ISSN: 2230-9926

Available online at http://www.journalijdr.com

IJDR

International Journal of Development Research
Vol. 10, Issue, 12, pp. 42644-42653, December, 2020
https://doi.org/10.37118/ijdr.20681.12.2020

RESEARCH ARTICLE OPEN ACCESS

A NEW SEGMENTED PLUME APPROACH FOR POLLUTANT DISPERSION MODELLING

Buske, D.[1*], Gonçalves, G.A.[1], Favero, C.[1], Quadros, R.S.[1] and Tirabassi, T[2]

[1]Federal Universityof Pelotas - PPGMMat, IFM/DME, Pelotas, RS, Brazil; [2]Federal University of Santa Maria, Santa Maria, RS, Brazil and Polytechnic University of Marche, Ancona, Italy

ARTICLE INFO

Article History:
Received 22nd September, 2020
Received in revised form
29th October, 2020
Accepted 17th November, 2020
Published online 30th December, 2020

Key Words:
Atmospheric dispersion; Analytical solution; Time-dependent advection-diffusion Equation; Plume segment

****Corresponding author: Buske, D.***

ABSTRACT

A segment approach is presented that allows to describe the temporal evolution of the dispersion of passive pollutants in non-stationary meteorological conditions. The methodology consists of a continuous series of source emissions integrated in time intervals whose result is a plume segment and has no numerical inversion, which refines earlier literature approaches. The dispersion of pollutants is subject to advection in horizontal direction and turbulent diffusion in all three directions, in an inhomogeneous and non-stationary atmospheric boundary layer. For validation, data from the Copenhagen experiment were used, but with a greater time resolution, considering meteorological data with 10 minutes averaged value. The numerical results show that the experimental data and other models from literature are compatible.

Citation: ***Buske, D., Gonçalves, G.A., Favero, C, Quadros, R.S. and Tirabassi, T.*** "A new segmented plume approach for pollutant dispersion modelling*", International Journal of Development Research*, 10, (12), 42644-42653.

INTRODUCTION

Air quality models are important tools in assessing the concentration of pollutants in the atmosphere and are used by regulatory agencies to estimate environmental impacts, risk analysis, and industrial plant planning. The complex dispersion process involves the transport and diffusion of the pollutant material and relies on the meteorological conditions varying according to the characteristics of the emission source and the terrain. Moreover, in cases of environmental accidents or even catastrophes one needs to implement fast procedures, which yield immediate results, such as to be aware of the ground level concentration of pollutants, especially the maximum concentration and its position. Numerical simulation approaches may still be slow in providing a map of concentrations in a short time, when immediate decision-making is imperative, despite the evolution of computing. The computational evaluation of numerical data of the concentration field for a set of position has to be a very fast task. In this regard, analytical models (models which use a solution or an approximation of the solution of the diffusion equation in the atmosphere) are very useful. Analytical solutions have the typical advantages of solutions and analytical formulas, such as they explicitly take into account all the parameters they consider.

But it is the solution of an equation, as well as the numerical models, which are an idyllic description of reality and therefore they suffer from such a characteristic. Numerical models are easier to introduce empirical corrections to mitigate this problem, as for analytical solutions are concerned, this is more delicate though. However, they are important because they help us to fully understand the meaning of the diffusion equation and the system they describe. They can also be used for numerical experiments and they are simpler to perform than field experiments. In scientific literature, there are countless models presented using an analytical expression for calculating the concentrations of airborne material. A concise history of these models can be found in Tirabassi *et al*. (2019). In scientific literature, there is a large number of air pollution models, Eulerian and Lagrangian models, complex models, such as WRF-Chem (Grell *et al*., 2005), and simpler models such as HYSPLIT (https://ready.arl.noaa.gov/HYSPLIT.php). Among analytical approaches, the steady-state Gaussian plume model is the most common approach to describe the three-dimensional concentration field generated by a point source. Its simplified description of the dispersion problem

is restricted to stationary meteorological and emission conditions. Nonetheless, in the last decades, due to the simplicity and easiness of Gaussian model application, research has advanced towards removing some constraints on the behalf of dealing with more realistic situations. In this context, some methods have been developed to calculate the function standard deviation of the Gaussian concentration distribution, sigma function, which are either based on measures of turbulence intensity or in semi-empirical calculations through the use of so-called stability classes of Pasquill. Among the Gaussian models, the best known is AERMOD (https://www. epa.gov/scram/air-quality-dispersion-modeling-preferred-and-recommended-models#aermod), whereas among Gaussian puff models is CALPUFF (http://src.com/). We introduce a solution that follows in the Gaussian footsteps along the horizontal directions, where the Gaussian approach has greater validity, whereas in vertical ones a well-known solution by integral transforms (Moreira *et al*., 2009) is applied. The novelty is represented by a new mathematical approach that comprises the three solutions now interdependent along the reference axes (which is not found that way in the classic Gaussian models). Furthermore, the solution is time-dependent in a discretized manner, thus describing an emission as a plume segment, a plume that as a whole it depends on the time made up of various stationary segments. In section 2 the proposed solution is presented. Experimental data and boundary layer parameterizations are presented in sections 3 and 4, respectively. In section 5, the numerical results and discussions are found. Finally, in section 6 the conclusions.

