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An automatic methodology for estimating eddy diffusivities from experimental data

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Summary. — A technique for estimating eddy diffusivities in a turbulent atmospheric layer is presented; the scheme adopted is based on an inverse-problem methodology. The inverse problem is formulated as a nonlinear constrained optimization problem, where the objective function is defined through the square differences between experimental and model data. The direct mathematical model is given by the advection-diffusion equation, which is solved by second-order finite-difference method. In the presence of noise it is necessary to use some regularization term; the Tikhonov function and an entropic regularization of zeroth, first and second orders are used in this paper. In addition, two inversion strategies are used: alternate and simultaneous eddy diffusivities estimation. Numerical experiments show a good performance of the proposed methodology.

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1. – Introduction

Turbulence has been a permanent challenge in science. A typically turbulent flow exists in the atmospheric boundary layer [1]. Many ideas have been proposed to understand and to represent the turbulence. An interesting approach is due to Osborne

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Reynolds: the flow is described as the sum of a mean stream plus a fluctuation term. In this regard, the turbulence contribution is constituted by the mean of the product between fluctuations, since individually the fluctuations have zero mean, according to Reynolds postulates. These products, also called covariances, are the new *unknowns* of the model, and represent the turbulent fluxes. Reynolds' hypotheses cannot be applied recursively, because it would lead to the appearance of higher-order correlations [2]; therefore, it is necessary to estimate the turbulence term or, in other words, to parameterize the turbulent fluxes.

In order to close the equation system in a turbulent flow, the K-theory assumes that the turbulent fluxes can be represented by means of the gradient-transfer assumption, *i.e.*, in the first-order closure the turbulence is modeled by a product between the gradient of the mean stream and a K diffusivity. However, these diffusivities still need to be determined.

Some approaches have been presented to estimate the turbulent diffusivities, based on semi-empirical theories, as the Monin-Obukhov similarity theory [1], Taylor's statistical theory of turbulence [3-5], and parameterizations using data from Large Eddy Simulation [6]. Some authors have proposed numerical procedures for estimating the diffusivities from the experimental data, such as described by Sorbjan ([7], p. 170) and Correa and Degrazia [8]. Another approach employing techniques of inverse problems has also been used [9-13].

In this work the estimation of the vertical and horizontal eddy diffusivities in an atmospheric stable boundary layer is done in such a way that an advection-diffusion equation model can well describe the dispersion process of pollutants. Two inversion procedures are considered: an *alternate strategy*, where at each iteration the value of the vertical eddy diffusivity is estimated before that of the horizontal diffusivity; and a *simultaneous strategy*, where both diffusivities are estimated in a unified fashion. In both inversion procedures the inverse model is an *implicit deterministic* inversion technique for function estimation from experimental measurements. However, inverse problems belong to the class of ill-posed problems, whose solutions are unstable in the presence of noise. It is well known that the presence of noise in the experimental data represents an unrecoverable loss of information that makes a perfect inversion impossible. Therefore, the observational data is often not sufficient to provide a physically feasible solution. The approach in this case is to restrict the class of admissible solutions (*i.e.*, the solutions that are consistent with the available data) by using a regularization operator [14].

The algorithm of the inverse problem is formulated as a constrained nonlinear optimization problem, in which the direct problem is iteratively solved for successive approximations of the unknown parameters. The objective function represents the least-square fit between experimental and model data, associated to a regularization operator. In the present paper six regularization methods are used: Tikhonov and entropic regularizations of zeroth, first and second orders.

2. – Formulation of the direct problem

The model described below was used to test some turbulent parameterization schemes [15, 16]. It represents a multidimensional steady state advection-diffusion equation. The system equation is expressed as

$$(1) \qquad U\frac{\partial c}{\partial x} = \frac{\partial}{\partial y}\left(K_{yy}\frac{\partial c}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_{zz}\frac{\partial c}{\partial z}\right) \qquad \begin{cases} \text{at } x > 0 \text{ and} \\ (y, z) \in (0, \ L_y) \times (0, \ h), \end{cases}$$

$$(2) \qquad c(x, y, z) = Q\delta(y - y_{\mathrm{F}})\,\delta(z - z_{\mathrm{F}}) \qquad \text{at } x = 0\,,$$

$$(3) \qquad K_{zz}\frac{\partial c}{\partial z} = 0 \qquad \text{at } z = 0 \quad \text{and} \quad z = h\,,$$

$$(4) \qquad \frac{\partial^2 c}{\partial y^2} = 0 \qquad \text{at } y = 0 \quad \text{and} \quad y = L_y,$$

where it is assumed that the transport in the x-directon is dominated by the advection, and the diffusivity tensor can be written in the orthotropic form. In eq. (1) $c(x, y, z)$ represents the mean concentration of pollutants; $K_{yy}(z)$ and $K_{zz}(z)$ are the horizontal and vertical eddy diffusivities, respectively; U is the mean wind speed; h is the height of the stable boundary layer. Equation (2) models a source located at $(x = 0, y = y_{\mathrm{F}}, z = z_{\mathrm{F}})$; this condition is similar to that used by Giordana *et al.* [11]. The boundary condition (3) does not permit exchange of vertical fluxes with the outside of the boundary layer, and expression (4) is the same condition used by Shir and Shieh [17].

Equation (1) is numerically solved using the Crank-Nicolson method in the x-direction and a centered finite-difference method for the diffusion operator. Therefore, the numerical solution can be expressed in a matrix form by

$$(5) \qquad (\mathbb{I} - \theta\mathbb{D}_z)\,\mathbb{C}_{i+1} = [\mathbb{I} + \mathbb{D}_y + (1 - \theta)\,\mathbb{D}_z]\,\mathbb{C}_i,$$

where $\mathbb{C} \equiv [\mathbf{C}_{i1}\mathbf{C}_{i2}\ldots\mathbf{C}_{i,N_y}]$ is the state vector, with $\mathbf{C}_{ij} \equiv [C_{ij1}C_{ij2}\ldots C_{i,j,N_z}]$, C_{ijk} being the approximate solution for mean concentration c at point (x_i, y_j, z_k); $\mathbb{I} \equiv I_y \otimes I_z$, with I_α the identity matrix of order $N_\alpha \times N_\alpha$ $(\alpha = y, z)$; $\mathbb{D}_y$ and $\mathbb{D}_z$ the finite-difference operator for horizontal and vertical diffusion as follows:

