A mathematical scheme to analytically solve the atmospheric diffusion equation with non-Fickian closure

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1. Introduction

Analytical solutions of advection-diffusion equations are of fundamental importance in describing and understanding dispersion phenomena, since all the parameters are expressed in a mathematically closed form and therefore the influence of individual parameters on pollutant concentration can be easily examined. Also, the analytical solutions make it easy to obtain asymptotic behaviors of the solutions, which are usually difficult to obtain through numerical calculations. The analytical solutions can also be used to improve the modeling of pollutant dispersion by evaluating the performances of sophisticated numerical dispersion models (which numerically solve the advection–diffusion equation), yielding results that can be compared not only with experimental data but, in an easy way, with the solution itself, to check numerical errors.

The most widely used mathematical model solves the closing of the advection-diffusion equation based on the gradient transport hypothesis that, in analogy with molecular diffusion, assumes that the turbulence is proportional to the magnitude of the concentration gradient average:

$$\overline{w'c'} = -K_x \frac{\partial \bar{c}}{\partial z} \tag{1}$$

where, in general, the eddy diffusivity K_x is a function of the typical length and velocity scales of the turbulence field and varies with height z.

Measurements collected in the Convective Boundary Layer (CBL) have shown that the flux of some quantities, such as potential temperature, can be counter to its mean vertical gradient (Lenschow, 1970; Warner, 1971). To account for this effect Deardorff (1972), Troen and Mahrt (1986) and Holtslag and Moeng (1991) proposed to include a countergradient correction term in Eq. (1):

$$\overline{w'c'} = -K_x \left(\frac{\partial \bar{c}}{\partial z} - \gamma_x\right) \tag{2}$$

The countergradient fluxes are characterized by larger scales of eddies in the boundary layer, as opposed to smaller scale eddies, such fluxes are often called non-local fluxes. A summary of countergradient expressions proposed in the literature is given by van Dop and Verver (2001). We aim to study the occurrence of countergradient fluxes for the variable concentration. For this, we use a generic equation for turbulent diffusion suggest by van Dop and Verver (2001), obtain an expression for the advection-diffusion equation depending on eddy diffusivity, skewness, Lagrangian time scale and vertical turbulent velocity. This equation is solved by the Laplace transform technique. The results show that the nonlocal closure affects the process and must be taken into account in dispersion calculations.

2. Solution of the advection-diffusion equation with the nonlocal closure

The advection-diffusion equation that describes the crosswind-integrated concentration arising from a continuous point source can be written as:

$$u\frac{\partial \overline{c}}{\partial x} = -\frac{\partial \overline{w'c'}}{\partial z} \tag{3}$$

where $\overline{c}$ is the crosswind-integrated concentration, u is the mean horizontal wind speed and $\overline{w'c'}$ is the vertical turbulent contaminant flux.

Using the generic equation for turbulent diffusion suggested by van Dop and Verver (2001), where the vertical turbulent contaminant flux can be written as (time independent):

$$\left(1+\left(\frac{S_k\sigma_w T_l}{2}\right)\frac{\partial}{\partial z}\right)\overline{w'c'} = -K_z\frac{\partial \overline{c}}{\partial z} \tag{4}$$

where S_k is the skewness, σ_w is the vertical turbulent velocity standard deviation and T_l is the Lagrangian time scale. The second term on the left hand side of Eq. (4) represents the nonlocal countergradient term.

In this work, Eq. (4) is substituted in Eq. (3), leading to:

$$u\frac{\partial \overline{c}}{\partial x} = \frac{\partial}{\partial z}\left(K_z\frac{\partial \overline{c}}{\partial z}\right) - \frac{\partial}{\partial z}\left(\beta\frac{\partial \overline{c}}{\partial x}\right) \tag{5}$$

where $\beta = 0.5 S_k\sigma_w T_l u$, for $0 < z < z_i$ and $x > 0$, subject to the boundary conditions (z_i is the CBL top):

$$K_z\frac{\partial \overline{c}}{\partial z} = 0 \qquad \text{at } z = 0, z_i \tag{6}$$

and a continuous source is assumed with rate of constant emission Q at the source height H_s:

$$\overline{c}(0,z) = \frac{Q}{u}\delta(z - H_s) \qquad \text{at } x = 0 \tag{7}$$

The advection-diffusion equation solution for the case when $S_k = 0$ (or $\beta = 0$) was obtained in the works of Moreira et al. (1999) and Mangia et al. (2002). It is observed that the second term on the right hand side of Eq. (5) is a diffusive term, where β has an eddy diffusivity (m^2/s) dimension.

Applying the Laplace transform to the above with respect to x, we obtain (with K_z, u and β independent of x):

$$\frac{d^2}{dz^2}\hat{\overline{c}}(s,z) - \frac{\beta s}{K_z}\frac{d}{dz}\hat{\overline{c}}(s,z) - \frac{us}{K_z}\hat{\overline{c}}(s,z) = -\frac{u}{K_z}\overline{c}(0,z) - \frac{\beta}{K_z}\frac{d}{dz}\overline{c}(0,z) \tag{8}$$

where $\hat{\overline{c}}(s,z) = L\{\overline{c}(x,z); x \to s\}$.

