IL NUOVO CIMENTO Vol. 28 C, N. 2 Marzo-Aprile 2005
DOI 10.1393/ncc/i2005-10187-0

Comparison of different dispersion models with tracer experiment(*)

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(ricevuto il 7 Febbraio 2005; approvato il 6 Giugno 2005)

Summary. — An intercomparison between three different models is presented. The simulated case is a tracer experiment performed in complex terrain. Two dispersion models are initialised with a meteorological model that can use as input the ECMWF analysis only or both these analysis and local measurements. The results demonstrate that the best performances are obtained by using the dispersion models coupled with a meteorological model. Moreover the Lagrangian model seems to slightly better perform when the local measurements are accounted for.

PACS 92.10.Lq – Turbulence and diffusion.
PACS 01.30.Cc – Conference proceedings.

1. – Introduction

The aim of this work is to assess the ability of different models in simulating pollutant dispersion in real complex terrain. The comparison between Gaussian, Puff and Lagrangian Particle models shows how they reproduce the measured ground level concentrations with the aim to select the best model for such a situation.

It is also a purpose of the paper to discuss the improvements due to the use of a meteorological circulation model to provide the flow and turbulence fields needed to the dispersion models. In fact the meteorological model should be able to compute both mean wind and turbulent fields on a three-dimensional domain and the dispersion model accounting for such a detailed input should correctly predict the concentrations of the considered pollutant.

(*) Paper presented at CAPI 2004, 8° Workshop sul calcolo ad alte prestazioni in Italia, Milan, November 24-25, 2004.

For this reason the comparison of the models performances with tracer experiment results and the inter-comparison between different models is of great importance.

Some simpler models can derive the input parameters simply from measurements made at or in the proximity of the pollutant source. Others, generally more sophisticated, need to be coupled with a circulation model reproducing the meteorological conditions on a large domain around the source point. The latter, obviously, require more computing resources but, in general, give better results. In this work we compare the results of three different models tested against tracer data gathered during an experiment, which constitutes a severe test due to the complex topographical and meteorological conditions. The comparison is performed by means of a model evaluation procedure based on statistical indexes calculated on the cross wind integrated concentrations.

In sect. **2** the models are presented, in sect. **3** the tracer experiments is described, in sect. **4** the simulations details are given and the results are shown, while sect. **5** contains the conclusions.

2. – Models description

The first modelling system consists in a coupled model based on the regional atmospheric model RAMS and the Lagrangian particle model SPRAY. RAMS (Regional Atmospheric Modeling System) is a well-known prognostic model, developed at the Colorado State University [1]. The coupling between the two models is made using an interface code, MIRS 2.0 [2], which receives RAMS outputs and calculates boundary layer and turbulence parameters for the Lagrangian dispersion model SPRAY, in particular the variables not directly provided by RAMS.

We performed meteorological simulations using the RAMS version 4.4 initialised with the ECMWF analysis and the measurements carried out during the tracer experiment. The turbulence model used is the Mellor and Yamada closure model [3], which provides the turbulence kinetic energy (E) to MIRS that in turn calculates the wind velocity standard deviations, and the Lagrangian Time Scales needed to the dispersion model as input by means of the following procedure.

The variances of the velocity fluctuation $\sigma^2_{u,v,w}$ are computed as

$$\sigma_u^2 = (1-2\gamma)q^2\,, \qquad \sigma_v^2 = \gamma q^2\,, \qquad \sigma_w^2 = \gamma q^2\,,$$

where $q^2 = 2E$, $\gamma \equiv 1/3 - 2(A_1/B_1)$ and A_1, B_1 are the constants which define two of the characteristic length scales introduced in the Mellor and Yamada model [3].

Then the Lagrangian time scales T_L are obtained from

$$T_{L_{x,y,z}} = \frac{K_{m_{x,y,z}}}{\sigma^2_{u,v,w}}\,,$$

where $K_{m_{x,y,z}}$ are the anisotropic diffusivities; the vertical component is calculated on the basis of the E equation from the Mellor and Yamada closure while the horizontal components are assigned from a deformational Smagorinsky-type scheme, based on the deformation strain tensor and the horizontal grid spacing.

Besides these quantities MIRS also provides to SPRAY the topography and the boundary layer height.

SPRAY [4] is a Lagrangian stochastic particle model designed to study the pollutants dispersion in complex terrain. It is based on the Langevin equation for the turbulent velocities [5], whose coefficients depend on a solution of the Fokker-Planck equation for a given Eulerian probability density function (PDF) of the turbulent velocity and on the inertial range turbulence theory, respectively. In the two horizontal directions the PDF is assumed to be Gaussian. In the vertical direction the PDF is assumed to be non-Gaussian, so to deal with convective conditions.