MODEL DESCRIPTION

The transient three-dimensional equation, advective in the horizontal directions and diffusive in the vertical direction, which describes the mean concentration, per unit of time, of pollutants in the atmosphere of a passive material, released by a source Q, at the initial time $t = 0$, is written as

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} + v\frac{\partial C}{\partial y} = \frac{\partial}{\partial z}\left(K_z\frac{\partial C}{\partial z}\right), \tag{1}$$

in which $C(t,x,y,z)$ is the mean concentration function (kg m^{-3}), $K_z = K_z(z)$ (m^2 s^{-1}) is the vertical eddy diffusion coefficient, u and v are the mean velocities (m s^{-1}) in the longitudinal and transverse directions respectively.

Equation (1) is subject to the usual conditions of null flux at the ground (or roughness), z_0, and at the top of the boundary layer, z_i,

$$K_z\frac{\partial C}{\partial z} = 0, \quad z = z_0 \quad \text{and} \quad z = z_i, \tag{2.a}$$

while the description of the source is formalized below with initial condition, $t = 0$,

$$uC(0,x,y,z) = Q(0)\delta(x)\delta(y)\delta(z - H_s) \tag{2.b}$$

and also, with the condition at $x = 0$,

$$uC(t,0,y,z) = Q(t)C_y(t,y)\delta(z - H_s), \tag{2.c}$$

in which δ represents the Dirac delta function, H_s (m) is the height of the source, Q (Kg m^{-2}s^{-1}) is the intensity of the source and $C_y(t,y)$ is the mean concentration distribution of the pollutant on the y-axis at time t.

The differential equation of the transient three-dimensional dispersion model, Eq. (1), initially considering u and v constants, and $K_z = K_z(z)$, presents solution given by the product of the solutions of the system of equations

$$\frac{d}{dt}T_{\kappa\lambda} = (\kappa - \lambda)T_{\kappa\lambda}, \tag{3.a}$$

$$u\frac{d}{dx}X_{\alpha\lambda} = (\alpha + \lambda)X_{\alpha\lambda}, \tag{3.b}$$

$$v\frac{d}{dy}Y_{\kappa} = -\kappa Y_{\kappa}, \tag{3.c}$$

$$\frac{d}{dz}\left(K(z)\frac{d}{dz}Z_{\alpha}\right) = \alpha Z_{\alpha}, \tag{3.d}$$

where $T_{\kappa\lambda}$, $X_{\alpha\lambda}$, Y_{κ} and Z_{α} are the eigenfunctions and k, λ, α are the respective eigenvalues. This solution can be written as

$$C_{k\lambda\alpha}(t,x,y,z) = [\psi_{\kappa}(t,y)][\phi_{\lambda}(t,x)][\varphi_{\alpha}(x,z)], \tag{4}$$

where each factor that makes up the solution is handledas

$$\psi_{\kappa}(t,y) = T_{\kappa}(t)Y_{\kappa}(y) = e^{-\frac{\kappa}{v}(y - vt)}, \tag{5.a}$$

$$\phi_{\lambda}(t,x) = T_{\lambda}(t)X_{\lambda}(x) = e^{-\lambda\left(t - \frac{x}{u}\right)}, \tag{5.b}$$

$$\frac{\partial}{\partial z}\left(K(z)\frac{\partial}{\partial z}\xi(x,z)\right) = u\frac{\partial}{\partial x}\xi(x,z) \ , \tag{5.c}$$

in which $\xi(x,z) = e^{\alpha x/u}Z_\alpha$. The average concentration solution C is a combination of these eigenfunctions, considering the continuous associated eigen values κ(m) and λ(s^{-1}), in the interval $[0,\infty)$, and the mean concentration is then expressed as:

$$C(t,x,y,z) = \psi(t,y)\phi(t,x)\xi(x,z) \ , \tag{6}$$

with:

$$\psi(t,y) = \int_0^\infty A(\kappa)\psi_\kappa(t,y)d\kappa, \tag{7}$$

$$\phi(t,x) = \int_0^\infty B(\lambda)\phi_\lambda(t,x)d\lambda, \tag{8}$$

where $A(\kappa)$ and $B(\lambda)$ are expansion coefficients and, in appendix 1, the solution for Eq. (7) and Eq. (8) are presented. The $\xi(x,z)$ function comes from the solution of problem (5.c) by integral transforms (Moreira *et al*. (2009), Buske *et al*. (2012)) and the details of the solution are given in appendix 2.

Consequently, the solution is given by the product of (A1.7), (A1.13) and (A2.4):

$$C(t,x,y,z) = Q\left(t-\frac{x}{u}\right)C_y(y-vt)\xi(x,z) \ . \tag{9}$$

Atthis point, considering $Q(t-\tau) = 2QH(t-\tau)$, in which H is Heaviside function,then $dQ(t-\tau) = 2Q\delta(t-\tau)d\tau$, and$C_y\big(y-v(t-\tau)\big) = \delta\big(y-v(t-\tau)\big)$. It follows from Eq. (9) that the mean concentration increment of the pollutant is given by

$$dC(t,x,y,z) = 2Q\delta\left((t-\tau)-\frac{x}{u}\right)\delta(v(t-\tau)-y)d\tau\ \xi(x,z) \ . \tag{10}$$

where

$$dC(t,\tau,x,y,z) = \frac{dC(t,\tau,x,y,z)}{d\tau}d\tau$$

Dirac delta functions can be represented by the limit of a Gaussian function

$$\delta\left((t-\tau)-\frac{x}{u}\right) = \lim_{K_x\to 0}\frac{u}{\sqrt{4\pi K_x(x/u)}}e^{-\frac{[u(t-\tau)-x]^2}{4K_x x/u}} \tag{11}$$

and,

$$\delta(v(t-\tau)-y) = \lim_{K_y\to 0}\frac{1}{\sqrt{4\pi K_y(x/u)}}e^{-\frac{[v(t-\tau)-y]^2}{4K_y\, x/u}} \tag{12}$$

