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IDENTIFICATION OF MICRO-METEOROLOGICAL PARAMETERS FOR THE CHARACTERIZATION OF ATMOSPHERIC BOUNDARY LAYERS

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Abstract – This paper deals with the use of inverse analysis techniques for the estimation of micrometeorological parameters required for the characterization of atmospheric boundary layers. The physical problem is formulated in terms of a transient two-dimensional advection-diffusion equation. Concentration measurements of a tracer are assumed to be available for the inverse analysis. The analysis of the sensitivity coefficients and of the determinant of the information matrix reveals the most appropriate sensor locations and duration of the experiment for the estimation of the unknown parameters. The parameter estimation problem is solved with the Levenberg-Marquardt method of minimization of the least squares norm.

1. INTRODUCTION

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The study of the dispersion of pollutants in the atmosphere is of extreme importance, because of the large number of industrial facilities and the effects of their emissions on the health of populations living in affected areas [1]. The atmosphere is the gaseous layer that surrounds the Earth. The atmosphere thickness is approximately 600 km and is sub-divided into 5 sub-layers. The troposphere is the sub-layer adjacent to Earth and is located within approximately 10 km of altitude. The troposphere concentrates 75% of the gases and 80% of the humidity of the atmosphere. The atmospheric boundary layer is the region of the troposphere that is directly affected by the Earth surface, where the response to thermal and mechanical phenomena takes place in a time scale of one hour or less. The thickness of the atmospheric boundary layer changes according to location and time, and can vary from hundreds of meters to few kilometers. The atmospheric boundary-layer thickness is influenced by several factors, including, among others, the daily cycle (heating and cooling of Earth's surface), the proximity to large water bodies and zones of high/low pressure [2]. Several recent turbulence models can be found in the literature for the atmospheric boundary layer [3-16].

In this paper, we examine the estimation of parameters appearing in a turbulence model for atmospheric flows, by using concentration measurements of a tracer released by a known source. The problem is assumed to be two-dimensional and is formulated by an advection-diffusion equation for the dispersion of the tracer in the atmosphere. The turbulence model proposed by Ulke [8] is used in this work. The direct problem is solved with the Generalized Integral Transform Technique, for which error-controlled solutions can be obtained [17-20]. The solution of the inverse problem was obtained by using the Levenberg-Marquardt method of minimization of the least-squares norm [21-24]. The identification of parameters for the characterization of atmospheric boundary layers in field experiments will permit the accurate control of areas affected by industrial emissions. In addition, the use of tracer concentration measurements for the identification of micro-meteorological boundary layer parameters will avoid the use of very expensive instruments required for such purpose.

2. PHYSICAL PROBLEM AND MATHEMATICAL FORMULATION

The physical problem considered in this work consists of the dispersion of a tracer in the atmosphere, as illustrated in Figure 1. The tracer is released into the atmospheric flow by a line source of constant strength *S*, located at the position (x_e, z_e) , and the tracer concentration in the atmosphere is assumed to be zero before the tracer is released. The wind velocity U(z) is supposed to be positive. The diffusive fluxes are assumed to be zero at the boundaries z=0, z=H and x=A, while the tracer concentration is supposed zero at the boundary x=0. The mathematical formulation for this problem is given by:

$$\frac{\partial c}{\partial t} + U(z)\frac{\partial c}{\partial x} = K_{xx}\frac{\partial^2 c}{\partial x^2} + \frac{\partial}{\partial z} \left[K_{zz}\frac{\partial c}{\partial z} \right] + S\,\delta(x - x_e)\,\delta(z - z_e) \qquad \text{in } 0 < x < A, 0 < z < H, \text{ for } t > 0 \quad (1.a)$$

= 0 at
$$z = 0$$
, $0 < x < A$, for $t > 0$ (1.b)

$$\frac{\partial c}{\partial z} = 0 \qquad \text{at } z = H, \ 0 < x < A, \text{ for } t > 0 \qquad (1.c)$$

$$c = 0$$
 at $x = 0$, $0 < z < H$, for $t > 0$ (1.d)

$$\frac{\partial c}{\partial x} = 0 \qquad \text{at } x = A , \ 0 < z < H, \text{ for } t > 0 \qquad (1.e)$$

$$c = 0$$
 for $t = 0$, in $0 < x < A$, $0 < z < H$ (1.f)

where c is the time-averaged tracer concentration, U(z) is the velocity profile and K_{xx} and K_{zz} are the diffusivities along the longitudinal and transversal directions, respectively. We note that the diffusivity was supposed to be constant in the longitudinal direction.



