IL NUOVO CIMENTO Vol. 28 C, N. 2 Marzo-Aprile 2005
DOI 10.1393/ncc/i2005-10188-y

Assessment of the numerical diffusion effect in the advection of a passive tracer in BOLCHEM(*)

M. D'Isidoro(1)(3)(**), A. Maurizi(1), F. Tampieri(1), A. Tiesi(2) and M. G. Villani(1)

(1) *ISAC-CNR - Bologna, Italy*
(2) *IMAA-CNR - Potenza, Italy*
(3) *Dipartimento di Fisica, Università di Ferrara - Via Paradiso 12, 44100 Ferrara, Italy*

(ricevuto il 7 Febbraio 2005; approvato il 27 Maggio 2005)

Summary. — The effects of the numerical scheme implemented in the advection equation of BOLCHEM have been quantified with reference to the diffusion of a passive tracer. An equivalent horizontal diffusion coefficient has been measured and is found to be dependent on wind field and resolution.

PACS 47.11.+j – Computational methods in fluid dynamics.
PACS 47.27.Qb – Turbulent diffusion.
PACS 92.60.Sz – Air quality and air pollution.
PACS 01.30.Cc – Conference proceedings.

1. – Introduction

Modelling of the spatial distribution and time evolution of the atmospheric minor components is a challenging step in the investigation, simulation and forecasting of air quality.

It is well recognized that the atmospheric composition results from the combined effects of emissions, transformations, transport and removal.

The present paper concentrates on some aspects of the overall problem, concerning the numerical simulation of transport and dispersion at the regional scale (namely, a space scale typically larger than a city, and a time scale of the order of more than one hour). At the space and time scales of interest, the transport is driven by the meteorological fields, and dispersion is treated as a "subgrid" process. Turbulent dispersion in the atmosphere is essentially a Lagrangian process, and therefore its simplified description is

(*) Paper presented at CAPI 2004, 8° Workshop sul calcolo ad alte prestazioni in Italia, Milan, November 24-25, 2004.
(**) E-mail: m.disidoro@isac.cnr.it

based on stochastic models mimicking the randomness of the process [10]. The simplified description is consistent with the above-defined scales, thus allowing to neglect time correlation of the velocity fluctuation (with respect to the resolved wind) and to use a Brownian-like description: the diffusion equation is therefore a consistent mathematical description of the process [11].

This stochastic method is not currently used as chemical transformations have to be treated so that the Eulerian equation with proper transformation term is solved.

The meteorological model we use does not solve the advection-diffusion equation, but implements a semi-Lagrangian scheme for the advection plus a ∇^4 operator necessary for numerical stability. This implementation contains two smoothing factors: the first is due to interpolation of the wind fields and the second to the ∇^4 operator.

The aim of this work is to investigate how the smoothing effect is able to reproduce the horizontal diffusion of a passive tracer in the atmosphere at different horizontal grid scales.

2. – Diffusion parameterization

We use the meteorological model BOLAM (BOlogna Limited Area Model) to drive the transport of passive tracers. The model is based on hydrostatic primitive equations, with wind components u and v, potential temperature θ, specific humidity q, and surface pressure P_s, as dependent variables. A more specific description of the model can be found in [2-4].

The passive tracer concentration field is computed using the Eulerian scheme implemented in BOLCHEM (BOLAM + CHEMistry) and a Lagrangian Stochastic Model solving the advection-diffusion equation.

2˙1. *Fourth-order diffusion.* – BOLAM implements a fourth-order diffusion scheme for the meteorological quantities with a semi-Lagrangian advection for the passive tracers. The computational stability of the semi-Lagrangian scheme allows for longer time steps and also mantains the values of conservative properties. It is therefore useful for accurately advecting passive tracers [8].

The fourth-order diffusion, selective for the small scales, has not a strict physical meaning but is useful in order to avoid an energy concentration over the grid step, thus mantaining the stability of the numerical scheme.