then results the equation

$$2Q\delta\left(t-\frac{x}{u}\right)\delta(vt-y) = \lim_{K_y\to 0}\lim_{K_x\to 0}\frac{2Qu}{\sqrt{16\pi^2K_xK_y(x/u)^2}}e^{-\frac{[u(t-\tau)-x]^2}{4K_x x/u}}e^{-\frac{[v(t-\tau)-y]^2}{4K_y x/u}}, \tag{13}$$

where x/u is the so-called travel time, K_x and $K_y$are respectively the diffusion coefficients in the *x* and *y*directions.However, to have physical significance the limit condition must be relaxed to cover diffusion in horizontal directions. Thus, the solution is posed as:

$$dC(t,x,y,z) = \frac{2Qu}{\sqrt{16\pi^2K_xK_y(x/u)^2}}e^{-\frac{[u(t-\tau)-x]^2}{4K_x x/u}}e^{-\frac{[v(t-\tau)-y]^2}{4K_y x/u}}d\tau\ \xi(x,z) \ . \tag{14}$$

If a problem with an arbitrary source $Q(t)$ emitting at an interval $(t_0,t)$is considered, the solution to the problem through the superposition principle is given by τ integration over interval $[t_0,t]$.

$$C(t,x,y,z) = \int_{t_0}^t dC(t,\tau,x,y,z) = \frac{2uQ}{\sqrt{16\pi^2K_yK_x(x/u)^2}}\int_{t_0}^t e^{-\frac{(v(t-\tau)-y)^2}{4K_y x/u}}e^{-\frac{(u(t-\tau)-x)^2}{4K_x x/u}}d\tau\ \xi(x,z). \tag{15}$$

It should be clear that in this solution the diffusion coefficients appear, K_x and K_y, so this is a diffusive solution in the horizontal directions.

After simple algebraic manipulation:

$$C(t,x,y,z) = 2Qu\frac{1}{\pi D}\int_{t_0}^{t} e^{-\frac{(A\tau^2+B\tau+E)}{D}} d\tau\ \xi(x,z), \quad (16)$$

in which

$$A = 4(x/u)(K_x u^2 + K_y v^2), \quad (17.a)$$

$$B = 8(x/u)[K_y u(x-ut) + K_x v(y-vt)], \quad (17.b)$$

$$D = 16K_x K_y (x/u)^2\ , \quad (17.d)$$

$$E = 4(x/u)[K_x(x-ut)^2 + K_y(y-vt)^2]\ . \quad (17.c)$$

The solution (16) is then posed as:

$$C(t,x,y,z) = \frac{Qu}{\sqrt{\pi A}} e^{\frac{(-4CA+B^2)}{4DA}}\left[erf\left(\frac{2At+B}{2\sqrt{AD}}\right) - erf\left(\frac{2At_0+B}{2\sqrt{AD}}\right)\right]\xi(x,z), \quad (18)$$

where *erf* is the error function.

It is possible to use the solution (18) in time intervals to simulate the concentration of pollutants in non-stationary meteorological conditions. Thus, for each time interval $\Delta t_j = [t_{j-1}, t_j]$, the source is composed of a set of plume segments:

$$Q(t) = \frac{2u}{\pi D}\int_0^t Qe^{-\frac{(A\tau^2+B\tau+E)}{D}}d\tau = \frac{2}{\pi}\sum_{j=1}^{N}\frac{u}{D}\int_{t_{j-1}}^{t_j} Qe^{-\frac{(A\tau^2+B\tau+E)}{D}}d\tau, \quad (19)$$

in which the index j designates the j_{th} interval, where $t_0 = 0$ and $t_N = t$. This formulation allows the simulation of different meteorological conditions measured at each interval $[t_{j-1}, t_j]$. The solution (19) will then be given by:

$$C(t,x,y,z) = \sum_{j=1}^{N}\frac{Q_j u_j e^{\frac{\left(-4E_jA_j+B_j^2\right)}{4D_jA_j}}}{\sqrt{\pi A_j}}\left[erf\left(\frac{2A_jt_j+B_j}{2\sqrt{D_jA_j}}\right) - erf\left(\frac{2A_jt_{j-1}+B_j}{2\sqrt{D_jA_j}}\right)\right]\xi_j(x,z)\ . \quad (20)$$

This equation represents the micrometeorological model that allows one to deal with temporal and spatial variations, such as wind speed, boundary layer height, and Monin-Obukhov length parameters.

EXPERIMENTAL DATA SET

To carry out a preliminary assessment of the model's performances we used the Copenhagen experimental data set (described by Gryning and Lyck (1984) and Gryning *et al*. (1987) and updated by Gryning and Lyck (2002)). In the Copenhagen experiment the tracer SF_6 was continuously released without buoyancy from a tower at a height of 115 m, and collected at ground level. The sampling units were positioned at the distances of 2 to 6 km from the point of pollutant release. The site was mainly residential with a roughness length of 0.6 m. The meteorological conditions during the dispersion experiments ranged from neutral to convective. The values of the maximum concentrationsof crosswind arc, normalized by the emission rate, from Gryning *et al*. (1987), were used. Generally, the distributed data set contains hourly mean values of concentrations and meteorological data. However, in this work we used data with a greater time resolution, meteorological data with10 minutes averaged value were used in particular. The data for experiment 6 is not available. Tables 1, 2 and 3 report the friction velocity (u_*) Monin-Obukhov length (L), the hourly average boundary layer height (z_i) and wind speed at 10m (only one value and direction for each trial), respectively which were used in the simulations.