Figure 1. Physical problem.

In this paper we have used the following expressions for the transversal eddy-diffusivity and velocity profile, respectively [8]:

$$K_{zz}(z) = k (u_*)_0 H\left(\frac{z}{H}\right) \left(1 - \frac{z}{H}\right) \left(1 - 22\frac{H}{L}\frac{z}{H}\right)^{\frac{1}{4}}$$
(2.a)

$$U(z) = \frac{(u_*)_0}{k} \left\{ \ln\left(\frac{z}{z_0}\right) + \ln\left[\frac{(1+\mu_0^2)(1+\mu_0)^2}{(1+\mu^2)(1+\mu)^2}\right] \right\} + \frac{(u_*)_0}{k} \left\{ 2 \left[\arctan\mu - \arctan\mu_0\right] + \frac{2L}{33H} \left[\mu^3 - \mu_0^3\right] \right\}$$
(2.b)

where the atmospheric condition was supposed to be unstable [8]. In eqns (2.a,b) k (=0.4) is Von Karman's constant, z_0 is the surface roughness and L is the Monin-Obukov length. The Monin – Obukov length (L) characterizes the atmospheric stability condition, where L < 0 for an unstable condition such as that under examination in this paper. The superficial friction velocity (u_*)₀ and the diffusivities influence the dispersion of the plume by the action of the wind field and turbulent diffusion, respectively. The surface roughness (z_0) represents the region of the atmosphere where the velocity of the wind is considered to be zero [3]. The parameters μ and μ_0 are given respectively by:

$$\mu = \left(1 - 22\frac{H}{L}\frac{z}{H}\right)^{\frac{1}{4}} , \quad \mu_0 = \left(1 - 22\frac{H}{L}\frac{z_0}{H}\right)^{\frac{1}{4}}$$
(3.a,b)

By defining the following dimensionless variables

$$X = \frac{x}{H}, Z = \frac{z}{H}, U^* = \frac{U}{(u_*)_0}, C = \frac{Hc(u_*)_0}{S}, \tau = \frac{t(u_*)_0}{H}, K^*_{zz} = \frac{K_{zz}}{(u_*)_0 H}, K^*_{xx} = \frac{K_{xx}}{(u_*)_0 H}, A^* = \frac{A}{H}$$
(4.a-h)

eqns (1.a-f) can be written in dimensionless form as:

$$\frac{\partial C}{\partial \tau} + U^*(Z) \frac{\partial C}{\partial X} = K_{xx}^* \frac{\partial^2 C}{\partial Z^2} + \frac{\partial}{\partial Z} \left[K_{zz}^* \frac{\partial C}{\partial Z} \right] + \delta(X - X_e) \delta(Z - Z_e) \quad \text{in } 0 < X < A^*, \ 0 < Z < 1, \ \text{for } \tau > 0 \quad (5.a)$$
$$\frac{\partial C}{\partial Z} = 0 \quad \text{at } Z = 0, \ 0 < X < A^*, \ \text{for } \tau > 0 \quad (5.b)$$

$$\frac{\partial C}{\partial Z} = 0 \qquad \text{at } Z = 1 , \ 0 < X < A^*, \text{ for } \tau > 0 \qquad (5.c)$$

$$\frac{\partial C}{\partial X} = 0 \qquad \text{at } X = A^*, \ 0 < Z < 1, \text{ for } \tau > 0 \qquad (5.e)$$

$$C = 0 \qquad \text{for } \tau = 0, \quad 0 < X < A^*, \quad 0 < Z < 1 \qquad (5.f)$$

3. DIRECT PROBLEM

The problem defined by eqns (5.a-f), with known initial and boundary conditions, source-term, velocity profile and diffusivities, constitutes a direct problem that is concerned with the determination of the transient concentration field $C(X,Z,\tau)$. The solution of the direct problem in this work was obtained with the hybrid analytic-numerical Generalized Integral Transform Technique [17-20]. The basic steps of such technique consists of: (i) Definition of an auxiliary eigenvalue problem; (ii) Definition of the pair transform/inverse; (iii) Transformation of the original problem into a system of infinite coupled differential equations; (iv) Solution of such system truncated to a finite number of equations; and (v) Use of the inversion formula to obtain the desired solution.

