Inverse Procedures to Reconstruct Turbulent Diffusivities

M.R. de Moraes¹, H.F. de Campos Velho^{1,2}, F.M. Ramos¹, G.A. Degrazia³ & D. Anfossi⁴

¹Laboratório Associado de Computação e Matemática Aplicada, (LAC-INPE), Brazil

²Department of Atmospheric Science, (CSU), USA

⁴ Instituto di Cosmo-geofisica, Torino, ITALY

Abstract

In this paper two inverse strategies for identifying the multidimensional eddy diffusivities are presented. In both strategies the eddy diffusivities are obtained through from a inverse problem methodology, i.e., eddy diffusivities are the most smooth that minimize the *distance* between the experimental and model data.

1 Introduction

In recent works have been presented a inverse methodology to estimate eddy diffusivities (Campos Velho and Ramos, 1996; M.R. Moraes et al., 1998a; M.R. Moraes et al. 1998b), for one and two dimensional problems. In this paper is studied two different inverse schemes for estimating vertical and horizontal eddy diffusivities.

The estimation of vertical and horizontal eddy diffusivities in an atmospheric stable boundary layer is done, in such way that an advection-diffusion equation model can well describe the dispersion process of pollutants. Two inversions procedures are considered: *alternate*, where the vertical eddy diffusivity is estimated and after it is got the horizontal diffusivity, with the alternate iteration proceeds until the convergence; *simultaneous*, where the parameter vector is composed by both diffusivities, estimating these diffusivities in an unified version. In both inversion procedures, the inverse model is an *implict* technique for parameter estimation from experimental measurements.

2 Advection-Diffusion Equation

The model described a multidimension steady state advection-diffusion equation. The system equation is expressed as

$$U\frac{\partial c}{\partial x} = \frac{\partial}{\partial y} \left(K_{yy} \frac{\partial c}{\partial y} \right) + \frac{\partial}{\partial z} \left(K_{zz} \frac{\partial c}{\partial z} \right)$$
(1)

$$c(x, y, z) = Q\delta(y - y_F)\delta(z - z_F) \quad at \quad x = 0;$$
⁽²⁾

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

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

where it is assumed that the transport in direction-*x* is dominated by the advection, and the diffusivity tensor can be written in the orthotropic form. In Eq. (1) *c* represents the mean concentration of pollutants; K_{yy} and K_{zz} are the horizontal and vertical eddy diffusivities, respectively; and *h* is the height of the stable boundary layer. The integration domain is $(x, y, z) \in (0, \infty) \times (0, L_y) \times (0, h)$.

The condition (2) informs that exists a source localized at $(x = 0, y = y_F, z = z_F)$, this condition is similar to that used by Giordana et al. The boundary condition (3) does not permit exchange of vertical fluxes with outside of boundary layer. The condition (4) means that the mass flux arriving on the

³Departamento de Física, (UFSM), Brazil

boundary is equal to the mass flux emerging from this boundary in direction-y.

Equation (1) is solved numerically using the Alternating Direction Implicit (ADI) method in the x direction and a centered finite difference method is applied to the diffusion operator. Therefore, the numerical procedure is second order in space. Additional details can be found in Campos Velho et al. (1997).

3 Implicit Inverse Model

The inverse methodology adopted is an implicit technique used by minimize a functional formed by a least square term and a regularization function. The regularization functions used in this paper are the same adopted by M.R. Moraes (1998a, 1998b).

In some inverse problems present different types of parameters to be estimated. These parameters can have a very different impact on direct model, for example in radiative transfer problems (Stephany, 1997; Stephany et al., 1997), where an alternate strategy was essential to obtain good results.

(a) Alternate Strategy:

1. Solve the optimization problem:

$$\min J_{\gamma_z}(K_z^n);$$

$$(K_z^n) = R(K_z^n) + \gamma_z \Omega(K_z^n);$$
(5)

2. Solve the optimization problem:

$$\min J_{\gamma_{y}}(K_{y}^{n});$$

$$J_{\gamma_{y}}(K_{y}^{n}) = R(K_{y}^{n}) + \gamma_{y}\Omega(K_{y}^{n});$$
(6)

3. If: $\left\|K_{\alpha}^{n} - K_{\alpha}^{n-1}\right\| / \left\|K_{\alpha}^{n}\right\| < \varepsilon$ stop! Other wise, come back item 1.

 J_{γ}

In the first estimative the value of \mathbf{K}_{y} is taken from the literature, for example the value used by Shir and Shieh (1974), in which the horizontal diffusivity is assumed as a simple scalar number.

