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Article

An Analytical Simple Formula for the Ground Level Concentration from a Point Source

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Abstract: The Advection-Diffusion Equation is solved for a constant pollutant emission from a point-like source placed inside an unstable Atmospheric Boundary Layer. The solution is obtained adopting the novel analytical approach: Generalized Integral Laplace Transform Technique. The concentration solution of the equation is expressed through an infinite series expansion. After setting a realistic scenario through the wind and diffusivity parameterizations, the Ground Level Concentration (GLC) is determined, and an explicit approximate expression is provided for it, allowing an analytically simple expression for the position and value of the maximum. Remarks arise regarding the ability to express value and position of the GLC as explicit functions of the parameters defining the Atmospheric Boundary Layer scenario and the source height.

Keywords: air pollution modeling; analytical solutions; advection-diffusion equation; maximum concentration

1. Introduction

Irreversible consequences of air pollution in the Atmospheric Boundary Layer (ABL) and instances of environmental accidents or even catastrophes demand increasing real time environmental monitoring and control as a routine instrument. In order to evaluate such scenarios one needs efficient procedures, which yield immediate results, for instance evaluating the ground level concentration of pollutants, and especially the maximum concentration and its position. Numerical simulation approaches may in fact still be too slow to provide a map of concentrations in real time, when immediate decisions are necessary. However, analytical solutions for theoretical models are independent of a specific situation and function by parameter estimation. The computational evaluation of numerical data of the concentration field or for a set of positions is an instant task. In view of this, the current work presents a derivation of compact phenomenological formula extracted from the analytical GILTT (Generalized Integral Laplace Transform Technique) [1] approach which permits determination of the ground level concentration in terms of physical parameters.

2. A Short Review of Solutions of the Advection-Diffusion Equation

The analytical solution of the Advection-Diffusion Equation (ADE) has been performed following different approaches based on Gaussian and non-Gaussian solutions. Gaussian solutions represent a rather easy operative tool to handle. Non-Gaussian analytical solutions represent a more realistic approach to represent atmospheric diffusion. However, solutions using non-Gaussian approaches are much harder to achieve, and are often restricted only to rather simple parameterization profiles. A short review in analytically solving the ADE is provided.

A two-dimensional (2-D) steady-state solution of the ADE is shown by [2] for ground source only. Parameterization of the ABL is realized through a power law for the wind $u(z)$ and the diffusivity $k_z(z)$, respectively. A solution for elevated sources has been provided by [3] but only considering linear profiles of the diffusivity. Van Ulden [4] presented a solution based on the Monin-Obukhov similarity theory, the ABL parameterizations of which follow power law profiles. Such a solution upgrades that given in [2] allowing it to be applied to higher source heights inside the surface layer. The solution was implemented in a Skewed Puff Model [5].

Another 2-D solution has been worked out by Smith [6] where both $u(z)$ and $k_z(z)$ follow a power law profile satisfying the conjugate law of Schmidt (that is: "wind exponent" = 1 − "$k_z(z)$ exponent"). An alternative solution uses constant $u(z)$ and a piecewise continuous power law function for $k_z(z)$ [7].

Scriven and Fisher [8] proposed a solution solving the stationary ADE for long-range distances. Results were provided for constant $u(z)$ and linear profiles of $k_z(z)$ inside the surface layer, and constant above, dry and wet deposition effects were included. References [9] and [10] presented 2-D solutions of the ADE for elevated source and with power profiles for both $u(z)$ and $k_z(z)$. However, the solution assumes infinite height of the ABL.

Demuth [11] provided a further solution with power law parameterizations with the more realistic assumption of a bounded ABL. Such a solution involves a series expansion of the concentration in terms of the Bessel functions. The solution has been implemented in the KAPPAG model [12].

Then [13] extended the solution of [11] with boundary conditions suitable for simulating dry deposition to the ground.

Nieuwstadt [14] presented a one-dimensional (1-D) time-dependent solution. A further extended solution accounting for a growing ABL height was given in terms of Jacobi polynomials [15].

Koch [16] developed a 2-D analytical solution for a ground level source with power law profiles for wind and eddy diffusion coefficients accounting for the effects of ground level absorption. The deposition term of the solution includes the Kummer function [17], which has the drawback that it requires continuous checking for computational overflow.

In the work [18], an analytical solution was proposed adopting a constant wind and a diffusivity depending on the horizontal distance from the source.

Due to the limitedness of generality and to the increasing development of Large Eddy Simulation (LES) models, analytical approaches to solve the ADE have been largely ignored. In this paper, a complete and coherent analytical solution of the ADE is presented. The solution is based on the GILTT method [1]. The solution in analytical closed form introduces progress in the field of the study of concentrations. Due to the non-explicit dependence on the set of variables defining the ABL scenario and the source features, an explicit analytical approximation would represent a useful reference when application purposes are required. Moreover, it provides a simple formula for the value and position of maximum ground level concentration in function of source characteristic and meteorological variables.