The following auxiliary eigenvalue problem along the Z direction was used in this work:

$$\frac{\partial}{\partial Z} \left(K_{zz}^* \frac{\partial \Psi_i}{\partial Z} \right) + \lambda_i^2 \Psi_i = 0 \qquad \text{in } 0 < Z < 1 \qquad (6.a)$$

$$\frac{\partial \Psi_i}{\partial Z} = 0 \qquad \text{at } Z = 0 \tag{6.b}$$

$$\frac{\partial \Psi_i}{\partial Z} = 0 \qquad \text{at } Z = 1 \qquad (6.c)$$

The solution of the eigenvalue problem (6.a-c) was obtained numerically with the sign-count method [17]. Based on the eigenfunctions Ψ_i , we define the following integral transform/inverse pair:

$$\overline{C}_{i}(X,\tau) = \int_{Z=0}^{1} \overline{\Psi}_{i}(Z) C(X,Z,\tau) dZ$$
 (Transform) (7.a)

$$C(X,Z,\tau) = \sum_{i=0}^{\infty} \overline{\Psi}_i(Z) \overline{C}_i(X,\tau)$$
 (Inverse) (7.b)

where

$$\overline{\Psi}_i(Z) = \frac{\Psi_i(Z)}{N_i^{1/2}}$$
(8.a)

$$N_{i} = \int_{Z=0}^{1} [\Psi_{i}(Z)]^{2} dZ$$
(8.b)

By operating on problem (5.a-f) with $\int_{Z=0}^{1} \overline{\Psi}_{i}(Z) dZ$ and performing some lengthy but straightforward manipulations [17], it reduces to:

$$\frac{\partial \overline{C}_i}{\partial \tau} + \sum_{j=0}^{\infty} B_{ij} \frac{\partial \overline{C}_j}{\partial X} = -\mu_i^2 \overline{C}_i + K_{zz}^* \frac{\partial^2 \overline{C}_i}{\partial X^2} + \delta(X - X_e) \overline{\Psi}_i(Z_e) \qquad \text{in } 0 < X < A^*, \text{ for } \tau > 0, i = 0, 1, 2, \dots$$
(9.a)

at
$$X = 0$$
, for $\tau > 0$, $i = 0, 1, 2, ...$ (9.b)

at
$$X = A^*$$
, for $\tau > 0, i = 0, 1, 2,...$ (9.c)

for
$$\tau = 0$$
, in $0 < X < A^*$, $i = 0, 1, 2,...$ (9.d)

where

 $\overline{C}_i = 0$

 $\overline{C}_i = 0$

 $\frac{\partial \overline{C}_i}{\partial X} = 0$

$$B_{ij} = \int_{Z=0}^{1} \overline{\Psi}_{i}(Z) \overline{\Psi}_{j}(Z) U^{*}(Z) dZ$$
(10)

After system (9.a-d) is truncated to a finite number of equations and solved, the inverse formula (7.b) is applied to obtain the concentrations $C(X,Z,\tau)$. The number of equations used for the solution of system (9.a-d) is the same number of terms retained in the series-solution given by the inverse formula; it is chosen so that convergence is obtained to a user-prescribed tolerance.

We note that a simpler eigenvalue problem with know analytical solution could be used, by making $K_{zz}^* = 1$ in eqn (6.a). However, the eigenvalue problem (6.a-c) results on an eigenfunction basis that better represents the original solution of problem (5.a-f) and faster computational solutions are then obtained.