Table 1. Friction velocity (m s^{-1}) for the different trials and time steps of the Copenhagen experiment. Every time step corresponds to 10 min

Time	Trial							
step	1	2	3	4	5	7	8	9
1	.36	.68	.46	.56	.58	.48	.65	.72
2	.37	.67	.45	.51	.52	.48	.79	.73
3	.40	.81	.47	.37	.51	.57	.67	.60
4	.43	.68	.39	.44	.58	.62	.67	.59
5	.35	.75	.39	.48	.59	.53	.68	.65
6	.34	.74	.40	.48	.52	.65	.65	.71
7	.42	.76	.40	.39	.52	.63	.68	.73
8	.43	.82	.41	.40	.45	.65	.67	.73
9	.40	.76	.31	.39	.44	.66	.73	.73
10	.37	.73	.34	.39	.44	.62	.73	.66
11	.35	.69	.39	.39	.44	.52	.75	.67
12	.36	.66	.40	.39	.43	.62	.69	.74

Table 2. Monin-Obukhov length (m) for the different trials and time steps of the Copenhagen experiment. Every time step corresponds at 10 min

Time	Trial							
step	1	2	3	4	5	7	8	9
1	-26	-178	-152	-75	-492	-71	-71	-793
2	-23	-227	-194	-42	-215	-80	-85	-471
3	-83	-311	-106	-23	-368	-64	-47	-202
4	-42	-160	-101	-32	-735	-111	-49	-366
5	-36	-203	-129	-71	-366	-177	-45	-633
6	-42	-286	-70	-80	-273	-67	-63	-13588
7	-47	-155	-83	-83	-273	-87	-41	-593
8	-38	-228	-60	-101	-262	-71	-47	-471
9	-83	-184	-106	-129	-395	-56	-70	-389
10	-21	-389	-42	-129	-395	-111	-64	-375
11	-32	-133	-101	-129	-395	-215	-52	-262
12	-29	-375	-70	-129	-759	-123	-39	-252

Table 3. Hourly average boundary layer height and wind speed measured at a 10 m height for the different trials of the Copenhagen experiment

	Trial							
	1	2	3	4	5	7	8	9
zi (m)	1980	1920	1120	390	820	1850	810	2090
u (m/s)	2.1	4.9	2.4	2.5	3.1	4.1	4.2	5.1

The vertical convective velocity (w_*) was evaluated from the 10 minute-averaged value of friction velocity and Monin-Obukhov length and the hour averaged boundary layer height standpoint using the formula $w_* = u_*(-z_i/kL)^{1/3}$, where κ is the von-Karman constant.

BOUNDARY LAYER PARAMETERIZATION

In order to investigate the performance of the present segment model, were selected two formulations for the turbulent diffusion coefficient for the vertical dispersion and one for the horizontal dispersions.

For the vertical dispersion, in the first formulation, during convective conditions at $\frac{z_i}{L} \leq -10$ the following relation is used (Pleim and Chang, 1992):

$$K(z) = kw_*z\left(1 - \frac{z}{z_i}\right), \tag{21}$$

while during stable and neutral conditions at $\frac{z_i}{L} \geq -10$:

$$K(z) = ku_*z\left(1 - \frac{z}{z_i}\right)^2/\emptyset_h \quad , \tag{22}$$

where $\emptyset_h = 1 + 5(z/L)$in stable conditions and $\emptyset_h = 1$ in neutral conditions. For the second formulation (Degrazia *et al*., 1997):

$$K(z) = 0.22\left(1 - e^{-4\frac{z}{z_i}} - 0.0003e^{8\frac{z}{z_i}}\right)z_i w_*\left(\frac{z}{z_i}\right)^{\frac{1}{3}}\left(1 - \frac{z}{z_i}\right)^{\frac{1}{3}} \quad , \tag{23}$$

in which w_* is the convective velocity scale.

The horizontal diffusion coefficients are given in the form(Willis and Deardorff ,1976):

$$K_h = 0.1w_*z_i. \tag{24}$$

In this study, the mean wind is parameterized assuming the power law representation (Panofsky and Dutton, 1984), because it is simple and valid for the whole atmospheric boundary layer. That is:

$$u(z) = U_{10}\left(\frac{z}{z_i}\right)^{\alpha} \quad , \tag{25}$$

where α is a function of stability (Irwin, 1979) which for the Copenhagen experiment is assumed to be equal to 0.1, andU_{10} is the standard wind speed at 10 meters above the ground.

Theseboundary layer parameterizations, chosen by the authors on an informed basis, are used as an example. In fact,a feature of the present methodologyis to accept any profile of the wind and of the turbulent diffusion coefficients.

NUMERICAL RESULTS AND DISCUSSION

In this study the eddy diffusivities and the wind profile described in section 4 were introducedin the newsegmentapproach (Eq. (18, 20)) to calculate the ground-level concentration of emissions released from an elevated continuous source point in an unstable/neutral atmospheric boundary layer. Following the work of Moreira *et al*. (2009), the number of eigenvalues used to truncate the summation of $\xi(x,z)$was n=100.

Application to different meteorological scenarios : In the sequence the behavior of the solution in different meteorological and turbulence scenarios is presented. In Fig.1, the non-dimensional concentration in function of the non-dimensional distance from the source (H_s=0.1z_i) for five different meteorological scenariosis presented, showing the influence of the atmospheric turbulence. In Tab. 4 are presented the exponent of the wind profile (α) associated with each inverse of Monin-Obukhov length (1/L) values for the different meteorological scenarios (Panofsky and Dutton, 1984). The eddy diffusivities (21), (22) and (24) are used. A graphical representation of the ground level concentrations predicted for different source heights in convective condition are shown in Fig. 2 showing the traditional behavior.