(b) Simultaneous Strategy:

In this case is solved only the follow optimization problem

$$\min J_{v}(K); \tag{7}$$

$$J_{\gamma_z}(K) = R(K) + \gamma \Omega(K);$$

$$K = \begin{bmatrix} K_y & K_z \end{bmatrix}^T$$
(8)

In the both strategies the parameter vector is the sampled eddy diffusivity function

$$K_{\alpha} = \begin{bmatrix} K_{\alpha,1} & K_{\alpha,2} \dots & K_{\alpha,N_{\alpha}} \end{bmatrix}^{T} \quad ; \quad where: \quad K_{n,\alpha} = K_{\alpha\alpha} (z_0 + n\Delta z_n). \tag{9}$$

In Eqs. (5)-(7) a smooth solution is obtained by choosing a function \mathbf{K}_{α} what optimize that functionals, where $\Omega(\mathbf{K})$ is a regularization function, γ 's are the positive numbers, and $R(\mathbf{K})$ is a norm l_2 of the difference between experimental and model data:

$$R(K) = \sum_{i=0}^{N_x} \sum_{j=0}^{N_y} \sum_{k=0}^{N_z} \left[C_{ijk}^{Exp} - C_{ijk}^{Mod}(K) \right]^2.$$
(10)

5 Numerical Results

In order to test the inverse strategies presented here, it was used a synthetic pollutant concentration data obtained from Eq. (1), corrupted with Gaussian noise, being the exact eddy diffusivities those derived by Degrazia and Moraes (1992). The physical and numerical parameters used in the simulations are given in the table 1.

The pollutant source is localized at $(0, L_y/2, h/4)$. Here will be shown only the results obtained with second-order Tikhonov regularization term, since it got the best the estimations with this regularization.

The Figs. 1 and 2 are depicted the results got with alternate and simultaneous strategy, respectively, for two levels of noise (1% and 5%). For 1% noise-data the results were very similar, while for 5% noise-data the K_{yy} eddy diffusivity presented less smooth for alternate than simultaneous strategy. Any way, the alternate strategy did not present any improvement for estimating eddy diffusivities, and it expends much more computational time.

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}

 Table 1: Numerical and physical parameters.

6 Conclusions

The entropic regularization presented very similar results for alternate and simultaneous strategy (no shown), being the best estimatives obtained with first-order entropy. However, better estimations were got using second-order Tikhonov regularization.

For this problem, multidimensional eddy diffusivity estimation, the alternate strategy did not give better results than simultaneous strategy. Actually, the estimation using second-order Tikhonov regularization results obtained with simultaneous strategy were better than alternate strategy, and in addition the alternate strategy has a bigger computational cost.

Acknowledgements

The authors regonize the role played by FAPESP, São Paulo State Foundation for Research Support, in supporting this piece of work through a Thematic Project grant (Proc. 96/07200-8). Author H.F. de Campos Velho acknowledges to the CNPq-Brasil (Proc. 200899/97-0) by the financial support for post-doctorate study.

References

1 H.F. Campos Velho and F.M. Ramos (1996): *Estimation of Turbulent Diffusivity by an Entropy-based Inversion Methodology*, Air Pollution and Acid Rain: The Candiota Program, Editors: O.L.L. Moraes, A.P. Oliveira, E.S. Caetano Neto, G.A. Degrazia, pp. 40-44, FAPESP, Bauru (SP), Brasil.
2 H.F. Campos Velho, M.R. Moraes, G.A. Degrazia (1997): *Um Modelo de Dispersão de Poluentes na Camada Estável*, Relatório Técnico, INPE, São José dos Campos, BRASIL.

3 M.R. Moraes, H.F. Campos Velho, F.M. Ramos, G.A. Degrazia, D. Anfossi (1998a): *Regularization Methods in Eddy Diffusivity Estimatiion*, submitted to **Air Pollution 98**, September 28-30, Genova, Italy.

4 M.R. de Moraes, H.F. Campos Velho, F.M. Ramos, G.A. Degrazia (1998b): Determination of the Vertical Turbulent Diffusivity Using an Implicit Inversion Technique, to be submitted to Brazilian

Journal of Geophysics.

5 SHIR, C.C. and SHIEH, L.J.; 1974: A Generalized Urban Air Pollution Model and Its Application to the Study of SO Distributions in the St. Louis Metropolitan Area, **Journal of Applied Meteorology**, **Vol.** 13, No. 2, pp. 185-204.

6 S. Stephany (1997a): *Reconstrução de Propriedades Óticas e de Fontes de Bioluminescência em Águas Naturais*, Tese de Doutoramento, CAP-INPE, São José dos Campos (SP), Brasil.

7 S. Stephany, H.F. Campos Velho, F.M. Ramos and C.D. Mobley (1997b): *Estimating Absortion and Scattering Coefficients and Internal Source Term in a Radiative Transfer Process*, **Proceedings of the XIV Brazilian Congress on Mechanical Engineering**, Abstract Book, page 28, available in CDROM (theme 22, code COB053), Baurú (SP), Brasil.

8 G.A. Degrazia and O.L.L. Moares (1992): A Model for Eddy Diffusivity in a Stable Boundary Layer, **Boundary-Layer Meteorol.**, 58, 205-214.

9 C. Giordana, M. Mochi and F. Zirilli (1991): *The Numerical Solution of an Inverse Problem for a Class of One-Dimensional Diffusion Equations with Piecewise Constant Coefficients*, **Siam J. Appl. Math**, 58, n.2, pp. 428-441.



Figure 1: Turbulent diffusivities by alternate strategy with Tikhonov second-order: (a) 1% and (b) 5% of noise-data.



Figure 2: Turbulent diffusivities by simultaneous strategy with Tikhonov second-order: (a) 1% and (b) 5% of noise-data.