4. INVERSE PROBLEM

For the inverse problem of interest here, the parameters K_{xx} , $(u_*)_0$, L and z_0 are regarded as unknown. For the estimation of such parameters, we consider available the transient concentration measurements Y_{km} taken at the locations (X_m, Z_m) m=1,...,M, and at times t_k , k=1,...,I. We assume the measurement errors to be additive, uncorrelated and normally distributed, with known and constant standard deviation and zero mean. With such hypotheses, the minimization of the least-squares norm results on minimum variance estimates [23]. Such a norm is written as:

$$S(\mathbf{P}) = [\mathbf{Y} - \mathbf{C}(\mathbf{P})]^T [\mathbf{Y} - \mathbf{C}(\mathbf{P})]$$
(11)

where

$$\mathbf{P}^{I} = [K_{xx}, (u_{*})_{0}, L, z_{0}]$$
(12.a)

$$[\mathbf{Y} - \mathbf{C}(\mathbf{P})]^{T} = [\vec{Y}_{1} - \vec{C}_{1}(\mathbf{P}), \vec{Y}_{2} - \vec{C}_{2}(\mathbf{P}), \cdots, \vec{Y}_{I} - \vec{C}_{I}(\mathbf{P})]$$
(12.b)

and each element $[\vec{Y}_{k} - \vec{C}_{k}(\mathbf{P})]$ is a row vector of length equal to the number of sensors *M*, that is,

$$[\vec{Y}_{k} - \vec{C}_{k}(\mathbf{P})] = [Y_{k1} - C_{k1}(\mathbf{P}), Y_{k2} - C_{k2}(\mathbf{P}), \cdots, Y_{kM} - C_{kM}(\mathbf{P})] \qquad \text{for } k = 1, \dots, I \qquad (12.c)$$

For the minimization of the least squares norm (11), we use the Levenberg-Marquardt Method [21-24]. The iterative procedure of such method is given by:

$$\mathbf{P}^{p+1} = \mathbf{P}^{p} + [(\mathbf{J}^{p})^{T} \mathbf{J}^{p} + \mu^{p} \Omega^{p}]^{-1} (\mathbf{J}^{p})^{T} [\mathbf{Y} - \mathbf{C}(\mathbf{P}^{p})]$$
(13)

where the superscript p denotes the number of iterations, μ^{p} is a positive scalar named damping parameter, Ω^{p} is a diagonal matrix and \mathbf{J}^{p} is the sensitivity matrix.

By performing a statistical analysis it is possible to assess the accuracy of \hat{P}_n , which are the estimated values for the parameters P_n , n = 1, ..., N, where N is the number of estimated parameters. By taking into account the statistical hypotheses described above, the *covariance matrix* for the ordinary least-squares estimator is given by [23]:

$$\mathbf{V} \equiv (\mathbf{J}^T \mathbf{J})^{-1} \sigma^2 \tag{14}$$

where σ is the standard deviation of the measurement errors, which is assumed to be constant. We note that eqn (14) is exact for linear estimation problems and is approximately used for nonlinear parameter estimation problems.

The standard deviations for the estimated parameters can thus be obtained from the diagonal elements of ${\bf V}$ as

$$\sigma_n \equiv \sqrt{\operatorname{cov}(\hat{P}_n, \hat{P}_n)} = \sqrt{V_{nn}} \qquad \text{for } n = 1, \dots, N$$
(15)

where V_{nn} is the n^{th} element on the diagonal of **V**.

Confidence intervals at the 99% confidence level for the estimated parameters can be obtained as

$$\hat{P}_n - 2.576 \,\sigma_n \le P_n \le \hat{P}_n + 2.576 \,\sigma_n \qquad \text{for } n = 1, \dots, N$$
 (16)

The joint confidence region for the estimated parameters is given by [23]:

$$(\hat{\mathbf{P}} - \mathbf{P})^T \mathbf{V}^{-1} (\hat{\mathbf{P}} - \mathbf{P}) \le \chi_N^2$$
(17)

where χ^2_N is the value of the chi-square distribution with N degrees of freedom for a given probability.