The advection-diffusion scheme is implemented in the following way:

$$\frac{\partial c}{\partial t} = -\mathbf{u} \cdot \nabla c - \alpha \nabla^4 c \,, \tag{1}$$

where $c\,(\mathbf{x}, t)$ is the passive tracer concentration. The first term on right-hand side represents the advection part where $\mathbf{u}$ is the horizontal wind field; the second acts as a smoothing term by means of the ∇^4 operator with a factor α. The coefficient α is calculated according to

$$\alpha = \beta\,(\Delta x)^2 \times 10^4 \,, \tag{2}$$

where β is a parameter fixed by the user and Δx is the grid step in km.

The semi-Lagrangian scheme has a diffusive effect due to the linear interpolation over the grid of the wind field at the starting point.

TABLE I. – *Summary of the performed simulations showing the horizontal grid resolution (HRES), time step length (Tstep) and the* β *parameter for the* ∇^4 *operator. For the four simulations with advection term added, NSTEPSL is the time interval (in time steps) between two calls to the semi-Lagrangian advection scheme.*

Diffusion	HRES (degrees)	Tstep (s)	β	NSTEPSL
∇^4	0.25	240	0.65	4
∇^4	0.20	200	0.6	4
∇^4	0.15	150	0.55	8
∇^4	0.10	100	0.4	8

2˙2. *Lagrangian Stochastic Model.* – The Lagrangian Stochastic Model (LSM) describes the statistics of the position of a passive tracer using the wind field from the BOLAM model. The LSM is based upon the implementation of the Langevin equation:

$$\mathrm{d}x_i = v_i \mathrm{d}t + \beta_{ij} \mathrm{d}W_j \, , \tag{3}$$

where x_i represents the i-th component of the single realization of the tracer particle trajectory, v_i the corresponding velocity component, $\mathrm{d}W_j$ is a Wiener process such that

$$\langle \mathrm{d}W_i\,(t)\rangle = 0, \langle \mathrm{d}W_i\,(t)\,\mathrm{d}W_j\,(s)\rangle = \delta_{ij}\,(t-s)\,\mathrm{d}s\mathrm{d}t \tag{4}$$

and β_{ij} represents the noise amplitude.

It is well known [9] that the *pdf* of the particle position is given by the Fokker-Plank equation

$$\frac{\partial p}{\partial t} = -\frac{\partial}{\partial z_i}(v_i p) + \frac{\partial^2}{\partial z_i \partial z_j}\left(\frac{\beta_{ij}^2}{2}p\right) \tag{5}$$

which also represents an equation for the mean tracer concentration $c(\mathbf{x}, \mathbf{t})$, because the *pdf* of the position and the concentration c differ only by a normalization constant (*i.e.* 1 for the *pdf*, the total concentration for $c(\mathbf{x})$).

Equation (5) can be rewritten in the more usual form, for a constant density flow [11]:

$$\frac{\partial c}{\partial t} + u_i \frac{\partial c}{\partial z_i} = \frac{\partial}{\partial z_i}\left(K_{ij}\frac{\partial c}{\partial z_j}\right) , \tag{6}$$

where the tracer velocity is identified as the mean flow velocity and the diffusion coefficient is defined as: $K_{ij} = \beta_{ij}^2/2$. This coefficient represents the effect of the unresolved scales of motion.

3. – Results

In order to assess the ability of BOLCHEM to reproduce the effect of the advection-diffusion scheme over a passive tracer field, two sets of experiments at different horizontal resolutions were performed. For these simulations only horizontal diffusion was allowed, setting vertical diffusion coefficient to zero. First, four simulations at 0.25, 0.20, 0.15 and