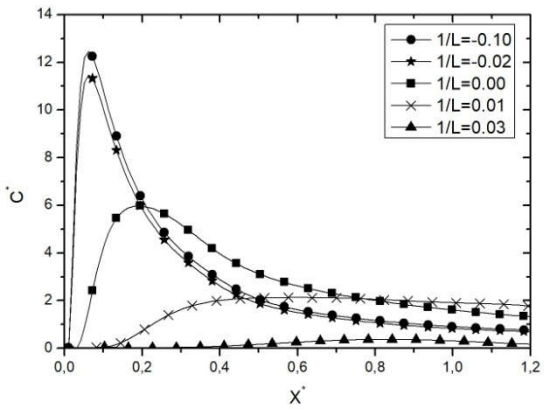

Figure 1. Non-dimensional concentration (C*= C uz_i^2/Q) in function of the non-dimensional distance (X*=xu*/uz_i) from the source (H_s=0.1z_i) for 5 different meteorological scenarios

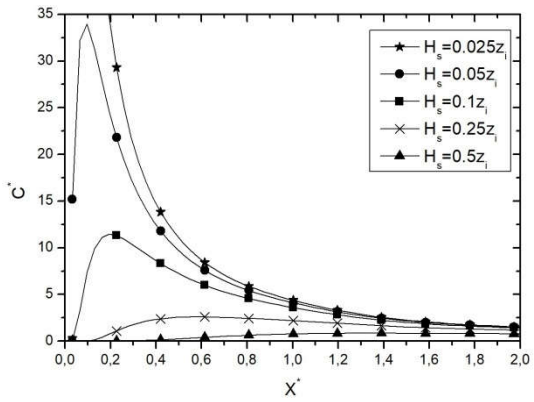

Figure 2. Ground level non-dimensional concentrationssolution (C*= C uz_i^2/Q) in function of the non-dimensional distance (X*=x u*/uz_i) for different source heights in convective conditions (1/L = −0.01 m^{-1})

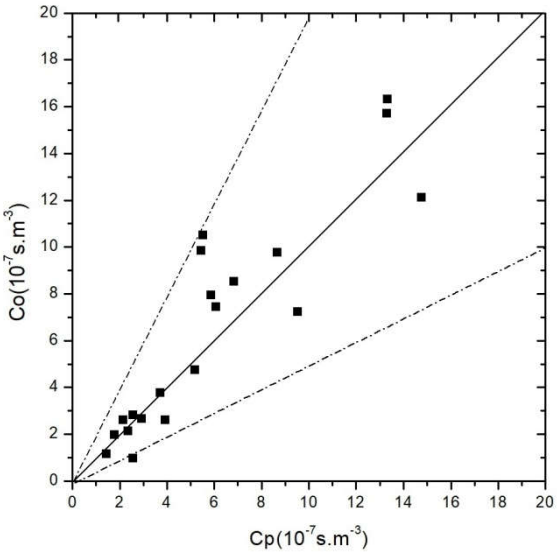

Figure 3. Observed and predicted scatter diagram of ground-level centerline concentrations using the new segment model (Eq. 20) for the Copenhagen experiment. Lines and dashes indicate a factor of two

Results of the segmentapproach for the Copenhagen experiment

The results obtained by the new segmentapproach are compared with the data set from the Copenhagen experiment.Eddy diffusivities (21), (23) and (24) are used. Figure 3show the comparison of segmentmodel concentrations against observed datain the Copenhagen experiments using observed and predicted scatter diagram of ground-level centerline concentrations. We can observe that the obtained concentrations reproduce the observed datareasonably well. Table 5 shows the hourly average concentrations observed in the Copenhagen experiment (C_o) and the concentrations obtained with the segment model using the parameterization suggested by Pleimand Chang (called here as C_1) and the ones obtained with the parameterization suggested by Degrazia (called as C_2), respectively Eq. (21) and Eq. (23) along with Eq. (24). In Tab.5 are also presented the results obtained by the GILTT model (presented as C_3) (Tirabassi *et al*., 2013).Whereas the present segment approach is based on three-dimensional description without numerical inversions, theintegral transforms approach GILTT, uses Gaussian Quadrature to numericallyinvert

the time variable(Tirabassi *et al*., 2013). The authors used the same data set, the parameterization suggested by Degrazia (Eq. (23)), as in solution (2), with a horizontal diffusion coefficient given by Degrazia et. al (1997):

$$K_y = \frac{\sqrt{\pi}\sigma_v}{16(f_m)_v q_v}, \tag{26}$$

with $\sigma_v^2 = \frac{0.98 c_v}{(f_m)_v^{2/3}} \left(\frac{\psi_\varepsilon}{q_v}\right)^{2/3} \left(\frac{z}{z_i}\right)^{2/3} w_*^2$; $\psi_\varepsilon^{1/3} = \left[\left(1 - \frac{z}{z_i}\right)^2 \left(-\frac{z}{L}\right)^{-2/3} + 0.75\right]^{1/2}$, $q_v = 4.16 \frac{z}{z_i}$ and

and $(f_m)_v = 0.16$ is the peak wavelength of the turbulent velocity spectra, σ_v is the Eulerian standard deviation of the longitudinal turbulent velocity, q_v is the stability function andψ_ε is the non-dimensional molecular dissipation rate function.