3. The Solution by GILTT

The two dimensional steady-state ADE for an emitting point-like source in a stationary ABL reads:

$$u(z)\frac{\partial C(x,z)}{\partial x} = \frac{\partial}{\partial z}\left(k_z(z)\frac{\partial C(x,z)}{\partial x}\right) \tag{1}$$

Where, along the x-direction, the longitudinal diffusion term has been neglected in respect to the advection term. In the above Equation (1), $C(x,z)$ represents the cross-wind integrated three-dimensional time-independent concentration:

$$C(x,z) = \int_{-\infty}^{+\infty} C(x,y,z)dy \tag{2}$$

The horizontal wind $u(z)$ is the horizontal mean wind and $k_z(z)$ is the vertical diffusivity. Both depend on the vertical coordinate z. The boundary conditions impose the flux to vanish at the extremes of the ABL ($z = 0, h$), and the source condition is set to represent the point-like source placed at the height h_S above the ground level, namely:

$$u(z)C(0,z) = Q\delta(z - h_s) \tag{3}$$

where Q is the constant rate of emission and $\delta(z - h_S)$ is the Dirac δ-function.

The GILTT technique provides a solution for Equation (1) which is written in terms of a converging infinite series expansion [1]:

$$C(x,z) = \sum_{i=0}^{\infty} \bar{c}_i(x)\varphi_i(z) \tag{4}$$

where $\varphi_i(z)$ are the eigenfunctions of an auxiliary problem, *i.e.*, solving the Sturm-Liouville equation, and $\bar{c}_i(x)$ are x-dependent functions. As a consequence of convergence the series can be truncated at a certain number N such that the rest $R_N(x,z)$ become negligible in respect of the partial sum. If one accepts an error not larger than 0.5% then $N = 190$, as shown in [19].

4. Turbulent Parameterization

The choice of the turbulent parameterization is set to account for the dynamic processes occurring in the ABL. In the following, we restrict our discussion to simple vertical profiles of wind and eddy diffusivity still a reasonably realistic, but more specifically for an unstable regime. For an extension including stable regimens we refer to a future work. The choice of the vertical profile for the wind $u(z)$ is set to follow a power law [20]:

$$\frac{u(z)}{u_1} = \left(\frac{z}{z_1}\right)^{\alpha} \tag{5}$$

where u_1 is the mean wind velocity at the height z_1, while α is an exponent related to the turbulence intensity [21]. On the quantitative side, results will be provided setting $\alpha = 0.1$, and the reference wind $u_1(0.01h) = 3ms^{-1}$; these values are quite consistent with the whole range of unstable regimes [22].

The vertical diffusivity parameterization is chosen according to reference [23], which for an unstable ABL is given as:

$$k_z(z) = kw_* z\left(1 - \frac{z}{h}\right) \tag{6}$$

where h is the height of the ABL, k is the von Karman constant which is set to 0.4, and w_* is the convective scaling parameter related to the Monin-Obukhov length L_{MO} and the mechanical friction parameter u_* as:

$$w_* = u_*\left(\frac{h}{L_{M0}}\right)^{1/3}. \tag{7}$$

For convective scenarios, L_{MO} is limited to values such that the relationship $\frac{h}{L_{MO}} < -10$ holds. Finally u_* is determined as [20,24]

$$u_* = u_1 k\left(\ln\frac{z_1}{z_0} - \psi(\xi)\right)^{-1} \tag{8}$$

where z_0 is the roughness ($10^{-5}h$). For an unstable ABL ψ defined as:

$$\psi(\xi) \cong \ln\left[\left(\frac{1+\xi^2}{2}\right)\left(\frac{1+\xi}{2}\right)^2\right] - 2\arctan\xi + \frac{\pi}{2} \tag{9}$$

and

$$\xi = \left(1 - 16\frac{z_1}{L_{M0}}\right)^{1/4} \tag{10}$$

The chosen profiles ensure simple functions whilst maintaining rather realistic horizontal wind $u(z)$ and diffusivity $k_z(z)$ inside and at both edges of the ABL.

5. Ground Level Concentration

From the solution of the ADE, the Ground Level Concentration (GLC) is obtained after setting $z = 0$ inside the solution $C(x,z)$. Results will be reported in terms of the dimensionless GLC as follows:

$$C_{GLC}(x) = C(x,0)\frac{<u>h}{Q} \tag{11}$$

where $<u>$ is the vertically averaged wind introduced in Equation (5)

$$<u> = \frac{1}{h}\int_0^h u(z)dz \tag{12}$$

If we consider the definition of u profile in Equation (5) we have $<u> = \frac{u_1}{\alpha+1}(h/z_1)^{\alpha}$.

Equation (11) has been introduced to obtain the unitary limit independent of a specific parameter choice

$$\lim_{x\to\infty} C_{GLC}(x) = 1 \tag{13}$$

according to the theoretical expectation for the two-dimensional ADE solution.