$$\mathbb{D}_y = D_y \otimes I_z, \qquad \mathbb{D}_z = I_y \otimes D_z,$$

where the matrices D_α are given by

$$D_\alpha = \begin{bmatrix} (\sigma^0_{bc})_{\alpha 1} & (\sigma^+_{bc})_{\alpha 1} & & & & \\ \sigma^-_{\alpha 2} & -\sigma^0_{\alpha 2} & \sigma^+_{\alpha 2} & & & \\ & \sigma^-_{\alpha 3} & -\sigma^0_{\alpha 3} & \sigma^+_{\alpha 3} & & \\ & \vdots & \vdots & \vdots & & \\ & & \sigma^-_{\alpha, N_\alpha - 1} & -\sigma^0_{\alpha, N_\alpha - 1} & \sigma^+_{\alpha, N_\alpha - 1} \\ & & & (\sigma^-_{bc})_{\alpha, N_\alpha} & (\sigma^0_{bc})_{\alpha, N_\alpha} \end{bmatrix} \qquad (\alpha = y, z).$$

The vertical boundary conditions are

$$\textit{Bottom}: \quad (\sigma^-_{bc})_{z,1} = (\sigma^-_{z,1} - \sigma^0_{z,1}), \qquad \textit{Top}: \quad (\sigma^-_{bc})_{z,N_z} = \sigma^-_{z,N_z},$$
$$(\sigma^+_{bc})_{z,1} = \sigma^+_{z,1}; \qquad\qquad (\sigma^0_{bc})^0_{z,N_z} = -(\sigma^0_{z,N_z} - \sigma^+_{z,N_z})$$

and for the y-direction: $(\sigma^0_{bc})_{\alpha 1} = (\sigma^+_{bc})_{\alpha 1} = (\sigma^-_{bc})_{\alpha, N_\alpha} = (\sigma^0_{bc})_{\alpha, N_\alpha} = 0$. More details can be found in Campos Velho *et al.* [15].

In the present simulation the eddy diffusivity is assumed to be a function of the vertical space variable only; however situations exist when this assumption is not valid [15, 18].

3. – Formulation of the inverse problem

The inverse methodology adopted is an implicit technique based on the least-square formulation, which can guarantee existence and uniqueness for the solution of the inverse problem, even though this solution can be unstable in the presence of noise in the experimental data, requiring the use of some regularization technique [14].

Some inverse problems require the estimaton of very different types of parameters (or functions). These parameters cause a very different impact on the direct model, as in radiative transfer problems [19, 20]. In the radiative process two phenomena occur simultaneously: the absorption and scattering of photons, which are respectively represented by their coefficient. However, the same percentual change for the absorption and scattering coefficient could give different outputs for irradiances, becoming difficult to estimate these coefficients in a unified inversion. In this case, it is possible to get good results only by adopting an alternate strategy.

The present estimation of eddy diffusivities will be applied for y and z directions, that is, K_{yy} and K_{zz} reconstruction, which can assume different values for each direction [4]. In order to verify the influence of each direction in the eddy diffusivities estimation two inversion strategies were elaborated:

a) *Alternate strategy*:

1. Solve the optimization problem:

$$\min \quad J_{\gamma_z}(\mathbf{K}^n_z); \qquad J_{\gamma_z}(\mathbf{K}^n_z) = R(\mathbf{K}^n_z) + \gamma_z \Omega(\mathbf{K}^n_z). \tag{6}$$

2. Solve the optimization problem:

$$\min \quad J_{\gamma_y}(\mathbf{K}^n_y); \qquad J_{\gamma_y}(\mathbf{K}^n_y) = R(\mathbf{K}^n_y) + \gamma_y \Omega(\mathbf{K}^n_y). \tag{7}$$

3. If: $\|\mathbf{K}^n_\alpha - \mathbf{K}^{n-1}_\alpha\| / \|\mathbf{K}^n_\alpha\| < \varepsilon$ stop! Otherwise, go back to step 1.

In the first estimation, the value of $\mathbf{K}_y$ is taken from the literature, for example the value used by Shir and Shieh [17], in which the horizontal diffusivity is assumed to be a simple scalar number.

b) *Simultaneous strategy*:

In this case only the follow optimization problem is solved:

$$\min \quad J_\gamma(\mathbf{K})\,; \tag{8}$$

$$J_{\gamma_z}(\mathbf{K}) = R(\mathbf{K}) + \gamma \;\; \Omega(\mathbf{K})\,; \tag{9}$$

$$\mathbf{K} = [\mathbf{K}_y \;\; \mathbf{K}_z]^{\mathrm{T}}.$$

In both strategies the vector of parameters is the sampled eddy diffusivity function

$$\mathbf{K}_\alpha = [K_{\alpha,\,1} \;\; K_{\alpha,\,2} \ldots K_{\alpha,\,N_\alpha}]^{\mathrm{T}}, \qquad K_{\alpha,\,n} = K_{\alpha\alpha}(z_0 + n\,\Delta z_n)\,. \tag{10}$$

In eqs. (6)-(8) a smooth solution is obtained by choosing a function $\mathbf{K}_\alpha$ that optimizes those functionals, where $\Omega(\mathbf{K})$ is a regularization operator, γ's are the Lagrange multipliers, $R(\mathbf{K})$ is a norm l_2 of the difference between experimental and model data:

$$R(\mathbf{K}) = \sum_{i=0}^{N_x} \sum_{j=0}^{N_y} \sum_{k=0}^{N_z} [C_{ijk}^{\mathrm{Exp}} - C_{ijk}^{\mathrm{Mod}}(\mathbf{K})]^2. \tag{11}$$

3˙1. *Regularization operators.* – As already mentioned, the least-square approach gives a unique solution for an inverse problem. However, ill-posed problems can yield stable solutions if sufficient *a priori* information about the true solution is available [14]; such information is added to the least-square approximation by means of a regularization term, in order to complete the solution for the inverse problem. The regularization operators used in this paper are described below.

3˙1.1. Tikhonov regularization. The regularization operator is expressed by [14]

$$\Omega(\mathbf{K}) = \sum_{m=0}^{p} \gamma_m \|\mathbf{K}^{(m)}\|_2^2, \tag{12}$$

where $\mathbf{K}^{(m)}$ denotes the m-th difference, and $\gamma_m \geqslant 0$ are regularization parameters. The effect of zeroth-order regularization is to reduce the amplitude of oscillations on the parameter vector (*smooth* function $K_{\alpha\alpha}(z)$), while first-order regularization acts on the difference $|\mathbf{K}_m - \mathbf{K}_{m-1}|$ (that is, $\mathbf{K}_m$ is constant in the limit of $\gamma_1 \to \infty$).