To solve the advection-diffusion equation for nonhomogeneous turbulence we must take into account the dependence of all parameters on the height variable (variable z). Therefore, to solve this kind of problem we have to perform a stepwise approximation of these coefficients. To reach this goal, we discretize the height z_i of the Atmospheric Boundary Layer (ABL) into N sub-intervals in such manner that inside each sub-region,

$K(z)$, $u(z)$ and $\beta(z)$ assume average values. Thus, after this procedure the equation (8) has a well known solution form for every sub-interval $z_n < z < z_{n+1}$:

$$\hat{\bar{c}}_n(s,z) = A_n e^{\left(F_n^* - R_n^*\right)z} + B_n e^{\left(F_n^* + R_n^*\right)z} + \frac{Q}{2R_n^* K_n}\left(e^{\left(F_n^* - R_n^*\right)(z-H_s)} - e^{\left(F_n^* + R_n^*\right)(z-H)}\right) \qquad (9)$$

for $n = 1 : N$.

Taking a closer look at the solution in equation (9), we promptly realize that 2*N* integration constants are present. To determine these integration constants, we impose (2*N*-2) interface conditions, namely the continuity of concentration and flux concentration at the interface. These conditions are expressed as:

$$\bar{c}_n = \bar{c}_{n+1} \qquad n = 1, 2, ...(N-1) \qquad (10)$$

$$K_n \frac{\partial \bar{c}_n}{\partial z} = K_{n+1}\frac{\partial \bar{c}_{n+1}}{\partial z} \qquad n = 1, 2, ...(N-1) \qquad (11)$$

Finally, applying the interface and boundary conditions we obtain a linear system for the integration constants. Henceforth the concentration is obtained by inverting numerically the transformed concentration $\hat{\bar{c}}$ by Gaussian quadrature scheme:

$$\bar{c}_n(x,z) = \sum_{j=1}^{8} \frac{p_j}{x} w_j \left[A_n e^{\left(F_n^* - R_n^*\right)z} + B_n e^{\left(F_n^* + R_n^*\right)z} + \frac{Q}{2R_n^* K_n}\left(e^{\left(F_n^* - R_n^*\right)(z-H_s)} - e^{\left(F_n^* + R_n^*\right)(z-H_s)}\right) H(z-H_s)\right] \qquad (12)$$

where $H(z-H_s)$ is the Heaviside function and,

$$R_n^* = \frac{1}{2}\sqrt{\left(\frac{\beta_n}{K_n}\frac{p_j}{x}\right)^2 + \frac{4u_n}{K_n}\frac{p_j}{x}} \quad ; \quad F_n^* = \frac{\beta_n}{2K_n}\frac{p_j}{x}$$

The solution is only valid for $x > 0$, as the quadrature scheme of Laplace inversion does not work for $x = 0$. The values of w_j (weights) and p_j (roots) of the Gaussian quadrature scheme are tabulated in the book by Stroud and Secrest (1966).

The classical statistical diffusion theory, the observed spectral properties and observed characteristics of energy-containing eddies are used to estimate the turbulent parameters in Eq. (12) (Degrazia et al. 1997, 2001).

3. Numerical results

The performance of the model has been evaluated against experimental data from dispersion experiments carried out in the northern part of Copenhagen, described in Gryning et al. (1987). To analyze the influence of the countergradient term in the turbulent transport, the simulation was made utilizing the data of experiment 8, which is strongly convective ($z_i/|L| > 10$).

Figures 1-a to 1-f show the effect of the nonlocal transport for different source heights on the ground-level concentration. It is quickly verified that the maximum concentration peak changes quantitatively (despite the maximum position does not vary).

In figure 1-a ($H_s/z_i = 0.025$) a pronounced peak near the source is observed for $S_k = 0.25$, approximately 15% larger than with $S_k = 0$. In the source, heights 0.05, 0.1

and 0.25, respectively, peaks are also observed, maintaining a significant difference in relation to the curve with $S_k = 0$, that is, (b) 20%, (c) 14% and (d) 8%. For negative skewness the difference between $S_k = 0$ is smaller and a reduction in the concentration peak happens: (a) 12%, (b) 11%, (c) 10% and (d) 7%. In figures 1-e and 1-f, that represent higher sources, the tendency of the negative skewness is altered in relation to the previous cases. The concentration with $S_k > 0$, in figure 1-e, grows quicker, but the maximum value is smaller than for $S_k < 0$. In figure 1-f, for $S_k < 0$, the concentration is practically null until a certain distance and begins to grow, reaching the same value that $S_k > 0$ in around $X \sim 3$.