Optimal experiments can be designed by minimizing the hypervolume of the confidence region of the estimated parameters, in order to ensure minimum variance for the estimates. The minimization of the

confidence region given by equation (17) can be obtained by maximizing the determinant of \mathbf{V}^{-1} , in the so-called *D-optimum design* [23]. Since the covariance matrix \mathbf{V} is given by equation (14), we can then design optimal experiments by maximizing the determinant of the so-called Fisher's Information Matrix, $\mathbf{J}^T \mathbf{J}$. Therefore, optimal experimental variables are chosen based on the criterion

$$\max \left| \mathbf{J}^T \mathbf{J} \right| \tag{18}$$

5. RESULTS AND DISCUSSIONS

In this section we discuss the analysis of the sensitivity coefficients and of the determinant of the information matrix, as well as we present the solution of the parameter estimation problem under investigation, by using simulated experimental data. In order to generate the simulated measurements and design the experiment, we used the parameters from Copenhagen's experiment number 3 [25,26], which is widely used for the analysis of micro-scale atmospheric dispersion. In this case, the values used for the parameters in the simulation were $(u_*)_0 = 0.38 \text{ m/s}$, L = -71 m and $z_0 = 0.6 \text{ m}$. The diffusivity in the longitudinal direction was assumed to be $K_{xx} = 50 \text{ m}^2/\text{s}$. The tracer was released at an altitude $z_e = 115 \text{ m}$, as in Copenhagen's experiment. The computational domain dimensions were taken as H = 1120 m and A = 6000 m. The longitudinal distance from the source to the origin was $x_e = 100 \text{ m}$. The sensors were assumed to be located 10 m above the ground, which is generally used in practice to collect meteorological data.

Figures 2.a-d present the contours of the normalized sensitivity coefficients with respect to the Monin-Obukov length, the superficial friction velocity, the longitudinal diffusivity and the surface roughness, respectively. The contours are presented with respect to the dimensionless time and the dimensionless longitudinal position. The normalized sensitivity coefficients were obtained by multiplying the original dimensionless sensitivity coefficients by the parameters that they are referred to. Figures 2.a-d show that the sensitivity coefficients with respect to all parameters attain large magnitudes at the time that the tracer plume reaches a specific longitudinal position. However, for X > 1 all the sensitivity coefficients decrease to very small values after the peak-value is reached. On the other hand, except for the superficial friction velocity (see figure 2.b), large magnitudes are observed for the sensitivity coefficients, even for large times, at some regions downstream the source position for X < 1. It is interesting to note that the sensitivity coefficients are null for the region upstream the source, i.e., for X < 0.1, except for the diffusivity along the longitudinal direction (K_{xx}). In fact, the regions upstream the source are affected by changes in this parameter because of longitudinal diffusion. An analysis of Figures 2.a-d reveals that the region 0.2 < X < 1 should be preferred for the location of sensors, because the sensitivity coefficients attain large magnitudes.

Figure 3 presents the transient variation of the concentration and of the normalized sensitivity coefficients with respect to the different parameters, at a longitudinal position X = 0.6. This figure shows that the sensitivity coefficients are of the same order of magnitude of the concentration. The sensitivity coefficient for the superficial friction velocity attains the largest magnitudes, but it tends to zero for large times (see also Figure 2.b). At this position, the sensitivity coefficients with respect to the longitudinal diffusivity also tends to zero for large times, but the sensitivity coefficients with respect to L and z_0 tend to constant values. We notice in Figure 3 that the sensitivity coefficients with respect to the surface roughness and with respect to the Monin-Obukov length tend to be linearly-dependent. Therefore, difficulties can be encountered for the simultaneous estimation of these two parameters.

The determinant of the information matrix for a sensor at the position X=0.6 is presented in Figure 4, for different sets of parameters. For the calculation of $|\mathbf{J}^T \mathbf{J}|$, the measurements were supposed to be taken in a fixed dimensionless time interval of 0.004, which corresponds to 12 s. Figure 4 shows that the smallest values for the determinant of the information matrix are obtained for the case involving the simultaneous estimation of the 4 parameters K_{xxx} , $(u_*)_0$, L and z_0 . In fact, we notice in Figure 4 that the determinant for the cases involving the simultaneous estimation of L and z_0 are at least one order of magnitude smaller than for the other cases. This is because of the tendency for linear dependence between the sensitivity coefficients for L and z_0 , as depicted in Figure 3. Figure 4 also shows that, for any set of parameters, the largest rate of increase in determinant of the information matrix takes place for $\tau < 2$. This is due to the fact that for larger times the sensitivity coefficients with respect to L and z_0 become constant.