It would be redundant to compare the GILTT results with experimental data as outcomes have already been extensively reported in the literature [25,26]. Instead, the scope of this paper is to provide a simple explicit expression for the maximum GLC $C_{MGLC}(x_M)$ occurring at the horizontal distance x_M as a function of the setting parameters for the ABL scenario and source emission. As previously mentioned, in fact, although Equation (4) represents the exact solution of the ADE (1) except for a round-off error, the series expansion misses manifest dependencies on ABL parameters and source height. On the other hand, the main advantage of the GILTT technique is that it allows the step from a differential-like approach, traditionally adopted to solve the ADE numerically, into a matrix algebra approach after applying the generalized Laplace transform. Then the core of the problem leads to the investigation of the behavior of the series (4) after setting $z = 0$, and using the property of the Sturm-Liouville eigenfunctions for which $\varphi_i(0) = 1$ regardless of the index i. An analysis of the behavior and properties of the series (4) will indicate how to synthesize the considerable expression into a more compact formula. The results based on such an approach are still profile-dependent and a general approximation is beyond the scope of the present work. Nevertheless, the choice of a profile-dependent approximation still maintains the advantage of simplicity and allows for a specific case for exploring the functional behaviors of the main physical parameters that drive atmospheric diffusion. To this end we introduce empirical parameters which are determined by fit procedures to best

reproduce the
exact solution.

Based on these facts, and bearing in mind the Gaussian solution and the GLC obtained with power low profile of wind and eddy diffusivity, the dimensionless GLC defined in Equation (11) can be approximated as follows:

$$C_{GLC}(x) = \left[1 + \left(\frac{\kappa h}{\lambda x}\right)^c\right]^b \exp\left[-\frac{\left(\pi h_S\right)^{1+2bc}}{h\left(\lambda x\right)^{2bc}}\right] \tag{14}$$

Due to the negative values assumed by the Monin-Obukhov length, it will be defined in the following calculations as the positive dimensionless parameter $\widetilde{L}_{M0} = -L_{M0}/h$. Parameters b, c, κ and λ have been determined by least squares fittings procedures in Equation (14) against the analytical solution. These are:

$$b = \widetilde{h}_s^{5/2} + 0.17 \tag{15}$$

$$c = -5.48\widetilde{h}_s^{0.87} + 4.73 \tag{16}$$

$$\kappa = \left(\frac{\alpha + 1}{0.4277}\right)^{2.62} \widetilde{h}_s^{0.41} \tag{17}$$

$$\lambda = (0.35u_1)^{-1}(\alpha + 1)^{-1.3} w_* \widetilde{h}_s^{0.47} \tag{18}$$

where the variables with $\widetilde{\ }$ are normalized with respect to the ABL height h (e.g., $\widetilde{h}_s = h_s/h$).

Equations (15)–(18) give the explicit dependency on the source height h_S, the wind parameters α (it compares in κ and λ), u_1 and the convection scaling parameter w_* (it compares in λ ,see Equation (18)) which is related to the Monin-Obukhov length L_{MO} and the friction parameter u_* by the relationship (7).

From the explicit approximation for $C_{GLC}(x)$ one may evaluate the position where the maximum GLC occurs. In fact, putting the derivative of Equation (14) equal to 0 with respect to x, and with the assumption that:

$$\left(\frac{\kappa h}{\lambda x}\right)^c >> 1 \tag{19}$$

we have:

$$x_M^{2bc} = 2\frac{(\pi\, h_s)^{1+2bc}}{(h\lambda)^{2bc}} \tag{20}$$

Finally, putting x_M in Equation (14), the corresponding Maximum Ground Level Concentration ($C_{MGLC}(x_M)$) is:

$$C_{MGLC}(x_M) = \left[1 + \left(\frac{2\kappa}{(2\pi\,\widetilde{h}_s)^{1+\frac{1}{2bc}}}\right)^c\right]^b e^{-1/2} \tag{21}$$

Two considerations are important here. Firstly, the expression for the position x_M is valid provided that it is in the range of horizontal distances where a position x_M occurs. Such approximation affects an error when high sources are concerned (above $\widetilde{h}_s \approx 0.35$), but high convection-driven turbulence enforces condition (19). Secondly, because no maximum is reached for any $\widetilde{h}_s > 0.5$, the position of maxima in these cases has to be expected at $x \to \infty$ (due to the predominant weight of the exponential function compared to the first factor in Equation (14)). For this reason, the study of the maximum GLC will be limited to sources placed below the ABL center level. The omission of maxima will be explicitly shown in Figure 1 (see next section).

6. Results

Figure 1 shows plots of the GLC *versus* the horizontal distance from the source $\widetilde{x}$ for near surface source ($\widetilde{h}_s = 0.01$), a low source ($\widetilde{h}_s = 0.1$) (at the top of the surface layer $\widetilde{z}_{sl} = 0.1$), center source ($\widetilde{h}_s = 0.5$), and high source ($\widetilde{h}_s = 0.7$) (above ABL center) with $\widetilde{L}_{M0} = 0.03$. Except for the plot $\widetilde{h}_s = 0.7$, all show a maximum, where the sharpness of the peak reduces as $\widetilde{h}_s$ increases, until a critical source height is reached (slightly above $0.5h$), then value 1 becomes an upper asymptote for the GLC. When the emitting source height decreases, the maximum GLC increases, and occurs at a closer distance, turning into a well-pronounced peak.