Results from the puff model ofSilva *et al*.(2013), a three-dimensional non-gaussian puff model, where the turbulent diffusion in the puffs is given by analytical solutions are also displayed in Tab. 5 as (C_4). The puff model usesthe Pleim and Chang parameterization (Eq. (21)) and horizontal coefficients given by Eq. (24).

Table 4. Exponent of power wind profile (α) and inverse of Monin-Obukhov length (1/L) values for different meteorological scenarios (Panofsky and Dutton, 1984)

Scenario	alpha	1/L
Unstable	0.07	-0.10
Unstable	0.10	-0.02
Neutral	0.15	0.00
Stable	0.35	0.01
Stable	0.55	0.03

Table 5. Observed (C_0) and predicted (C_p) maximum concentrations of crosswind arc,normalized by the emission rate (10^{-7}s.m^{-3}) at different distances from the source (m) for the segment approach with Pleim and Chang parametrization (C_1), segment approach with Degrazia parametrization (C_2), non-gaussian GILTT model (C_3) and non-gaussian puff model (C_4)

			C_p			
Run	Distance	C_o	1	2	3	4
1	1900	10.50	4.96	5.53	8.50	3.68
1	3700	2.14	2.23	2.36	2.90	1.64
2	2100	9.85	4.96	5.45	5.08	3.13
2	4200	2.83	2.30	2.56	1.88	1.64
3	1900	16.33	12.78	13.31	12.41	10.24
3	3700	7.95	5.74	5.85	4.26	4.57
3	5400	3.76	3.74	3.71	2.18	3.68
4	4000	15.71	13.52	13.28	6.71	15.75
5	2100	12.11	14.63	14.75	11.69	17.39
5	4200	7.24	9.45	9.52	4.46	7.59
5	6100	4.75	5.26	5.17	2.40	3.68
7	2000	9.48	5.50	6.08	5.68	3.47
7	4100	2.62	1.96	2.13	1.95	1.47
7	5300	1.15	1.35	1.43	1.25	1.00
8	1900	9.76	8.58	8.67	6.74	10.96
8	3600	2.62	3.99	3.91	2.55	5.80
8	5300	0.98	2.64	2.55	1.44	3.43
9	2100	8.52	6.56	6.82	5.51	3.71
9	4200	2.66	2.58	2.93	2.11	1.85
9	6000	1.98	1.59	1.78	1.15	1.06

Table 6. Statistical comparison between models using the Copenhagen dataset

	NMSE	COR	FA2	FB	FS
Segmented model – Eq. (21)	0.14	0.89	0.90	0.14	0.15
Segmented model –Eq. (23)	0.11	0.91	0.95	0.11	0.15
GILTT	0.30	0.90	0.95	0.36	0.35
Puff GILTT	0.36	0.75	0.67	0.21	-0.03
SPM	0.32	0.58	0.78	-0.23	0.00
INPUFF	0.50	0.49	0.74	0.12	---

Further, standard statistical indicesare used in order to compare the quality of the new approach against other models. Table 6 present some performances evaluations of the model results using the statistical evaluation procedure described by Chang and Hanna (2004) and defined in the following way:

NMSE (normalized mean square error) = $\overline{(C_o - C_p)^2} / \overline{C_p}\,\overline{C_o}$,

FA2 = fraction of data (%, normalized to 1) for $0.5 \leq (C_p/C_o) \leq 2$,

COR (correlation coefficient) = $\overline{(C_o - \overline{C_o})(C_p - \overline{C_p})} / \sigma_o \sigma_p$,

FB (fractional bias) = $(\overline{C_o} - \overline{C_p})/0.5(\overline{C_o} + \overline{C_p})$,

FS (fractional standard deviations) = $(\sigma_o - \sigma_p)/0.5(\sigma_o + \sigma_p)$,

where C is the concentration, $\sigma$the standard deviation and the subscripts *o* and *p*refer to observed and predicted quantities, respectively, and the overbar indicates an averaged value. The statistical index FB says whether the predicted quantities underestimate or overestimate the observed ones. The statistical index NMSE represents the model values dispersion in respect to data dispersion. The best results are expected to have values near to zero for the indices NMSE, FB and FS, whereasnear to 1 for the indices COR and FA2. The statistical indices point out that a reasonable agreement is obtained between experimental data and the new model. The analysis of the statistical evaluation shows a reasonable agreement (displayed in lines 1 and 2 of Tab.6) between the computed values against the experimental ones. Furthermore, in Tab.6, we compared the model with other models from the literature: GILTT (Tirabassi *et al*., 2013), Puff GILTT (Silva *et al*., 2013), INPUFF (Petersen *et al*., 1984) and SPM (Tirabassi and Rizza, 1995). The first two models are non-gaussian models and were described above, INPUFF is a Gaussian puff model and SPM utilizes approximate solutions proposed by van Ulden(1992) for a dispersion of a skewed cloud of passive contaminant released from a source in the surface layer. Tables 5 and 6 allow to assert that the presented model and the results previously obtained with the GILTT method are very similar. The advantage in the presented model is to avoid to perform the numerical inversion in the time which allows us to obtain the final result more quickly.

