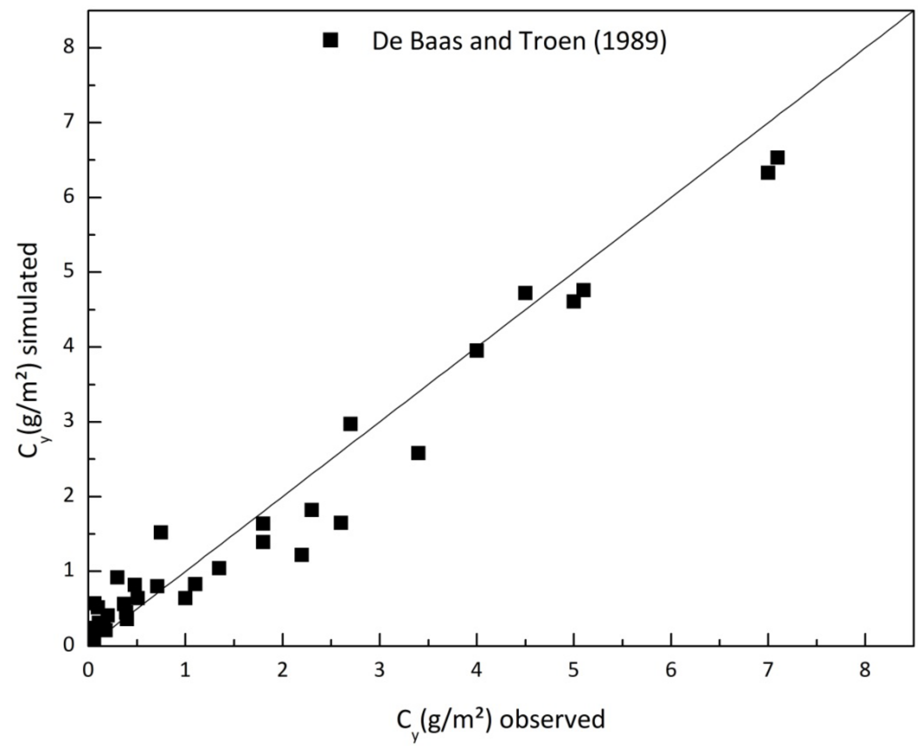

Figure 2. *Scatter diagram between observed and predicted cross-wind integrated concentrations for the Prairie Grass data set. Simulation results employing the third moment of the vertical velocity of De Baas and Troen (1989) - Equation (2).*