It can be noted that as $\gamma_m \to 0$ the least-square term in the objective function is over-estimated, and this might not give good results in the presence of noise. On the other hand, if $\gamma \to \infty$, all consistency with the information about the system is lost.

3˙1.2. Entropic regularization. The maximum entropy principle was first proposed by Jaynes [21] on the basis of Shannon's information theory [22]. Similar to the Tikhonov approach, this general inference method searches for a *global* regularity, yielding the smoothest solution which is consistent with the available data.

Recently, a higher-order entropic regularization has been proposed [23-27].

A generic expression for entropic regularization can be written as

$$\Omega(\mathbf{K}) = \sum_{m=0}^{p} \gamma_m S^m(\mathbf{K}); \qquad S^m(\mathbf{K}) \equiv - \sum_{q=1}^{N_q} s_q \log(s_q), \tag{13}$$

where

$$s_q = r_q^{(m)} \Big/ \sum_{l=1}^{N_q} r_l^{(m)} \tag{14}$$

and $r_q^{(m)}$ represents the m-th difference among the vector of parameters, for example the three first differences:

$$r_q^{(m)} = \begin{cases} K_q & \text{if } m = 0, \\ |K_q - K_{q-1}| + \zeta & \text{if } m = 1, \\ |K_{q-1} - 2K_q + K_{q+1}| + \zeta & \text{if } m = 2. \end{cases} \tag{15}$$

Here ζ is a small positive constant, which assures that entropies of higher order will always have a definite value. The function S^m attains its global maximum when all the r_q are the same, *i.e.*, a uniform distribution with $S_{\max} = \log(N_q)$; in contrast, the lowest entropy value $S_{\min} = 0$ is reached when all the elements r_q but one are set to zero [28].

3·2. *Optimization algorithm.* – There are many techniques to solve an optimization problem, as conjugate gradient method [29, 30], techniques based on fuzzy theory [31] and stochastic methods, such as genetic algorithms [32, 33] or simulated annealing [34]. In the present paper, the problem given by eqs. (6)-(8) is iteratively solved by a quasi-Newtonian optimizer E04UCF routine from the NAG Fortran Library [35]; this algorithm is designed to minimize an arbitrary smooth function subject to constraints (simple bound, linear or nonlinear constraints), using a sequential programming method.

The approach used here has been sucessfully adopted in other works [23, 36-38]. In addition, Afonso and Horowitz [39] have investigated four different sequential quadratic programming algorithms for structural shape optimization procedure; the NAG routine was the only one that solved all the examples presented.

4. – Numerical results

The two inversion strategies presented in the previous section were tested with *synthetic data* generated by the direct numerical model and corrupted by white Gaussian noise with different levels of noise, being the exact eddy diffusivities given by Degrazia and Moraes [4]:

$$\frac{K_{zz}}{u_* h} = \frac{0.32(1 - z/h)^{\alpha_1/2}(z/h)}{1 + 3.7(z/h)(h/\Lambda)}, \tag{16}$$

$$\frac{K_{yy}}{u_* h} = \frac{0.55(1 - z/h)^{\alpha_1/2}(z/h)}{1 + 3.7(z/h)(h/\Lambda)}, \tag{17}$$

TABLE I. – *Numerical and physical parameters.*

N_x	Δx	N_y	Δy	N_z	Δz	L	u_*
100	20 m	40	2.5 m	40	2.5 m	60 m	0.09 m s^{-1}

where u_* is the friction velocity, h is the height of the stable boundary layer, z is the height above the ground, Λ is the local Monin-Obukov length given by

$$\frac{\Lambda}{L} = \left(1 - \frac{z}{h}\right)^{3\alpha_1/2 - \alpha_2}; \tag{18}$$

L is the surface Monin-Obukov lenght, $\alpha_1 = 3/2$ and $\alpha_2 = 1$ are used for fully developed stable boundary layer (SBL), as observed in the Cabaw experiment [4]. The physical and numerical parameters are given in table I, where: $L_x = N_x \Delta x$, $L_y = N_y \Delta y$, $h = N_z \Delta z$; being L_x the maximum.

The pollutant source is located at $(0, L_y/2, h/4)$. The SBL height is a typical value for this layer [40], and it is lying in the interval $0 < h/L < 2$ that is representative for a stable layer.

Figure 1 shows the reconstruction of the diffusivities for the simultaneous strategy without regularization ($\gamma = 0$ in eqs. (8)), where $K_{\alpha\alpha\_\mathrm{re}}$ $(\alpha = z, y)$ is the real value given by eq. (16) and eq. (17), and $K_{\alpha\alpha\_\mathrm{mo}}$ is the diffusivity obtained with the inversion model. Clearly, some spurious spikes appear in the estimation, indicating that some regularization is needed. In the next sections different regularization operators will be tested, in the context of both the alternate and simultaneous strategies.

The influence of noise is clearly noted in fig. 1, where the increase in the level of noise implies an amplification of the spikes. Although the tests had been performed for two levels of noise, the results are shown only for data with 5% of noise, but the numerical values of the Lagrange multipliers for 1% and 5% are indicated.

4$\cdot$1. *Alternate strategy.* – The regularization parameters for these estimations are determined by numerical experiments and are presented in table II; the number of iterations to reach the final result is shown in tables III and IV for 1% and 5% of noise, respectively.

Results using objective functions (6) and (7) are shown below. The estimation using zeroth-order regularization is shown in figs. 2a for Tikhonov and 2b for entropic approaches. The entropic regularization reduced the oscillations in comparison to the reconstruction displayed in fig. 1. The Tikhonov approach yielded smoother results than the entropic method, but near to the ground ($z/h < 0.3$) the estimation was not sufficiently effective.

First-order regularization methods are plotted in figs. 3a for Tikhonov and 3b for entropic regularizations, respectively. The worse results are obtained for the Tikhonov method, mainly on the top of the boundary layer; but we do not have significant difference related to the zeroth-order Tikhonov estimation. The entropic scheme does not present any improvement.