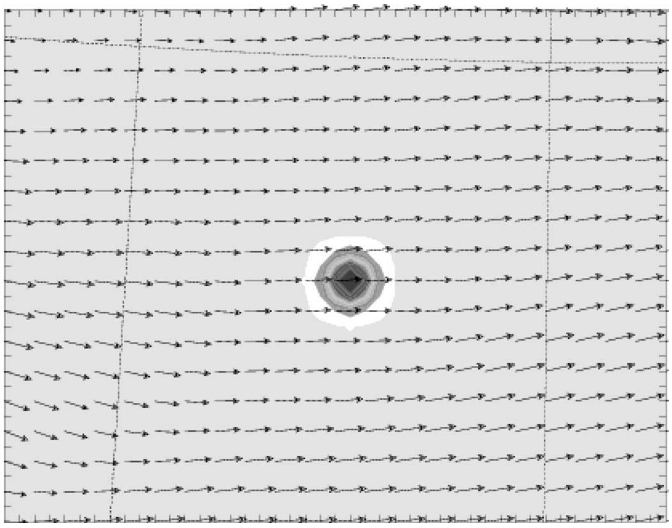

Fig. 1. – Initial concentration distribution and wind field used for the experiments. The wind field was considered only for the simulations with the semi-Lagrangian advection scheme.

0.10 degrees resolution were carried out to test the impact of the ∇^4 term, neglecting the effect of the wind field. The same simulations were then repeated considering also the advection term computed by means of the semi-Lagrangian scheme. For both experiments a common initial condition for the passive tracer was used. The tracer was released with a Gaussian concentration having a half-amplitude σ of 0.2° with a cut beyond 3σ (fig. 1).

3˙1. ∇^4 *diffusion.* – Four 12 hour simulations at different resolutions were performed with the parameters summarized in table I.

Figures 2 a and b represent the variance of the concentration distribution as a function of the integration time along the longitude component x and the latitude component y, respectively. In the figures the straight lines are superimposed in order to compare the results with the exact solution of the diffusion equation.

It can be seen that apart for the coarse resolution for the y direction, the variance increases according to t^α, with $0 < \alpha < 1$ for small times, and the higher the resolution the greater this feature. In general for longer times the variance increases roughly linearly with the time. In the range that displays a diffusive behaviour, an equivalent horizontal diffusion coefficient is estimated by fitting the diffusion relationship $\langle x^2 \rangle = 2kt$ on data.

The values are reported in table II.

3˙2. *Diffusive effect of the semi-Lagrangian advection.* – A second set of experiments was performed in order to evaluate the contribution of the semi-Lagrangian advection term to the diffusion. In this perspective the same four 12 hour simulations described in the previous section were carried out, adding the wind field to take into account the advective part (first term on the right-hand side of eq. (1)).

In order to assess this effect in realistic but rather homogeneous conditions for the model, a particular case was chosen. Simulations started on 8 September 2002 06 UTC, in a geographical domain located in the eastern sub-tropical Atlantic Ocean; here, in the chosen period of time, the wind field presented suitable features at a level of about