In Figure 2a–2c, the GLC *versus* $\widetilde{x}$ is shown for three values of $\widetilde{h}_s$ ($\widetilde{h}_s = 0.01, 0.05, 0.1$). For each source height, two extreme Monin-Obukhov lengths are used with $\widetilde{L}_{MO} = 0.001, 0.099$ (empty squares and triangles, respectively). The second value for $\widetilde{L}_{MO}$ reflects the limit imposed by the Pleim and Chang diffusivity introduced in Equation (6). The GILTT-based GLC are superimposed on the approximation of Equation (14) (dotted lines). The plots show that for near surface sources there is a slight difference between points and lines near the source position. Where the horizontal gradient is most pronounced, a logarithmic scale enhances such a discrepancy.

Figures 3a–3c refer to higher sources with $\widetilde{h}_s = 0.25, 0.4, 0.5$. These plots show well-matching results as well as a good reproduction of the position where the maximum GLC occurs. As the emitting source height $\widetilde{h}_s$ increases, the approximated function slightly underestimates the GILTT-based maximum. This discrepancy reflects the fact that condition (19) is no longer satisfied. Nonetheless, through the whole range of source heights $0 < \widetilde{h}_s \le 0.25$ the function $C_{GLC}(x)$ reproduces the GILTT results fairly well.

Figures 4 and 5 show plots of the maximum GLC $C_{MGLC}(x_M)$ and its position x_M for several source heights $\widetilde{h}_s$ and for a selection of turbulence parameters $\widetilde{L}_{MO}$. In both figures the GILTT results (points) are superimposed on the approximations (20) (dotted lines). Figure 5 depicts the position where the maximum occurs for low sources, where GILTT results (dotted lines) and our approximations (solid lines) show well-matching results, regardless of the turbulence regime. When higher sources are considered, a difference is visible and increases as convective turbulence reduces its strength. This fact follows from the condition of (19). The turbulence dependency shows that, for a fixed $\widetilde{h}_s$, the strength of convection causes x_M to get closer to the source. From the physics point of view this result agrees with the mixing effect of turbulence.

Figure 1. GILTT (Generalized Integral Laplace Transform Technique) Ground Level Concentration (GLC) *versus* the horizontal distance from the source $\widetilde{x} = x/h$. Four different source heights are selected: $\widetilde{h}_s = 0.01, 0.1, 0.5, 0.7$ and $\widetilde{L}_{MO} = 0.03$. A maximum GLC occurs only for sources below the Atmospheric Boundary Layer (ABL) middle level.