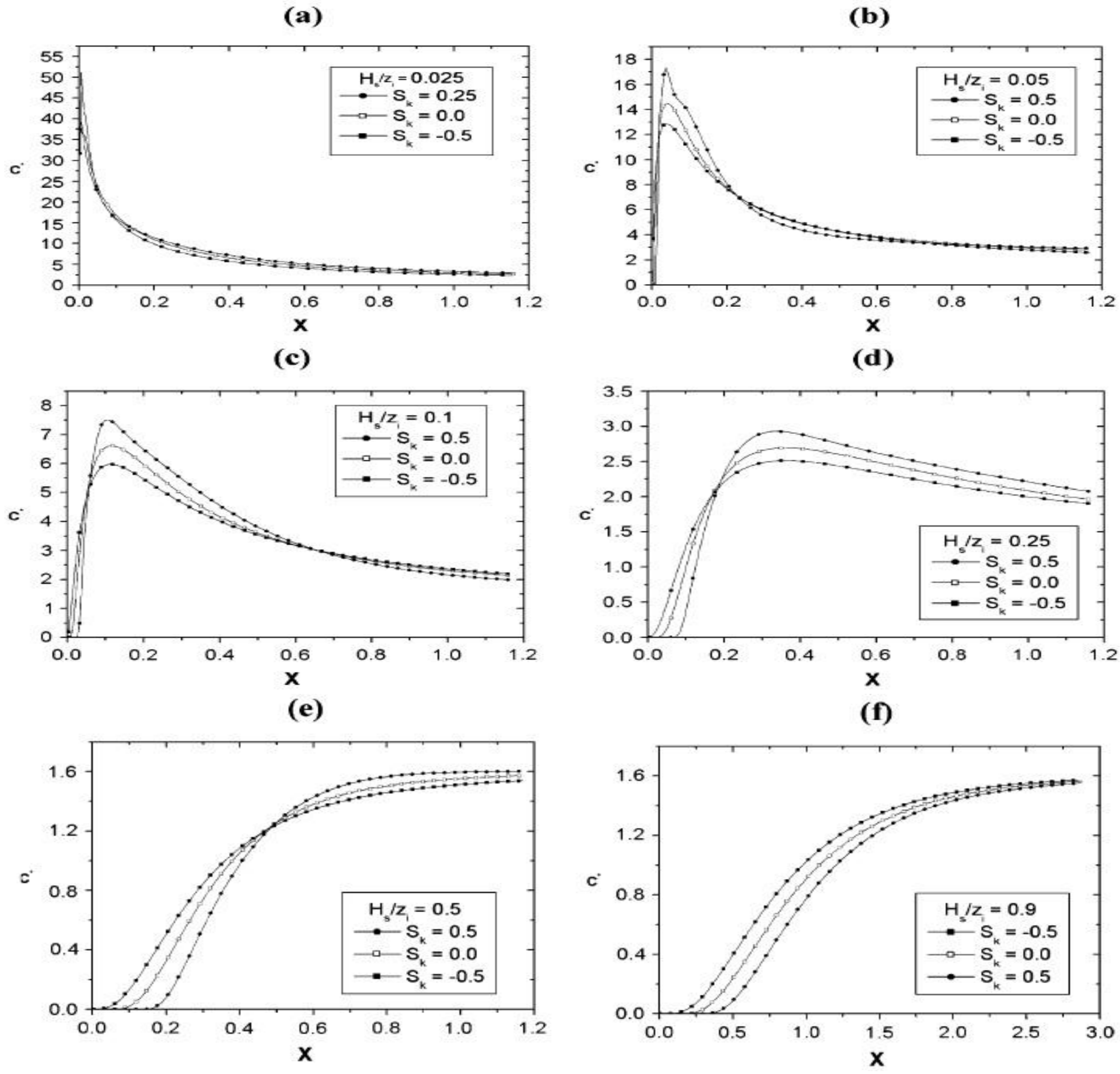

Figure 1: Nondimensional ground-level concentration $C^* = \bar{c}uz_i/Q\theta$ as a function of the nodimensional distance ($X = xw_*/uz_i$) for different nondimensional source heights H_s/z_i: (a) 0.025, (b) 0.05, (c) 0.1, (d) 0.25, (e) 0.5 and (f) 0.9.

4. Conclusions

This work describes the analytical solution of a model that considers the nonlocal closure of the turbulent diffusion in the advection-diffusion equation. The countergradient term in the turbulence closure made an additional term appear in the advection-diffusion equation. This term is related to the asymmetrical transport in the CBL. The nonlocal character was introduced in previous works in the eddy diffusivity, but now it is done as a new term of the differential equation. We verified that the skewness was more effective in the distance of the peak concentration, altering the value of the maximum. This is an important result because the determination of the maximum in the ground-level concentration is one of the most important aspects to be considered in the control of the quality of the air. Additionally, the incorporation of the countergradient term didn't generate larger computational effort in relation to the original problem. We will focus our future attention on a comparison with the dataset of the classic tank experiment obtained in the work of Misra (1982).

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