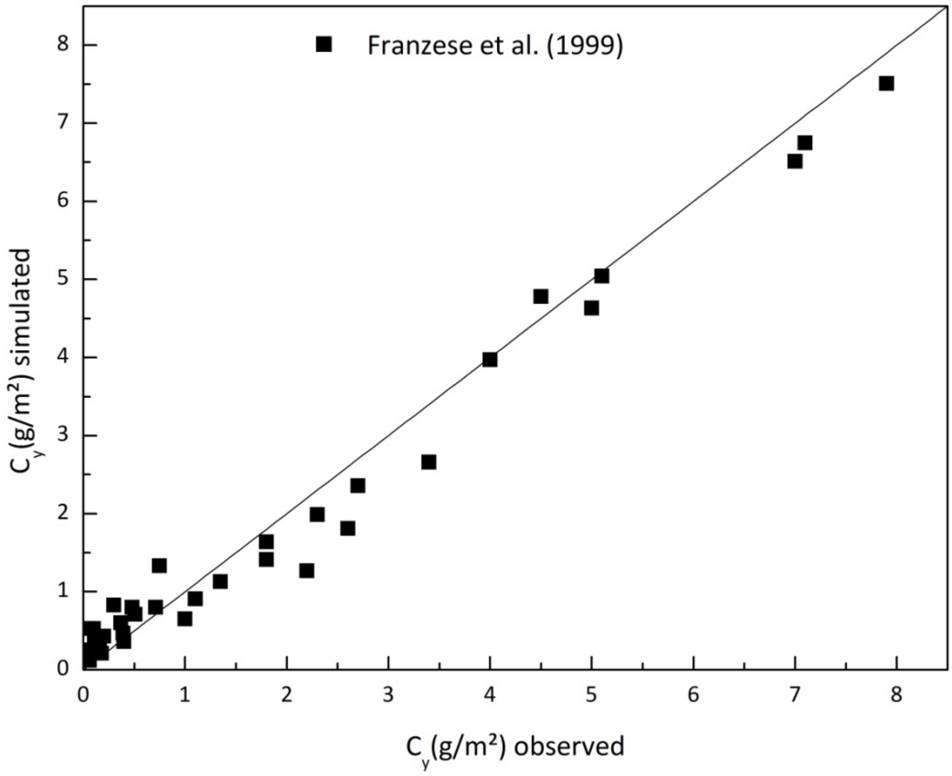

Figure 3. *Scatter diagram between observed and predicted cross-wind integrated concentrations for the Prairie Grass data set. Simulation results employing the third moment of the vertical velocity of Franzese et al. (1999) - Equation (3).*

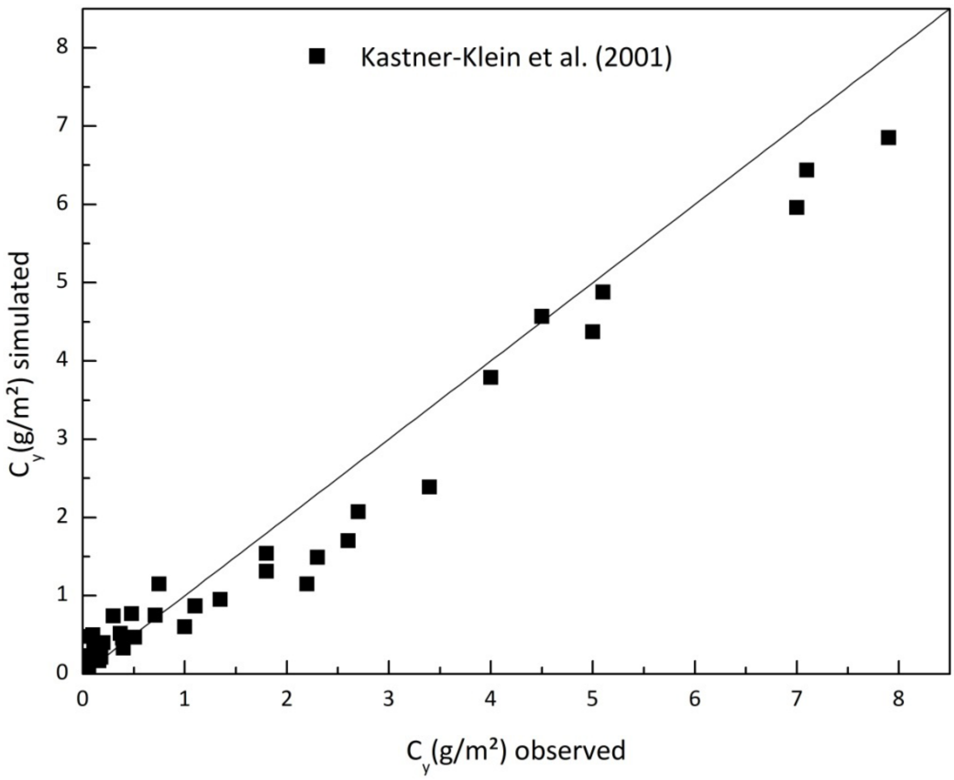

Figure 4. *Scatter diagram between observed and predicted cross-wind integrated concentrations for the Prairie Grass data set. Simulation results employing the third moment of the vertical velocity of Kastner-Klein et al. (2001) – Equation (4).*