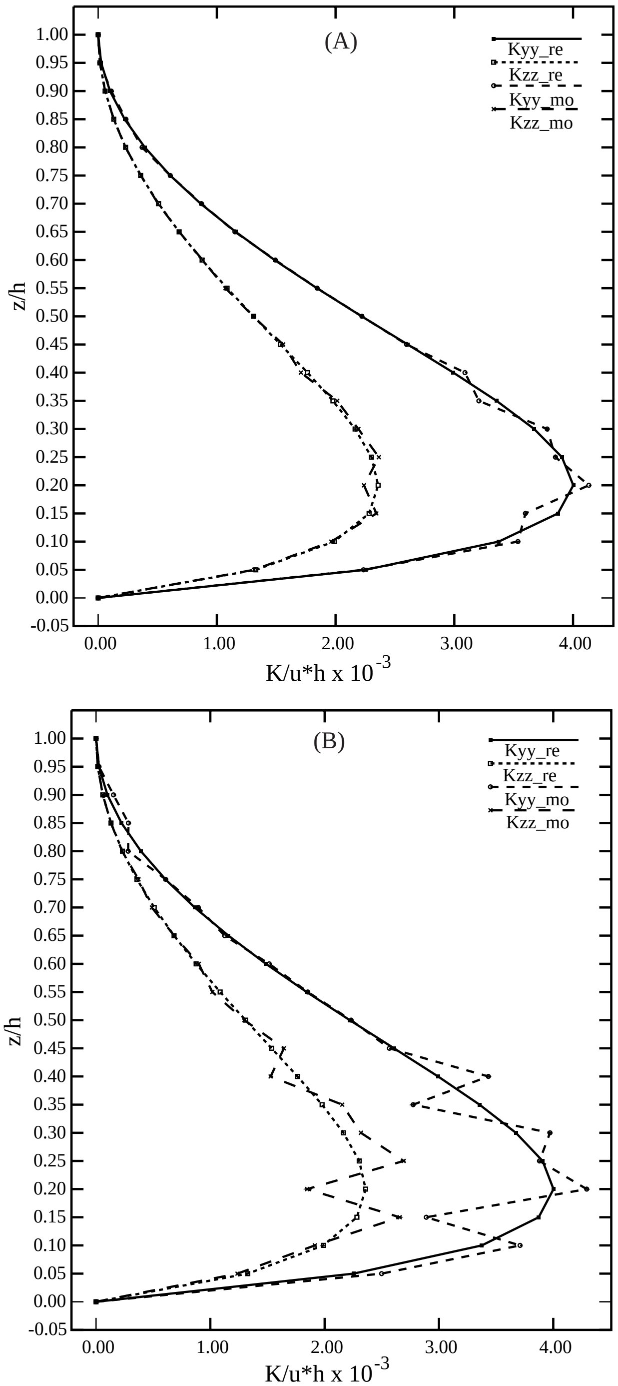

Fig. 1. – Eddy diffusivity estimation without regularization: (A) 1% and (B) 5% of noise data.

TABLE II. – *Regularization parameters* (γ_m) *in alternate strategy, for entropic—eq.* (13)*—and Thikhonov—eq.* (12)*—regularizations.*

	Entropy-0	Entropy-1	Entropy-2	Tikhonov-0	Tikhonov-1	Tikhonov-2
1% noise	$1\cdot10^{-4}$	$1\cdot10^{-4}$	$7\cdot10^{-4}$	0.6	0.2	0.08
5% noise	$1\cdot10^{-4}$	$1\cdot10^{-5}$	$7\cdot10^{-4}$	1.3	1.5	1.0

TABLE III. – *Number of* (*glocal*, G.) *iterations* (iter.) *up to the convergence for 1% of noise.*

$\Omega(\mathbf{K})$	Entropy-0		Entropy-1		Entropy-2		Tikhonov-0		Tikhonov-1		Tikhonov-2	
G. iter.	K_{yy}	K_{zz}	K_{yy}	K_{zz}	K_{yy}	K_{zz}	K_{yy}	K_{zz}	K_{yy}	K_{zz}	K_{yy}	K_{zz}
1	85	68	74	43	81	43	43	27	59	34	58	34
2	99	39	71	63	110	71	91	56	86	74	81	58
3	110	45	97	42	121	46	48	57	54	45	47	59
4	68	40	49	38	43	37	26	48	28	40	27	53
5	26	30	47	35	36	33	23	28			24	43
6	26	23	32	31	27	26	22	28			20	37
7	22	28	28	36	22	29	20	20			21	39
8	22	33	27	30	19	28	19	19			19	33
9	22	32	23	36	19	27	19	18			19	34
10	22	30	24	36	20	25	16	19			18	21
11											19	21
12											16	30
13											15	14
14											17	19
15											17	17
16											19	27
17											16	26
18											16	14
19											10	29
20											11	11

TABLE IV. – *Number of* (*global*, G.) *iterations* (iter.) *up to the convergence for* 5% *of noise.*

$\Omega(\mathbf{K})$	Entropy-0		Entropy-1		Entropy-2		Tikhonov-0		Tikhonov-1		Tikhonov-2	
G. iter.	K_{yy}	K_{zz}	K_{yy}	K_{zz}	K_{yy}	K_{zz}	K_{yy}	K_{zz}	K_{yy}	K_{zz}	K_{yy}	K_{zz}
1	69	73	75	44	88	64	38	34	57	28	61	40
2	117	42	56	75	111	67	66	66	68	62	61	64
3	105	54	92	46	101	45	45	57	41	40	36	47
4	75	37	44	41	50	27	28	39			25	41
5	27	36	38	31	47	33	25	23			25	36
6	25	28	32	28	32	32	23	21			23	39
7	25	37	29	33	27	30	21	22			24	33
8	25	31	25	34	25	27	20	22			22	20
9	23	26	24	26	24	27	15	19			23	29
10	23	29	23	24	22	24	16	20			22	21