Figure 2. Normalized sensitivity coefficients for (a) Monin-Obukov length, (b) superficial friction velocity, (c) longitudinal diffusivity and (d) surface roughness.



Figure 3. Transient variation of the normalized sensitivity coefficients at the position X=0.6.



Figure 4. Determinant of the information matrix for different sets of parameters.

We now consider the estimation of the unknown parameters by using simulated experiments taken at the longitudinal position X=0.6, with a frequency of 1 measurement every dimensionless time interval of 0.004 (12 s in physical time). The duration of the experiment was considered as $\tau = 1.2$, which corresponds to 1 hour. For the results presented below, the initial guess for the Levenberg-Marquardt method was taken as: $K_{xx}^0 = 5 \text{ m}^2/\text{s}$, $(u_*)_0^0 = 1 \text{ m/s}$, $L^0 = -20 \text{ m}$ and $z_0^0 = 1 \text{ m}$. Two different levels of measurement errors were examined in this work: $\sigma = 0$ (errorless measurements) and $\sigma = 0.01 C_{max}$, where C_{max} is the maximum measured concentration.

For errorless measurements, the unknown parameters were exactly recovered with the Levenberg-Marquardt method for any set of parameters for which the determinant of the information matrix was examined in Figure 4. On the other hand, the simultaneous estimation of the 4 parameters was not possible with simulated measurements containing random errors. In fact, for such case the iterative procedure of the Levenberg-Marquardt method stalled at the bounds imposed for the parameters, probably because of the linear-dependence between the sensitivity coefficients for L and z_0 (see Figure 3). Since the surface roughness can be identified through other experiments [3], we decided to consider this parameter as exactly known for the inverse analysis hereafter and then examined the simultaneous estimation of $\mathbf{P}^T = [K_{xx}, L, (u_*)_0]$.

Figures 5.a-c present the estimated values for the longitudinal diffusivity, Monin-Obukov length and superficial friction velocity, respectively, obtained with different runs of the inverse problem analysis. For each run, a different set of random numbers was used to generate the simulated noisy measurements. Figures 5.a-c show that quite accurate estimates could be obtained for the unknown parameters by using the Levenberg-Marquardt method. The averaged values for the estimated parameters and their respective 99% confidence intervals are presented in Table 1. This table shows that the longitudinal diffusivity is not as accurately estimated as the other parameters. This is a result of the lower magnitude of its sensitivity coefficient as compared to those for the other parameters, as can be seen in Figure 3. In fact, longitudinal diffusive effects are small compared to advective ones for the case under investigation.



Figure 5.a. Estimation of the Monin-Obukov length.



Figure 5.b. Estimation of the longitudinal diffusivity.



Figure 5.c. Estimation of the superficial friction velocity.

Table 1. Averaged estimates with correspondent 99% confidence intervals

Parameter	Exact Value	Initial Guess	Estimated	99% Confidence
				Interval
K_{xx} (m ² /s)	50	5	50.2	(39.6; 60.7)
<i>L</i> (m)	-71	-20	-71.0	(-73.0,-69.1)
$(u_{*})_{0}$ (m/s)	0.38	1	0.38	(0.37, 0.39)

6. CONCLUSIONS

In this paper we examined the possibility of estimating micro-meteorological parameters appearing in the formulation of atmospheric boundary layer flows, by using simulated measurements of the concentration of a tracer released by a known source. The problem was assumed to be two-dimensional and the turbulence closure equations from Ulke [8] were used for the velocity profile and for the vertical eddy-diffusivity. The Generalized Integral Transform Technique was used for the solution of the direct problem, while the Levenberg-Marquardt method of minimization of the least-squares norm was applied for the parameter estimation.

The analyses of the sensitivity coefficients and of the determinant of the information matrix revealed the most appropriate sensor locations and duration of the experiment, as well as which of the parameters could be simultaneously estimated. Results obtained with simulated experimental data, for the simultaneous estimation of the longitudinal diffusivity, Monin-Obukov's length and superficial friction velocity, were quite accurate and stable with respect to measurement errors.

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