CONCLUSIONS

Analytical solutions of equations are of fundamental importance in understanding and describing physical phenomena. They explicitly take into account all the parameters of a problem so that their influence can be reliably investigated, which is usually difficult to generate through numerical calculations. Moreover, the maximum ground level concentration can be easily obtained. We present a new non-gaussian solution of the advection-diffusion equation.The novelty of the solution compared to similar models in literature (Moreira *et al*. (2009); Buske *et al*. (2012); Tirabassi *et al*. (2013); Silva *et al*. (2013)) demands less computational effort once no numerical inversions are made to obtain the final concentration solution, and therefore suitable for environmental problems where a fast response is required. The solution is time-dependent, but a continuous series of source emissions are integrated in time intervals whose result is a plume segment. In the plume segment approach, the plume is broken up into independent sections whose initial feature and time dynamics are functions of time-varying emissions conditions and local time-varying meteorological conditions encountered. Furthermore, the statistical evaluation of the performance of the model was carried out, using two different parametrizations, and both gave good results, comparable to that of other models known in the scientific literature. This article can be considered a preliminary evaluation and we plan to extend the validation of other experimental datain the future.Finally, we wish to stress that rather than a model, we wanted to present a methodology to be used by anyone to assemble models, being able to use other parameters of the boundary layer.In fact, the solution presented is general in the sense that it accepts any wind and eddy diffusion coefficients profile.

APPENDIX 1

Development of functions $\psi(t,y)$ and $\phi(t,x)$ from Eq. (7) and Eq. (8).

To determine the eigenfunctions, the initial condition and the condition at $t = 0$ are used. First, the initial condition imposed on the problem is used:

$$uC(0,x,y,z) = u\psi(0,y)\phi(0,x)\xi(x,z) = Q(0)\delta(x)C_y(0,y)\delta(z - H_s), \quad \text{(A1.1)}$$

and equalities can be established:

$$\begin{cases} \psi(0,y) = C_y(0,y) \\ \phi(0,x) = Q(0)\delta(x) \\ u\,\xi(x,z) = \delta(z - H_s) \end{cases} . \quad \text{(A1.2)}$$

The unit of the solution factors are: ψ (dimensionless), ϕ (kg m^{-2} s^{-1}) and ξ (s m^{-1}). With the equalities established in (A1.2), the integral relative to the continuous eigenvalue κ can be find.

To solve the integral appearing in (7), the following development using (5.a) is made:

$$\psi(t,y) = \int_0^\infty A(\kappa)\psi_\kappa(t,y) = \int_0^\infty A(\kappa)e^{-\frac{\kappa}{v}(y - vt)}d\kappa \, . \quad \text{(A1.3)}$$

After some algebraic manipulation and a transformation of variables ($\eta = \frac{\kappa}{v}; d\eta = \frac{1}{v}d\kappa; vA(\kappa) = D(\eta)$):

$$\psi(t,y) = \int_0^\infty D(\eta)e^{-\eta(y - vt)}d\eta, \quad \text{(A1.5)}$$

For $t = 0$,

$$\psi(0,y) = C_y(0,y) = \int_0^\infty D(\eta)e^{-\eta y}d\eta \quad \text{(A1.6)}$$

this means that $C_y(0,y)$ is a Laplace transform. Therefore $D(\eta) = L^{-1}\{C_y(0,y), y \to \eta\}$, in which L^{-1} means the inverse Laplace transform. So,

$$\psi(t,y) = \int_0^\infty L^{-1}\{C(0,y), y \to \eta\} e^{-\eta(y-vt)} d\eta = C_y(y-vt) \quad \text{(A1.7)}$$

Now using the condition in $x = 0$,

$$uC(t,0,y,z) = Q(t)c_y(t,y)\delta(z-H_s) = u\psi(t,y)\phi(t,0)\xi(0,z), \quad \text{(A1.8)}$$

and since $\psi(t,y) = C_y(y-vt)$, the problem to be solved is:

$$Q(t)\delta(z-H_s) = \phi(t,0)u\xi(0,z), \quad \text{(A1.9)}$$

Then, once again is possible to establish the equalities:

$$\begin{cases} \phi(t,0) = Q(t) \\ u\,\xi(0,z) = \delta(z-H_s) \end{cases} . \quad \text{(A1.10)}$$

Following a similar procedure, done previously to find $\psi(\mathrm{t},y)$, the solution of Eq. (8) is given by

$$\phi(t,x) = \int_0^\infty B(\lambda)\phi_\lambda(t,x)d\lambda = \int_0^\infty B(\lambda)e^{-\lambda(t-\frac{x}{u})}d\lambda \ , \quad \text{(A1.11)}$$

considering x = 0, and using Eq.(A1.9),

$$\phi(0,t) = Q(t) = \int_0^\infty B(\lambda)e^{-\lambda t}d\lambda, \quad \text{(A1.12)}$$

this means that $Q(t)$ is a Laplace transform and so $B(\lambda) = L^{-1}\{Q(t), t \to \lambda\}$. Therefore,

$$\phi(t,x) = \int_0^\infty L^{-1}\{Q(t), t \to \lambda\} e^{-\lambda\left(t-\frac{x}{u}\right)}d\lambda = Q\left(t-\frac{x}{u}\right). \quad \text{(A1.13)}$$

APPENDIX 2

Here the solution of Eq. (5c) by integral transforms is presented. Details about this well-known solution derivation are found in Moreira *et al*. (2009) and Buske *et al*. (2012).