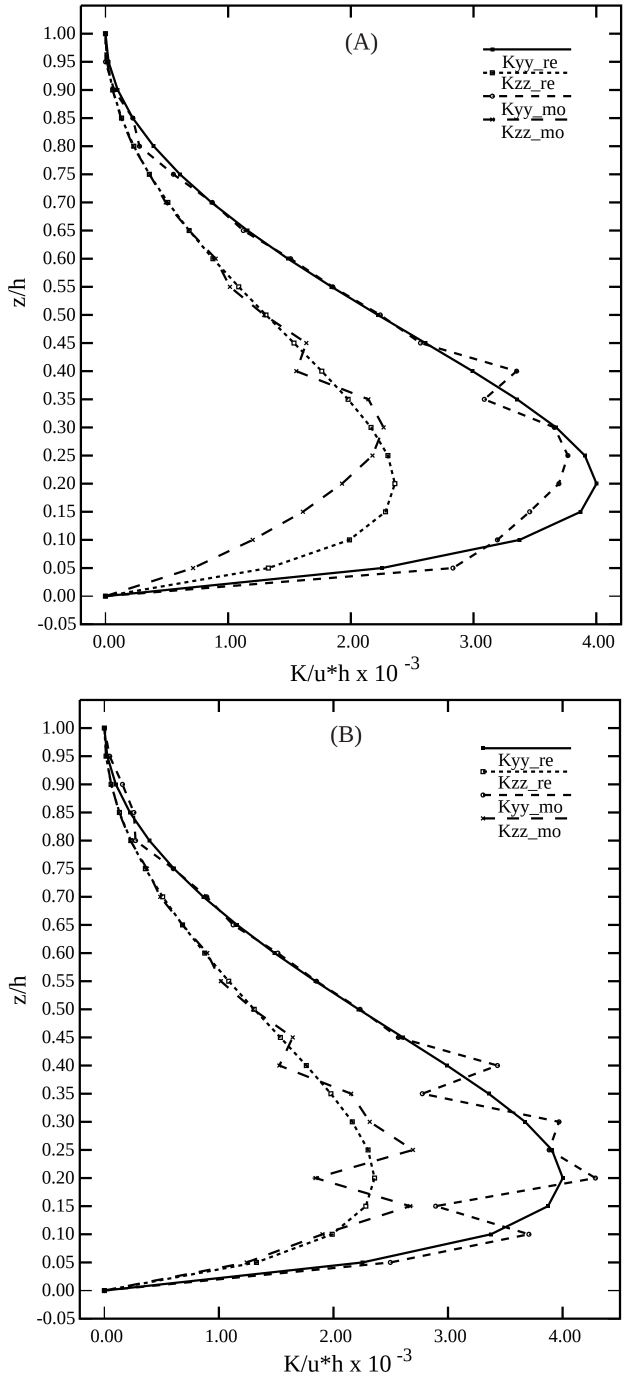

Fig. 2. – Turbulent diffusivities by alternate strategy with zeroth-order regularization: (A) Tikhonov and (B) entropic.

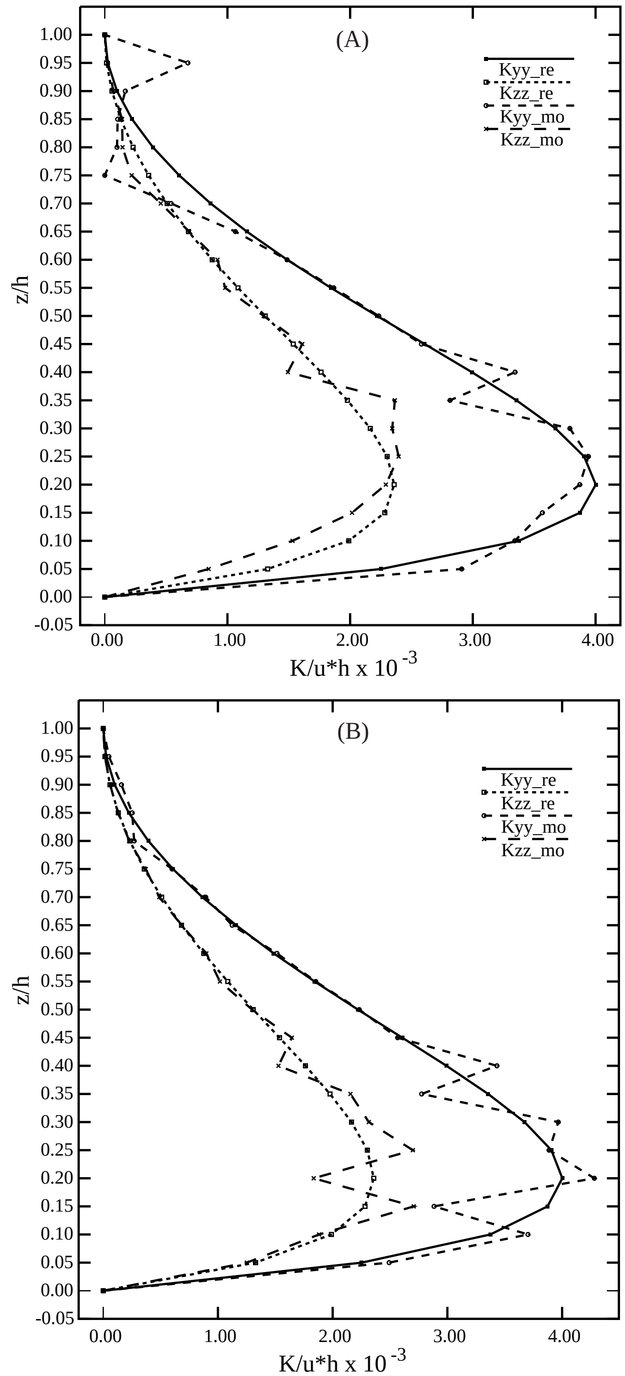

Fig. 3. – Turbulent diffusivities by alternate strategy with first-order regularization: (A) Tikhonov and (B) entropic.