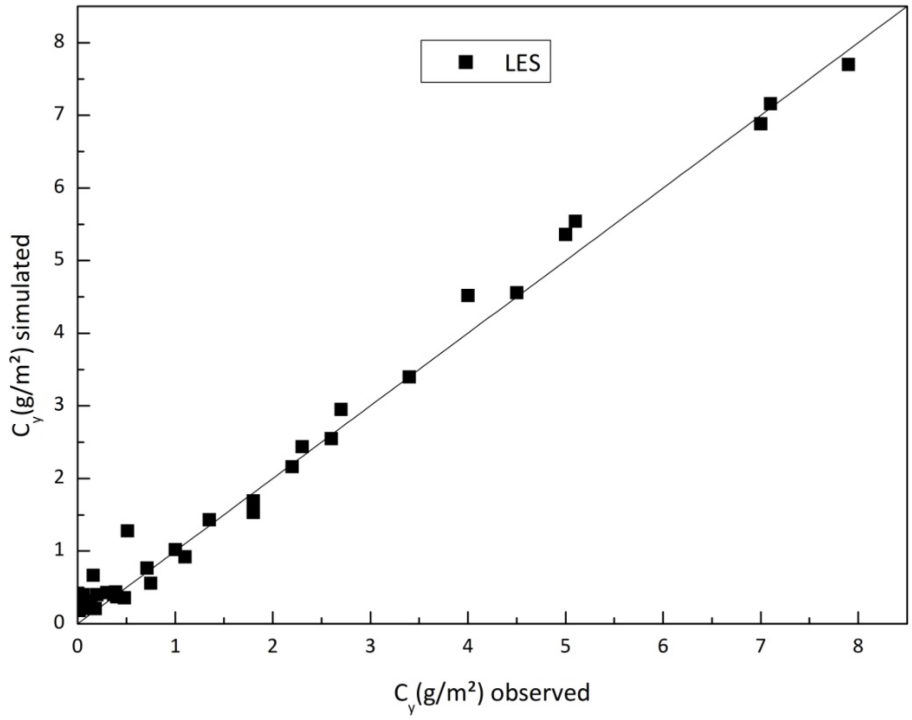

Figure 5. *Scatter diagram between observed and predicted cross-wind integrated concentrations for the Prairie Grass data set. Simulation results employing the third moment of the vertical velocity obtained from LES data – Equation (6).*

Table 2. *Statistical evaluation of model results for cross-wind integrated concentration*

Formulations for $\overline{w^3}$	NMSE	R	FA2	FB	FS
LES	0.02	0.99	0.80	-0.03	0.02
De Baas and Troen (1989)	0.06	0.98	0.77	0.02	0.05
Franzese et al. (1999)	0.04	0.99	0.80	0.02	0.08
Kastner-Klein et al. (2001)	0.07	0.99	0.83	0.11	0.14
$\overline{w^3} = 0$	0.71	0.89	0.57	-0.34	-0.41

From this statistical viewpoint we may promptly conclude that the LAMBDA model utilizing the Equations (2), (3), (4), (6), representing the phenomenon of the pollutants dispersion, in general simulates fairly well the concentration experimental data in a convective PBL. It is important, at this point, to stress that the results from the present study have a different character from the others to which they are compared. The skewness profiles used in the studies from De Baas and Troen (1989), Franzese et al. (1999) and Kastner–Klein (2001) were all obtained from fitting expressions to experimental data, while in the present case the data arise from a LES simulation. The importance of this difference lies in the fact that experimental data of higher–order moments are fairly difficult to obtain, especially considering that the observations must span the depth of the CBL. Not many of such observations are, therefore, available, and for this reason, LES constitutes quite a useful tool for that purpose. The present study has, therefore, shown that such approach is possible and that it, indeed, leads to good results. Furthermore, LES outputs have some advantages over the other methods used. Particularly, it allows better spatial representation, not restrained to vertical levels where the observations are taken. On the other hand, one must argue that being simulations, the LES results have a larger uncertainty, especially near the ground, where they tend to perform poorer. This is the reason why an adaptable vertical grid was used, such that smaller eddies are explicitly modeled near the ground, diminishing such limitation. It is also interesting to notice that the experimental results on which the other formulations are based show quite a large scattering, as can be seen in Figure 1. Naturally, therefore, those formulations also present an appreciable uncertainty associated with them. In that sense, the present study based on alternative, more detailed data, may be used to validate those results, as they all performed similarly well.

To emphasize the importance of including the third moment in the LAMBDA model, the Prairie Grass dispersion experiment has also been simulated without considering its physical effect, by forcing $\overline{w^3}$. The Lagrangian simulations results from this case are shown in Figure 6. The quality of the comparison between simulated and observed concentrations is worse than in any of the cases in which a formulation for the third moment was considered, as can be also seen from the statistical evaluation of results (Table 2, last line). The employment of the third moment is meant to represent the non–homogeneous character of the turbulence. From a physical viewpoint, $\overline{w^3} \neq 0$, means incorporating the special transport pattern associated with the existence of updrafts and downdrafts in the estimation of the pollutants concentration. The statistical analysis (Table 2) shows that the third moment of the turbulent vertical velocity must be considered to correctly describe the contaminant dispersion in a CBL.