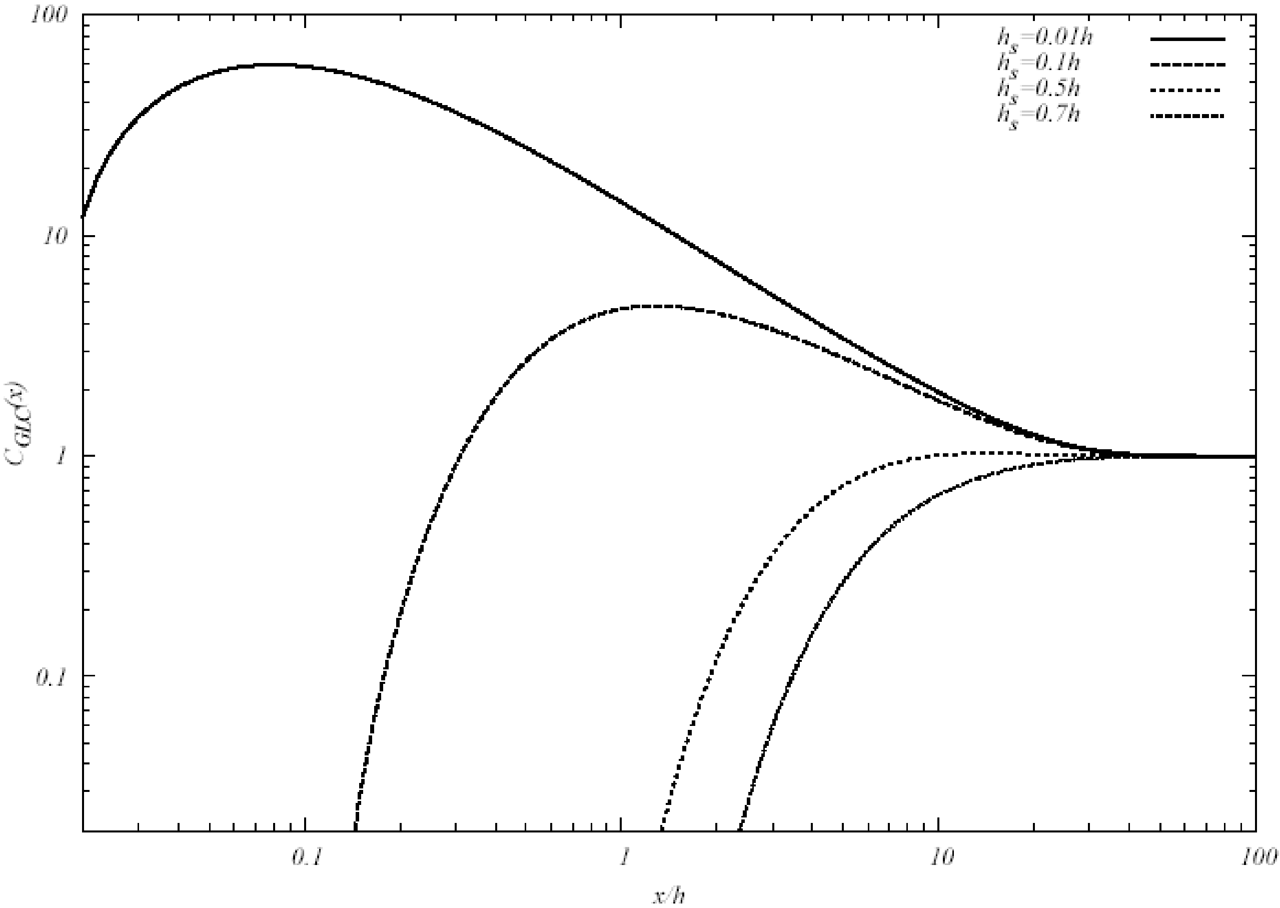


Figure 2. GLC *versus* $\widetilde{x}$ for (**a**) $\widetilde{h}_s = 0.01$, (**b**) $\widetilde{h}_s = 0.05$, and (**c**) $\widetilde{h}_s = 0.1$. Points refer to the GILTT results, and dotted lines refer to the approximation function of Equation (14). Empty squares indicate $\widetilde{L}_{MO} = 0.001$, empty circles $\widetilde{L}_{MO} = 0.099$.