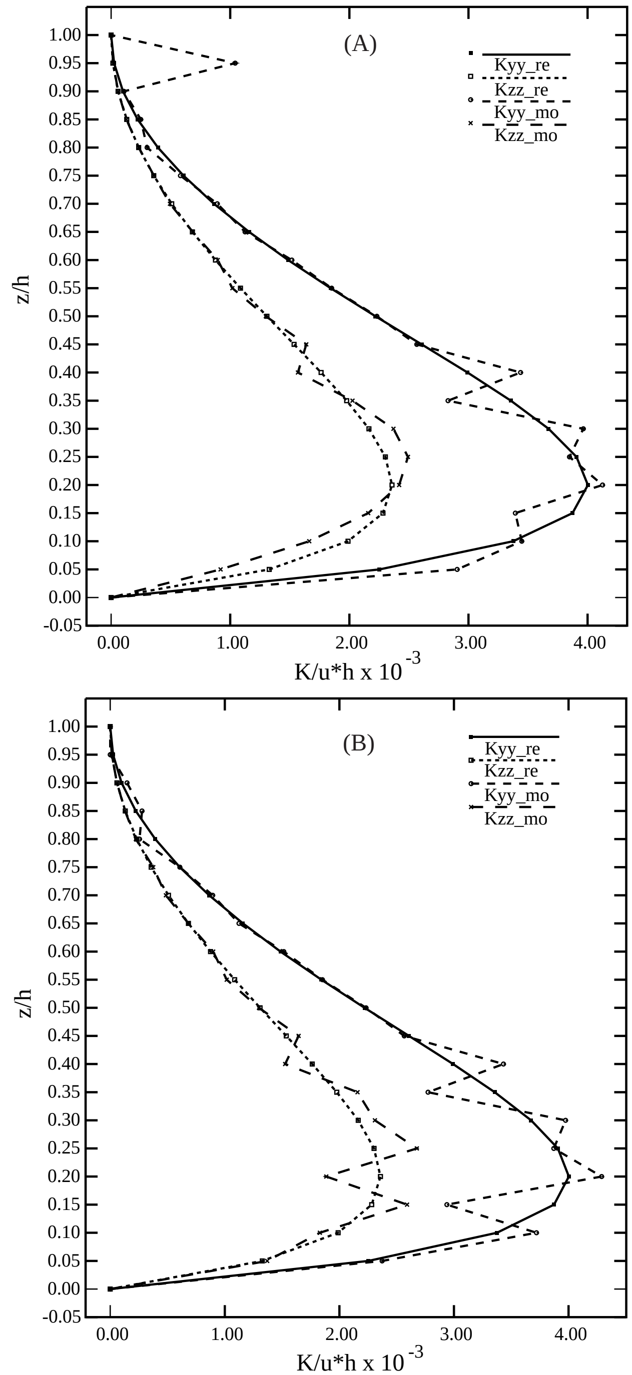

Fig. 4. – Turbulent diffusivities by alternate strategy with second-order regularization: (A) Tikhonov and (B) entropic.

TABLE V. – *Regularization parameters* (γ)—*eqs.* (13) *and* (12)—*and number of iterations in simultaneous strategy for* 1% *and* 5% *of noise.*

		Entropy-0	Entropy-1	Entropy-2	Tikhonov-0	Tikhonov-1	Tikhonov-2
1%	γ	$1\cdot10^{-6}$	$1\cdot10^{-7}$	$5\cdot10^{-8}$	0.01	0.09	0.1
	iter.	136	118	118	75	49	50
5%	γ	$1\cdot10^{-6}$	$1\cdot10^{-6}$	0.09	0.1	0.7	0.8
	iter.	112	116	58	72	52	52

Figure 4 shows the estimation for second-order Tikhonov and entropic regularizations method. The result for Tikhonov method is close to that obtained with first order, but some oscillations on the top of boundary layer, were persistent. The entropic scheme presented the same performance of previous cases.

Tables III and IV show the number of iterations needed to reach the convergence. As in the alternate strategy the eddy diffusivity is found for each direction, in which the estimation is also done through an iterative process. Therefore, two iteration cycles occur: a *global iteration* (a complete cycle of estimation of eddy diffusivities) and an *internal iteration* in order to solve the optimization problem. The first column in tables III and IV refers to the former iteration, while other columns denote the local iterations for each regularization method.

From all these results the entropic regularization showed a better fit (see table VI); the smallest for second-order approach. However, the Tikhonov regularization presented a smoother solution.

4˙2. *Simultaneous strategy.* – In sect. **3** the estimation of the eddy diffusivities was presented as being a unique problem: the simultaneous estimation strategy, where the unknown parameter vector is formed by both diffusivities.

Figure 5 shows the estimation for zeroth-order regularization. This reconstruction is better than that presented in fig. 2 with the alternate strategy for Tikhonov regularization. Nevertheless, better results are obtained with first-order (fig. 6) and second-order (fig. 7) Tikhonov regularizations, being second-order a little bit better.

The entropic scheme presented the same results than those shown in the alternate strategy, except for second-order approach, with significant improvement.
Table V shows the regularization parameters used and the number of iterations needed to the convergence.

4˙3. *Influence of the boundary conditions.* – Although the boundary conditions (3) and (4) are more adequate in a pollutant dispersion problem, in order to investigate the robustness of the present methodology an inversion for other boundary conditions was performed, *i.e.*, the Dirichelet conditions:

$$c(x, y, z) = 0 \quad \text{at } y = z = 0 \quad \text{and} \quad y = L_y, \qquad z = h\,. \tag{19}$$

This reconstruction was carried out only with 1% of noise with simultaneous strategy. It was also tested with six regularization functions, but fig. 8 shows the estimation with the second-order Tikhonov regularization only. It can be seen that there is a good agreement between the exact solution and the vertical eddy diffusivities estimated. For horizontal eddy diffusivity the solution was not so good for $z/h < 0.25$.