Considering the two-dimensional advection-diffusion problem,

$$\frac{\partial}{\partial z}\left(K(z)\frac{\partial}{\partial z}\xi(x,z)\right) = u\frac{\partial}{\partial x}\xi(x,z), \quad \text{(A2.1)}$$

and subject to the boundary and initial conditions:

$$K_z\frac{\partial\xi(x,z)}{\partial z} = 0 \text{at } z = 0, z_i \quad \text{(A2.2)}$$

$$u\,\xi(0,z) = \delta(z-H_s) \qquad \text{at } x = 0 \quad \text{(A2.3)}$$

Following the work of Moreira *et al*. (2009) we pose that the solution of problem (A2.1) has the form:

$$\xi(x,z) = \sum_{n=0}^{N}\bar{\zeta}_n(x)\Psi_n(z), \quad \text{(A2.4)}$$

where $\Psi_n(z)$ are the eigenfunctions of the associated Sturm-Liouville problem, we mean, $\Psi_n(z) = cos(\alpha_n z)$ where $\alpha_n = \frac{n\pi}{h}$ (*n=0,1,2,...*) are the respective discreet eigenvalues.

To determine the unknown coefficient $\bar{\zeta}_n(x)$ we replace Eq. (A2.4) in Eq. (A2.1), and taking moments it come out with the result in matrix form like:

$$Y'(x) + FY(x) = 0, \quad \text{(A2.5)}$$

subject to the condition:

$$Y(0) = \bar{\zeta}_n(0). \quad \text{(A2.6)}$$

Here *Y(x)* is the vector whose components are $\bar{\zeta}_n(x)$ and $= R^{-1}.S$; $R = \{r_{n,m}\}$ and $S = \{s_{n,m}\}$ are the matrices whose entries are respectively:

$r_{n,m} = -\int_0^h u\Psi_n\Psi_m\, dz$ and $s_{n,m} = \int_0^h K'_z\Psi_n'\Psi_m\, dz - \alpha_n^2 \int_0^h K_z\, \Psi_n\Psi_m dz$.

For the source condition (Eq. (A2.3)), after a similar procedure, we have:

$\bar{\zeta}_n(0) = \Psi_m(H_s)P^{-1}$, (A2.7)

where $P^{-1}$is the inverse matrix of A given by $p = \int_0^h u\, \Psi_n(z)\Psi_m(z)\, dz$.

Finally, the transformed problem represented by the Eq. (A2.5) can be solved by the Laplace Transform technique and diagonalization.

Acknowledgments: The authors would like to thank CNPq (Conselho Nacional de DesenvolvimentoCientífico e Tecnológico) and Regione Marche (Italy) for the partial financial support of this work.

REFERENCES

Buske, D., Vilhena, M.T., Tirabassi, T., Bodmann, B., 2012. Air pollution steady-state advection-diffusion equation: The general three-dimensional solution. J. Environ. Protection, 3, 1124-1134.

Chang, J.C., Hanna, S.R., 2004. Air quality model performance evaluation. Meteorol. Atmos. Phys. 87, 167–196.

Degrazia, G.A., Campos Velho, H.F., Carvalho, J.C., 1997. Nonlocal exchange coefficients for the convective boundary layer derived from spectral properties. Contr. Atmos. Phys., 57-64.

Grell, G.A., Peckham, S.E., Schmitz, R., McKeen, S.A., Frost, G., Skamarock, W.C., Eder, B., 2005. Fully coupled 'online' chemistry in the WRF model. Atmos. Environ. 39, 6957-6976.

Gryning, S.E., Holtslag, A.A.M., Irwin, J.S., Siversten, B., 1987. Applied dispersion modelling based on meteorological scaling parameters. Atmos. Environ. 21, 79–89.

Gryning, S.E., Lyck, E., 1984. Atmospheric dispersion from elevated source in an urban area: comparison between tracer experiments and model calculations. J. Appl. Meteor. 23, 651–654.

Gryning, S.E., Lyck, E., 2002. The Copenhagen tracer experiments: reporting of measurements. Riso National Laboratory, 74 pp.

Irwin, J. S. 1979: A theorical variation of the wind profile power-law exponent as a function of surface roughness and stability, 13,191-194.

Moreira, D. M., Vilhena, M. T., Buske, D., Tirabassi, T., 2009. The state-of-art of the GILTT method to simulate pollutant dispersion in the atmosphere. Atmos. Research, 92, 1-17.

Panofsky, H.A., Dutton, J.A., 1984. Atmospheric turbulence. John Wiley & Sons, New York.

Petersen, W.B., Catalano, J.A., Chico, T., Yuen, T.S., 1984. INPUFF – a single source Gaussian puff dispersion algorithm. EPA-600/8-84-027, U.S. Environmental Protection Agency, Raleigh (NC –USA).

Pleim, J., Chang, J.S., 1992. A Non-Local Closure Model for Vertical Mixing in the Convective Boundary Layer. Atmos. Environ. 26 (6), 965–981.

Silva, E.J.G.,Tirabassi, T., Vilhena, M.T., Buske, D. , 2013. A puff model using a three-dimensional analytical solution for the pollutant diffusion process. Atmos. Research, 134, 131-136.

Tirabassi, T., Rizza, U., 1995. A practical model for the dispersion of skewed puffs. J. Appl. Meteor. 34, 989–993.

Tirabassi, T., Silva, E.J.G.,Buske, D. and Vilhena, M.T. 2019. A solution of the time-dependent advection-diffusion equation, Int. J. Environment and Pollution, 65, 211–228.

Tirabassi, T., Vilhena, M.T., Buske, D., Degrazia, G.A., 2013.An Analytical Air Pollution Model with Time Dependent Eddy Diffusivity. J. Environ. Protection, 4, 16-23.

van Ulden, A. P., 1992. A surface-layer similarity model for the dispersion of a skewed passive puff near the ground. Atmos. Environ., 26A, 681–692.

Willis, G.E., Deardorff, J.W., 1976. A laboratory model of diffusion into the convection planetary boundary layer. Quart. J. Royal Meteor. Soc., 102, 427-445.

****