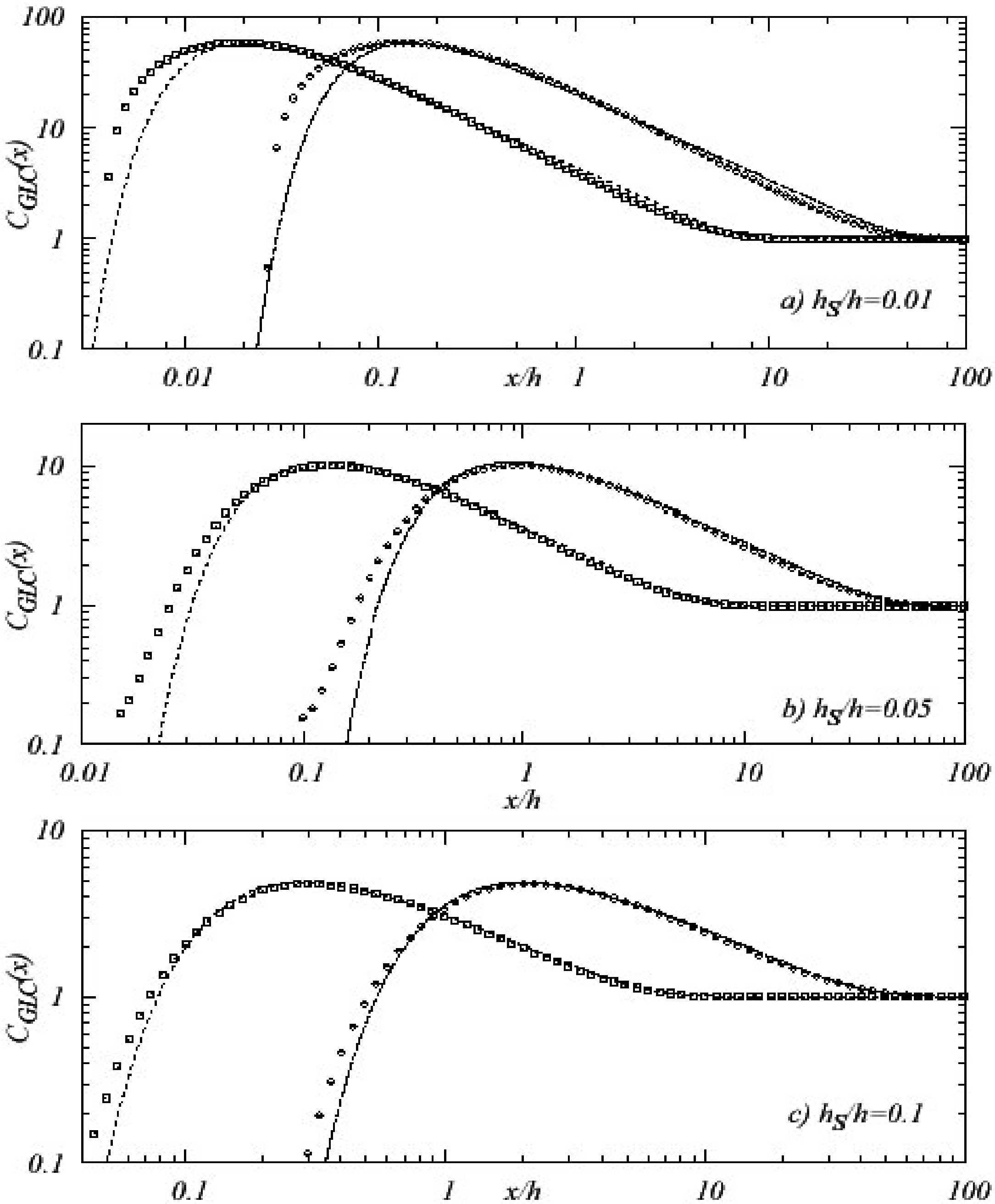


Figure 3. GLC *versus* $\widetilde{x}$ for (**a**) $\widetilde{h}_s = 0.25$, (**b**) $\widetilde{h}_s = 0.4$, and (**c**) $\widetilde{h}_s = 0.5$. Points refer to the GILTT results, and dotted lines refer to the approximation function of Equation (14). Empty squares indicate $\widetilde{L}_{MO} = 0.001$, empty circles $\widetilde{L}_{MO} = 0.099$.

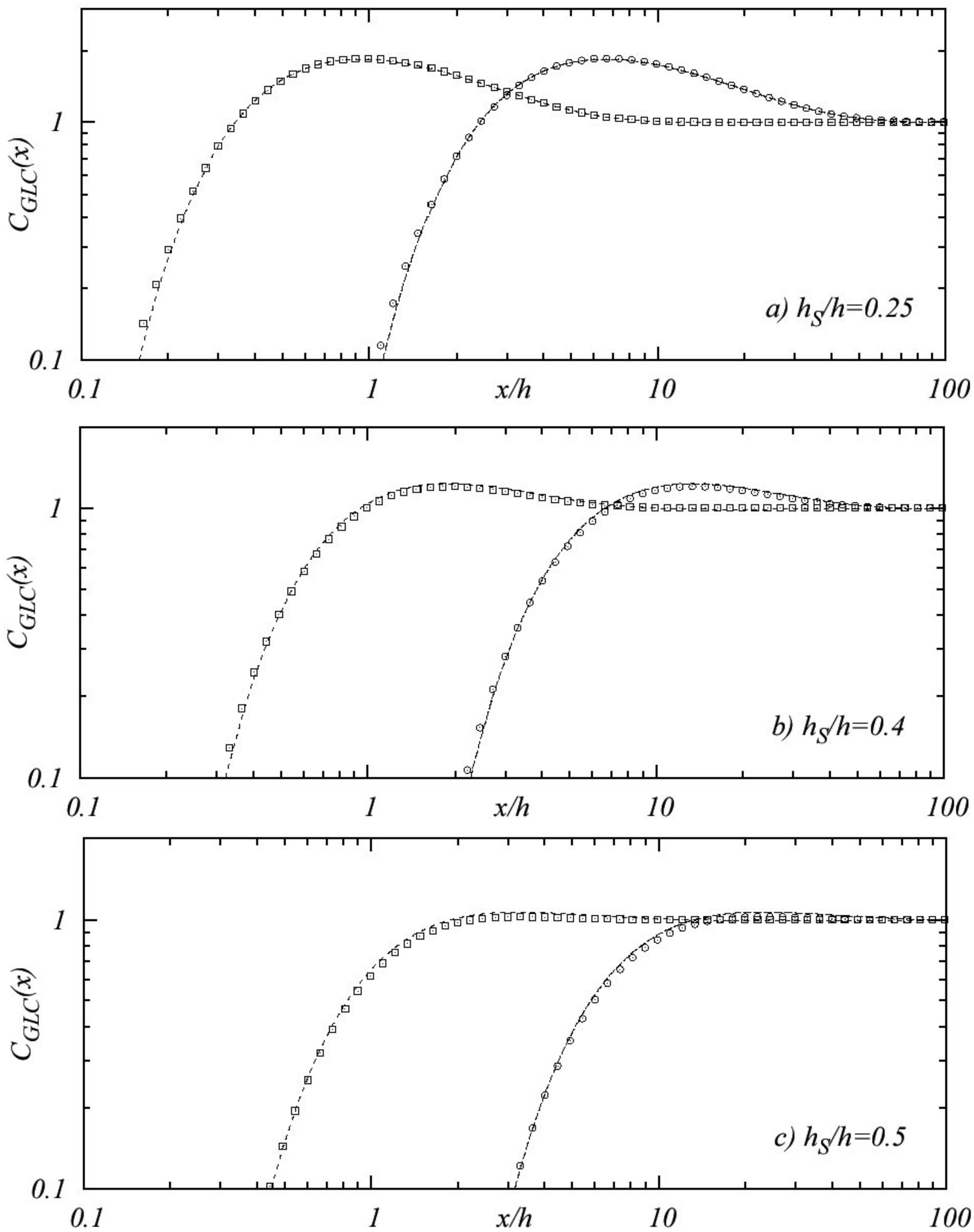


Figure 4. Position of the maximum GLC *versus* the source height $\widetilde{h}_s = h_s / h$. Points refer to the GILTT results, dotted lines refer to Equation (20).