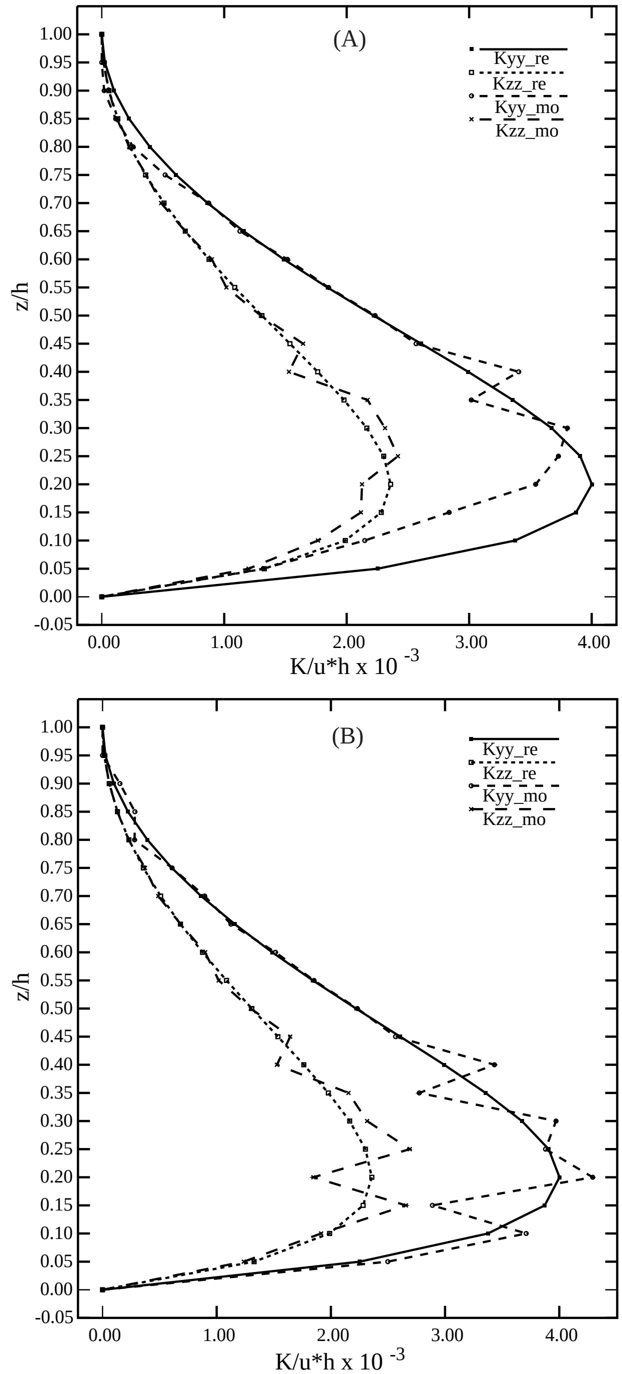

Fig. 5. – Turbulent diffusivities by simultaneous strategy with zeroth-order regularization: (A) Tikhonov and (B) entropic.

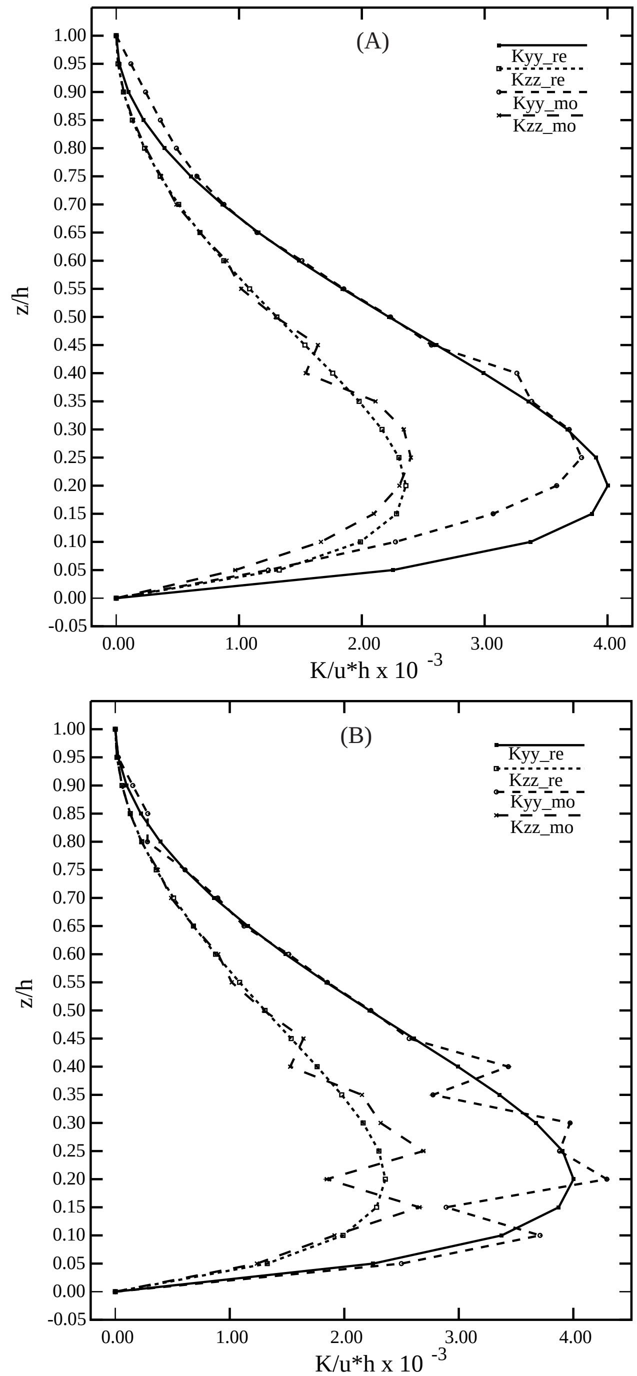

Fig. 6. – Turbulent diffusivities by simultaneous strategy with first-order regularization: (A) Tikhonov and (B) entropic.

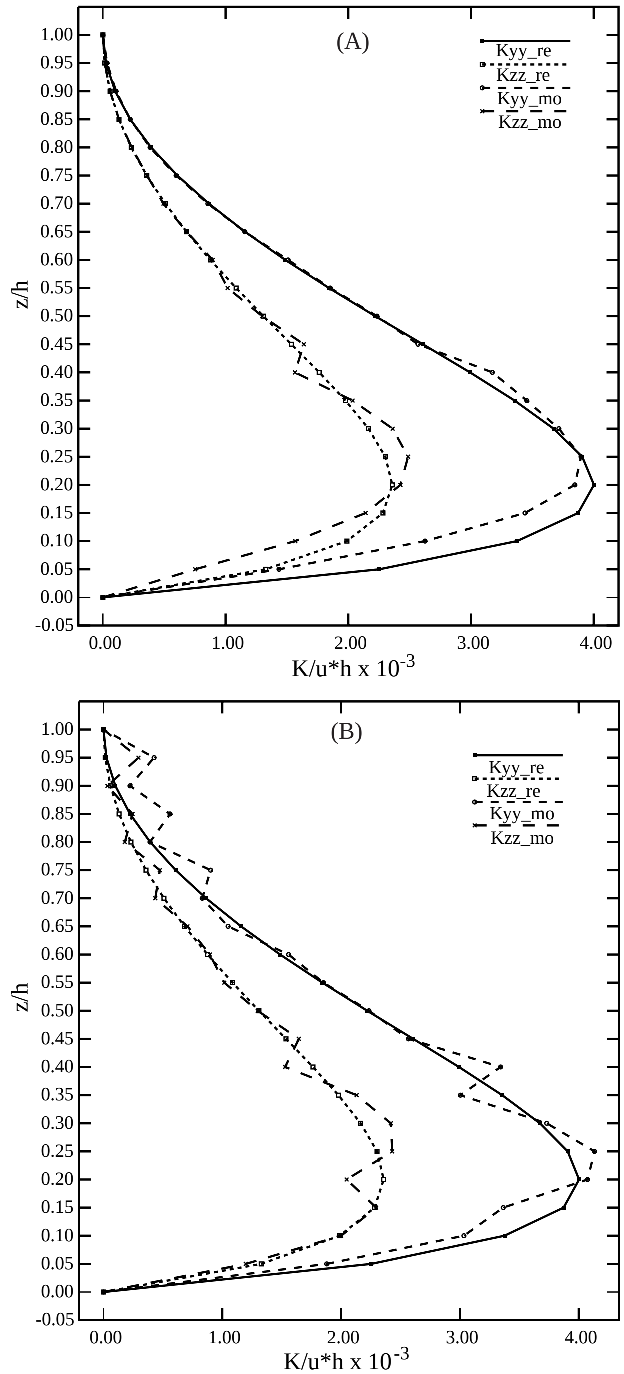

Fig. 7. – Turbulent diffusivities by simultaneous strategy with second-order regularization: (A) Tikhonov and (B) entropic.