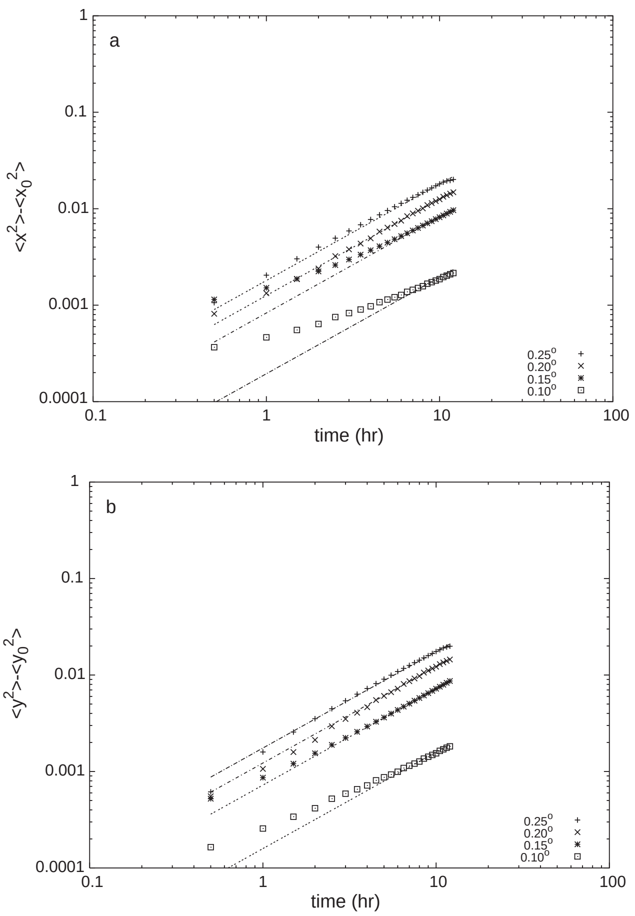

Fig. 2. – Variance (degrees squared) of the concentration distribution along the x (a) and y (b) directions calculated every time step for the simulations using the ∇^4 diffusion at different resolutions (see symbols). Variances at the initial instant have been subtracted. Axes in logarithmic scale.

TABLE II. – *Equivalent horizontal diffusion coefficients for x (K_x) and y (K_y) directions calculated from the simulations performed with the ∇^4 operator.*

Fourth-order diffusion		
Resolution (degrees)	K_x(m^2/s)	K_y (m^2/s)
0.25	3095	3005
0.20	2162	2100
0.15	1425	1240
0.10	334	272

TABLE III. – *As in table II, for the simulations performed using the* ∇^4 *diffusion combined with the semi-Lagrangian advection scheme.*

Fourth-order diffusion + semi-Lagrangian advection		
Resolution (degrees)	K_x (m^2/s)	K_y (m^2/s)
0.25	17877	10571
0.20	11654	7038
0.15	6439	3137
0.10	975	2529

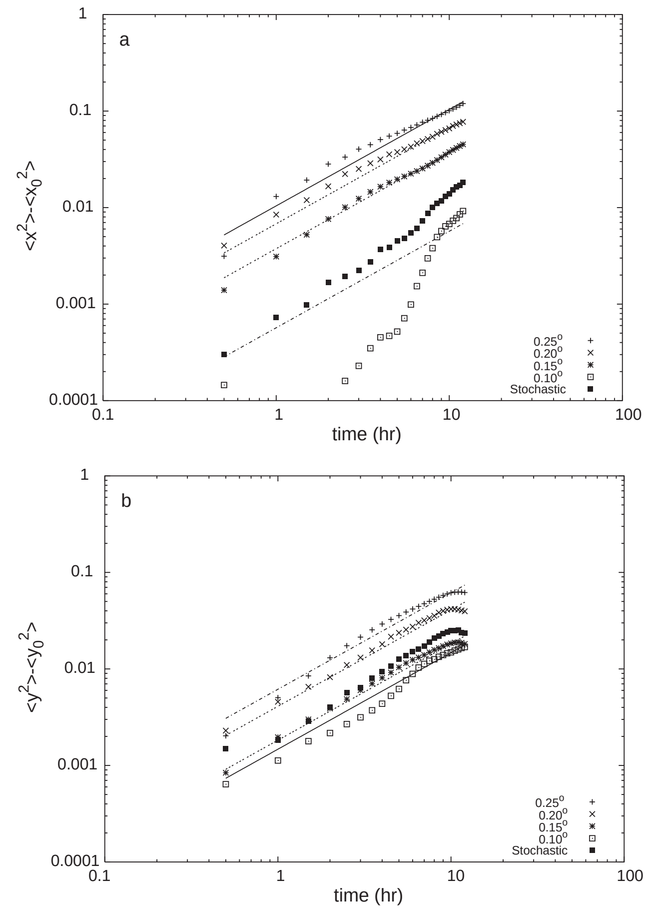

Fig. 3. – Variance (degrees squared) of the concentration distribution along the x (a) and y (b) directions calculated every time step for the simulations summarized in table I. Solid squares for the LSM simulation, other symbols for the fourth-order diffusion with the semi-Lagrangian advection scheme at different resolutions. Variances at the initial instant have been subtracted. The straight lines are superimposed in order to compare the linear behaviour of the diffusion on logarithmic axes.