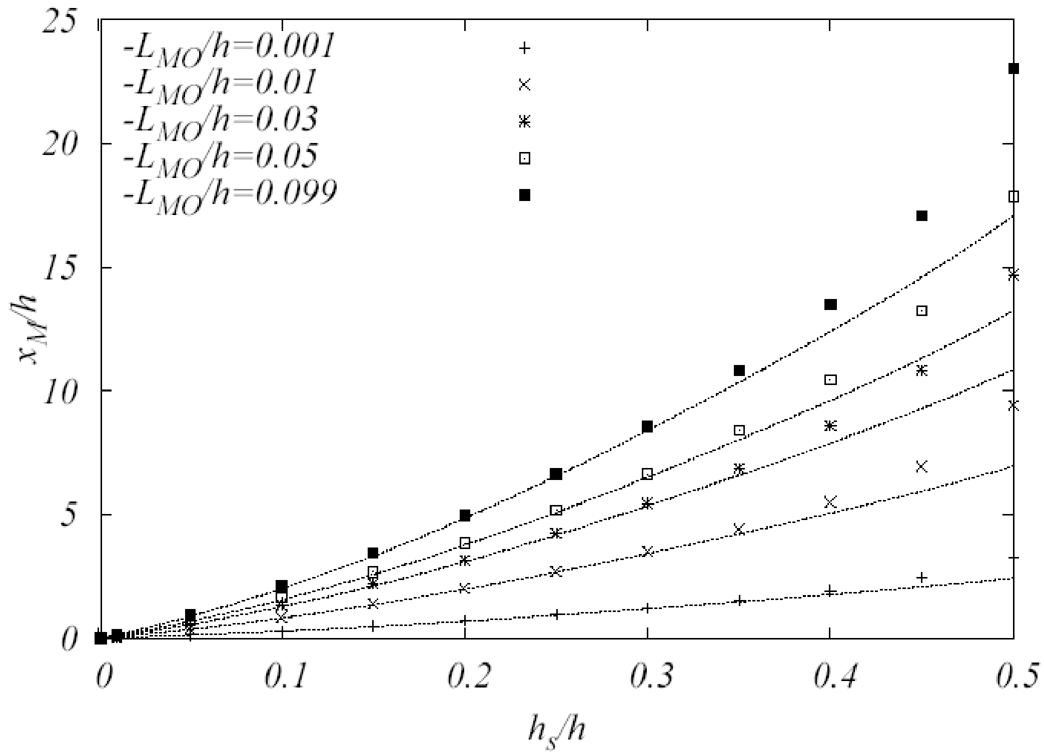
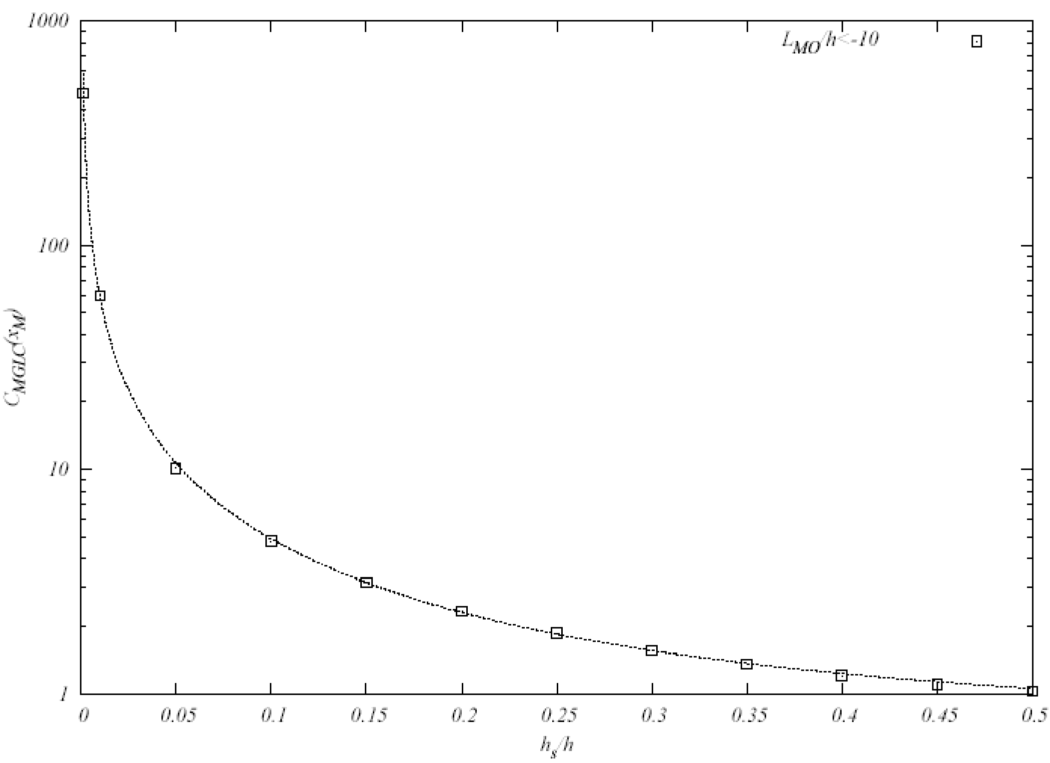


Figure 5. Value of the maximum GLC *versus* the source height $\widetilde{h}_s = h_s / h$. Points refer to the GILTT results, dotted lines refer to Equation (21).