4. Conclusion

The third moment of the vertical velocity is a statistical quantity of great interest for dispersion modeling associated to the turbulence study. Normally, mathematical expressions for this higher order statistical moment are obtained from observational data measured in laboratory (wind tunnel, water–tank) and in the PBL. In this study, we employed LES data to obtain an algebraic formulation that provides the vertical profile of the third moment of the vertical velocity in a CBL. Such formulation is derived from Equation (1), in which the vertical velocity skewness and variance were extracted directly from LES. Furthermore, our analysis showed that there is a fairly good agreement between the simulated vertical velocity third moment with those measured in different experiments. Therefore, Equation (6), that provides the

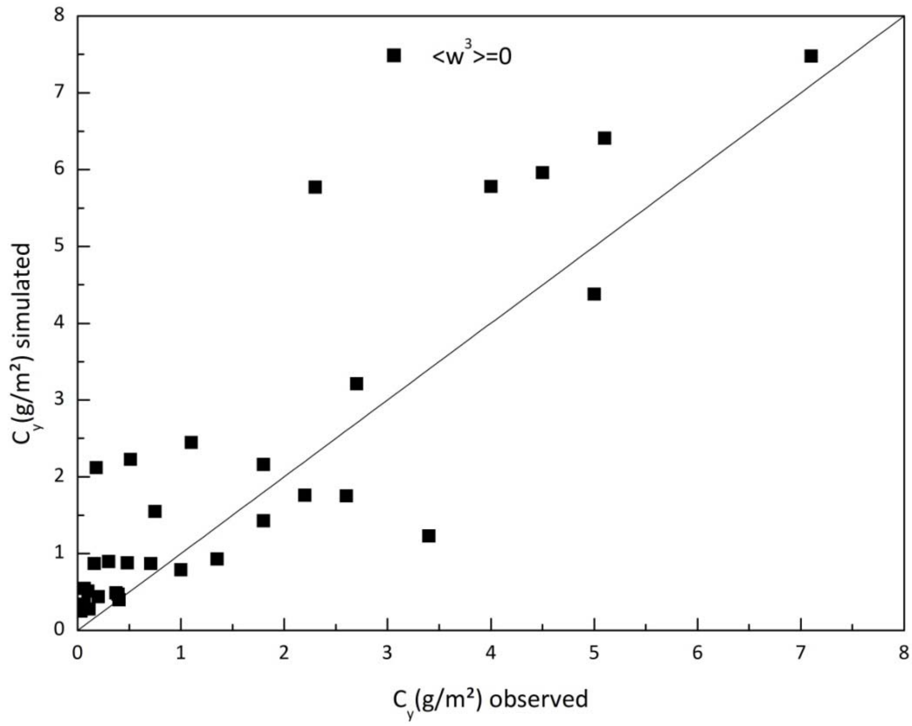

***Figure 6**. Scatter diagram between observed and predicted cross-wind integrated concentrations for the Prairie Grass data set. The Lagrangian simulation results employing* $\overline{w^3} = 0$.

third moment of the vertical velocity from LES data, is well–behaved and is described in the form of a similarity profile using the convective velocity scale and the inversion height. As a test of the new formulation for this third moment, we included this parameterization in a Lagrangian stochastic dispersion model and, utilizing concentration data from dispersion field experiments, we compared it with the expressions suggested by De Baas and Troen (1989) [Equation (2)], Franzese et al. (1999) [Equation (3)] and Kastner–Klein et al. (2001) [Equation (4)]. On analyzing the results and related statistics we can see that the LAMBDA dispersion model reproduces adequately the experimental concentration measurements with the vertical velocity third moment parameterizations utilized. Very good results for the ground–level cross–wind integrated concentrations are obtained with the parameterization proposed from LES data and formulated by the algebraic representation given by Equation (6). This fact shows that when LES–derived Equation (6) is employed in a dispersion model, results are equivalent to those obtained from field experiment measurements. The main difference lies in the fact that LES outputs provide more detail and do not depend on quite difficult observations, which are also somewhat uncertain. In this sense, the present study is a validation of previous experimental efforts. The high quality of the performance of Lagrangian models using both the LES–originated skewness profile or those obtained experimentally suggests that either of these expression may be used with similar results. Although this is certainly a true inference from the analysis presented here, the LES–derived expression has the advantages of relying on data with less uncertainty.

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