3000 m, where the initial concentration distribution was placed. The initial (see fig. 1) and boundary conditions were derived from the ECMWF fields interpolated over the model grid. All the simulations were performed with constant zero boundary conditions for the passive tracer concentration. Table I summarizes the performed simulations, showing the parameters used for each experiment.

In order to make a comparison between the BOLCHEM diffusion and a ∇^2 diffusion, an additional simulation with the LSM was carried out, in which the passive tracer was driven by the evolving wind field interpolated from the 0.2° resolution BOLAM grid. A time step of 200 seconds was used in the LSM, together with a horizontal diffusion coefficient of 2300 m^2s^{-1}, estimated from satellite observations of aerosol originating from the Etna volcano during the eruption of October-November 2002. This value is in agreement with the range $0.5–6\times10^4$ m^2s^{-1} resulting from [1, 6, 7].

Figures 3 a and b represent the variance of the concentration distribution in the x and y directions, respectively, as a function of the time integration. For each simulation the NSTEPSL number of time steps between two calls to the semi-Lagrangian advection scheme is reported in table I.

It can be observed that the introduction of the semi-Lagrangian scheme produces a larger diffusion. Furthermore, the small time behaviour can be fairly well represented by a diffusion process in contrast to the case of the ∇^4 only solution.

Examining the equivalent horizontal coefficient values, it can be observed that they are generally larger for semi-Lagrangian advection simulations.

Moreover, the higher the resolution the larger the impact of the specific wind field used, as can be seen in particular from the 0.1 degrees resolution simulation in x direction (fig. 3-a).

These results are in qualitative agreement with [5].

4. – Conclusions

The ∇^4 operator introduces a two regime growth of the variance and exhibits a diffusive behaviour for long times. The addition of the semi-Lagrangian advection scheme causes greater diffusion and induces an anisotropy between along wind and across wind directions. In general, the diffusion effect of the advection scheme is expected to depend on the wind field. In the present work the effective horizontal diffusion coefficients have been estimated as a function of resolution, using values for parameter β that are commonly adopted in meteorological practice. The estimated values lie in the range suggested by literature for the troposphere. In modelling passive tracers the value of diffusion coefficient is expected to be dependent on meteorological conditions. Therefore further investigations are necessary in order to model the dispersion effects independently of the resolution adopted.

* * *

This work has been partially supported by ACCENT NoE. We gratefully acknowledge Dr. P. Malguzzi for suggestions and comments.

REFERENCES

[1] Barr A. and Gifford F. A., *Atmos. Environ.*, **21** (1987) 1737.
[2] Buzzi A., D'Isidoro M. and Davolio S., *Q. J. R. Meteorol. Soc.*, **129** (2003) 1795.

[3] Buzzi A. and Foschini L., *Meteorol. Atmos. Phys.*, **72** (2000) 131.
[4] Buzzi A., Fantini M., Malguzzi P. and Nerozzi P., *Meteorol. Atmos. Phys.*, **53** (1994) 137.
[5] Chevenez J., Baklanov A. and Sørensen J. H., *Meteorol. Appl.*, **11** (2004) 265.
[6] Gifford F. A., *Atmos. Environ.*, **16** (1982) 505.
[7] Gifford F. A., *Boundary Layer Meteorol.*, **30** (1984) 159.
[8] Holton J. R., in *An Introduction to Dynamic Meteorology* (Academic Press) 1992, pp. 445-446.
[9] Risken H., in *The Fokker-Planck Equation. Methods of Solution and Applications* (Springer-Verlag) 1989.
[10] Thomson D. J., *J. Fluid. Mech.*, **180** (1987) 529.
[11] Thomson D. J., *Atmos. Env.*, **29** (1995) 1343.