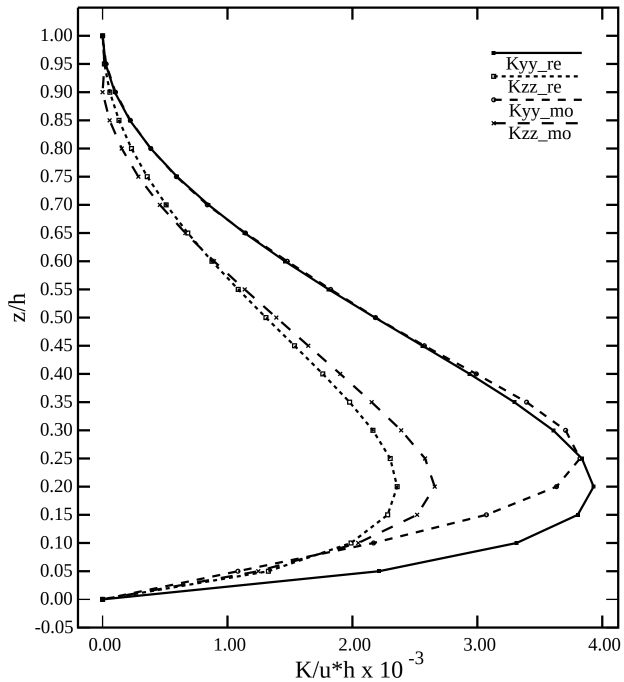

Fig. 8. – Estimation of eddy diffusivity with Dirichelet boundary condition, using second-order Tikhonov regularization with 1% of noise: vertical eddy diffusivity K_{zz} and horizontal eddy diffusivity K_{yy}.

TABLE VI. – *Square differences sum between exact and estimated values for alternate* (Alter.) *and simultaneous* (Simul.) strategies: $\sum_{i=0}^{N_z} [K_{yy,i}^{\text{Exact}} - K_{yy,i}^{\text{Estim.}}]^2 + [K_{zz,i}^{\text{Exact}} - K_{zz,i}^{\text{Estim.}}]^2$.

		Entropy-0	Entropy-1	Entropy-2	Tikhonov-0	Tikhonov-1	Tikhonov-2
1%	Alter.	$1.35 \cdot 10^{-5}$	$1.45 \cdot 10^{-5}$	$1.27 \cdot 10^{-5}$	$4.49 \cdot 10^{-5}$	$4.38 \cdot 10^{-5}$	$1.51 \cdot 10^{-5}$
	simul.	$2.31 \cdot 10^{-6}$	$3.50 \cdot 10^{-6}$	$3.02 \cdot 10^{-6}$	$7.00 \cdot 10^{-6}$	$9.68 \cdot 10^{-6}$	$3.92 \cdot 10^{-6}$
5%	Alter.	$1.50 \cdot 10^{-4}$	$1.51 \cdot 10^{-4}$	$1.41 \cdot 10^{-4}$	$7.10 \cdot 10^{-5}$	$1.61 \cdot 10^{-4}$	$1.85 \cdot 10^{-4}$
	simul.	$5.76 \cdot 10^{-5}$	$6.13 \cdot 10^{-5}$	$5.00 \cdot 10^{-5}$	$1.42 \cdot 10^{-4}$	$6.71 \cdot 10^{-5}$	$3.46 \cdot 10^{-5}$

5. – Conclusions and comments

A methodology for estimating the eddy diffusivities from experimental data based on the minimization of the difference between experimental and model data, added to a regularization operator, was presented. The use of alternate and simultaneous strategies yielded good reconstructions for the eddy diffusivities.

Looking at tables III and IV it is seen that for the present simulations the simultaneous strategy needed smaller computational effort than the alternate strategy. In both strategies the Tikhonov regularization operator presented smoother results. Moreover, on the whole, the present analysis shows that the best results and lowest computatonal cost were achieved with the second-order Tikhonov regularization with simultaneous strategy (see table VI). The entropic approach presented a poorer smoothness, since the regularization parameter must be very small (less than 10^{-5} for the alternate strategy, and 10^{-6} for the simultaneous strategy—except for second-order entropy with 5% of noise, see tables II and V) and then unable to efficiently reduce the noise effect in the experimental data. It is believed that the entropic method of high order requires more study for a definitive opinion.

This methodology is robust in the sense that it can be applied for different boundary conditions. In addition, it can be extended for estimating parameters for other types of phemomena, such as momentum and energy transport. The inversion scheme presented can also be used for the different descriptions of dispersion pollutant problem. For example, the Lagrangian direct model can be coupled to the inverse problem, but in the Lagrangian modeling other parameters must be estimated, as the decorrelation time scale [41] and the Kolmogorov constant [42]. It is also important to note that every improvement in the direct model can be immediately incorporated with this inverse formulation. However, simplified direct models could be useful in the sense that it is possible to get a good first approach for more complex models, because a more suitable first guess tends, in principle, to decrease the number of iterations required to get the solution for the optimization problem.

Another interesting application of this methodology would be the use to determine a more adequate parameterization scheme, when many turbulence models and experimental data are available. Other applications to this inversion method in the turbulent flows could be the identification of the counter-gradient term [43], where the turbulent flux is expressed by

$$\overline{w'\phi'} = K_{zz}(z)\left[\frac{\partial\phi}{\partial z} - \chi_z(z)\right].$$

Finally, other promising techniques deserve to be investigated for inversion, as neural networks [44] and Kalman filter scheme [45].

* * *

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