A final remark should be made in regard to Figure 5. Both GILTT and Equation (21) confirm that the maximum GLC value depends on the source height, regardless of the turbulence. Based on the Equation (21) and the parameters definitions (15)–(16) for b, c and κ, the leading term for the maximum GLC results:

$$C_{MGLC}(x_M) \approx \tilde{h}_s^{-1} \tag{22}$$

where the exponent −1 is a lower bound for the source term. These results broaden the well-known result obtained with the Gaussian approach for an unbounded ABL. Furthermore, this agrees with the two-dimensional Gaussian result that the maximum for the GLC is:

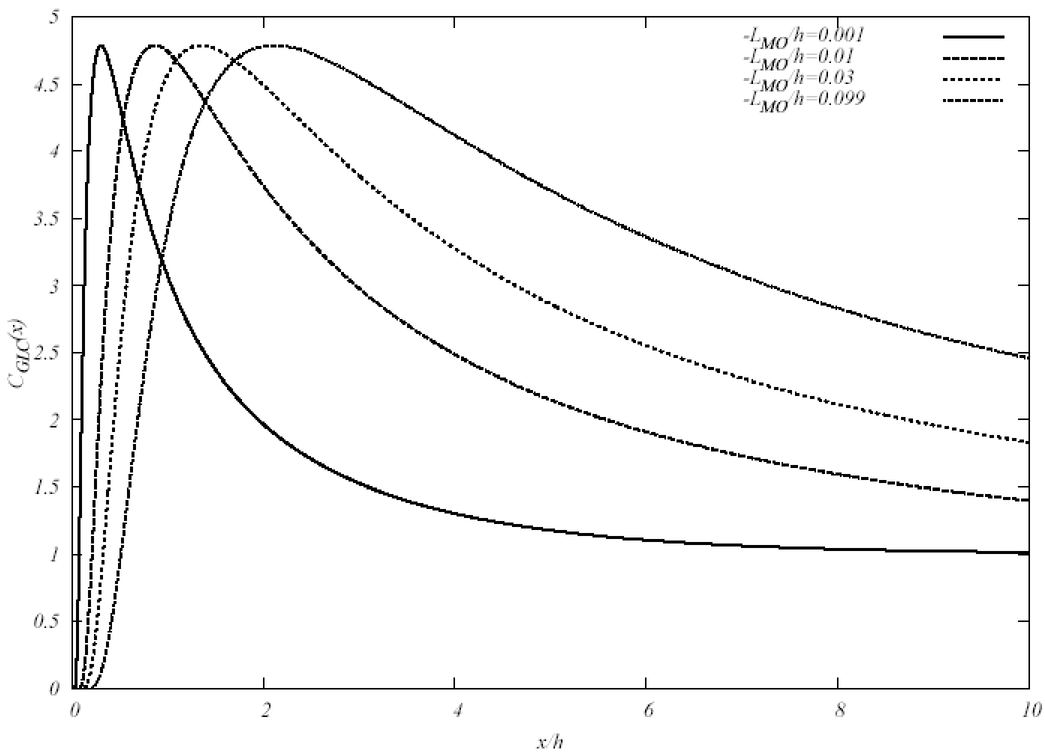
$$C_{MGLC}(x_M) = \left(\frac{2}{e\pi}\right)^{1/2} \tag{23}$$

Note that for the three-dimensional case this is no longer true. It is evident that diffusive parameters do not play a part and it confirms that turbulence has the only effect that determines the distance where maximum GLC occurs. The results shown above can be generalized (see Figure 6 as an example) to the case of vertical diffusivities defined with a multiplicative Monin-Obukhov length:

$$k_z(z) \approx F(L, u_*, w_*)G(z) \tag{24}$$

where F and G are two functions.

Figure 6. Ground level concentration *versus* the horizontal distance from the source. The source height has been set to $\tilde{h}_s = h_s / h = 0.1$. The value of the maximum GLC does not change as the turbulence varies.



7. Conclusions

The results presented in this paper show the possibility of expressing the GLC from an emitting point-like source in a steady convective ABL by a compact analytical expression. The function was determined analyzing the behavior of the series expansion provided by the GILTT solution, the predictive power of which has been extensively demonstrated in the literature when applied to several experimental data sets. Despite the simplifications due to restricting only to unstable ABL regimes, the analysis allows a high level of understanding of the form of the ground level concentration.

The main progress worth emphasizing is the following: for a function given in Equation (14), within the setting choice for the ABL parameter set, the maximum GLC depends only on the source height, regardless of the Monin-Obukhov length. However, turbulence can still affect the position where the maximum GLC occurs, which is also confirmed by the GILTT solution. A further notable point shown in the result that no maxima occurs for all sources placed above the ABL center level; the limit becomes an upper-bound limit. The existence of a non-zero limit is one of the main properties of the two-dimensional ADE.

From the operative point of view, Equation (14) and its related features are useful as an additional tool for decisional as well as emergency responses.

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