The vertical dispersion calculation is based on the generalised Langevin equation [5]. The equations prescribing the evolution of the vertical velocity fluctuation w and the displacement z are the following:

$$\mathrm{d}w = a(z,w)\mathrm{d}t + \sqrt{C_0 \varepsilon \mathrm{d}t}\mathrm{d}\mu\,,$$

$$\mathrm{d}z = w\mathrm{d}t\,,$$

where $\mathrm{d}\mu$ has zero mean and unit variance, C_0 is a constant and ε is the dissipation rate of the turbulent kinetic energy. $a(z,w)$ must be determined by solving the Fokker-Planck equation, obtaining

$$a\,(z,w) = \frac{1}{P}\left(B_0 \frac{\partial P}{\partial w} + \Phi\right)\,,$$

where $B_0 = (1/2)C_0\varepsilon$ and, as suggested by Thomson [5],

$$\Phi \;=\; -\frac{\partial}{\partial z}\int\limits_{-\infty}^{w} wP(z,w)\,\mathrm{d}w\,.$$

$P(z,w)$ is the PDF that must be prescribed from the available measurements or parameterisations. In the present work, we have used the Gram-Charlier PDF [6]. The model makes use of the Gaussian assumption in the horizontal directions. The assumed steady conditions (as in the case of the other models considered) are not a limitation in this kind of applications, which are performed at the small scales where the meteorological conditions can be considered the same during the dispersion process.

The second modelling system used is the CALMET-CALPUFF chain. The wind field produced by RAMS 4.4 is processed by CALMET that also computes the turbulence variables necessary for CALPUFF. CALPUFF [7] is a multi-layer, multi-species non-steady-state puff dispersion model, which can simulate the effects of time- and space-varying meteorological conditions on pollutant transport, transformation, and removal, developed and distributed by Earth Tech, Inc.

The model has been adopted by the U.S. Environmental Protection Agency (U.S. EPA) in its Guideline on Air Quality Models as the preferred model for assessing long-range transport of pollutants and their impacts on Federal Class-I areas and on a case-by-case basis for certain near-field applications involving complex meteorological conditions.

The modelling system consists mainly of CALMET (a diagnostic three-dimensional meteorological model) and CALPUFF (an air quality dispersion model). Advection is carried out by a three-dimensional wind field and the dispersion coefficients are computed from internally calculated wind standard deviations using CALMET micrometeorological variables (u_*, w_*, L, etc.)

The third model used in this work is ISC3 (Industrial Source Complex Model) [8], a steady-state Gaussian plume model which can be used to assess pollutant concentrations from a wide variety of sources associated with an industrial complex. This model accounted in our simulations for plume rise as a function of downwind distance and was driven by the hourly meteorological data measured by the tower near the stack.

3. – Bull Run data set

The models have been applied to the Bull Run experiment [9, 10] and the results compared. The Bull Run steam plant is located in the broad Tennessee River valley (about 60 km wide) surrounded by mountains rising over 1700 m of altitude. Close to the plant, the ridges are approximately 100 m and the region is covered by forests. The Melton Hill Lake cuts perpendicular across the ridges near the Bull Run steam plant.

The meteorological measurements were collected from a 122 m TVA tower, located near the crest of a 70 m ridge about 2 km west of the stack, the central observing station, located at about the same elevation as the stack base in a field near the river about 5 km northwest of the stack, one acoustic sounder about 1 km east of the stack, the National Weather Service (NWS) stations at Knoxville and Nashville, Tennessee.

The tracer (FS_6) was released from the 243 m high plant stack and measured on 200 monitors deployed on arcs from 0.5 to 50 km, during two 5-week periods. The locations of the monitors were changed following the forecasted meteorological conditions in order to catch the wind direction and depending on the forecasted maximum ground level concentration. In particular during the day chosen for the simulations (5 October 1982) 187 receptors were located on 4 circles of radius 0.5, 2, 5, 10 km around the source position. The tracer was released for 12 hours starting at 9 LST (Local Standard Time) and the hourly measurements have been performed for 9 hours since 11 LST. In fig. 1 the topography, the receptors and the source position are shown. October 5th, 1982 was a sunny day with low winds with very variable directions as shown in fig. 2.

4. – Simulations and results

RAMS was run using three horizontal nested grids corresponding to domains of extension 1248×1248 km^2, 328×328 km^2 and 82×82 km^2, with horizontal resolution equal to 32000 m, 8000 m, 2000 m, respectively. In the vertical direction a stretched grid of 32 levels up to 18000 m, with a minimum grid size equal to 50 m and a maximum of 1200 m, was considered. The integration time steps for the three grids were 50 s, 16 s, and 8 s, respectively.

Two RAMS simulations were carried out for a period of 24 hours from 5 October 00 UTC until 6 October 00 UTC. During the first simulation the initial and boundary conditions were provided only by the ECMWF analysis data, while, during the second simulation, the necessary meteorological fields were obtained by the assimilation of the ECMWF data with the measurements performed near the source during the experiment. A nudging procedure was applied in both cases. In figs. 3 a and b are shown the horizontal cross-sections at 250 m of wind speed computed by the two RAMS simulations at 15 LST. It is possible to see that the up-slope thermal winds in the NW and SE parts of the domain are well reproduced even if the assimilation of the measured data reduces the intensity of this phenomenon slowing down the wind speed.

The results of the model evaluation are presented in table I, for the crosswind-integrated concentrations. It may be useful to stress that the simulations were performed

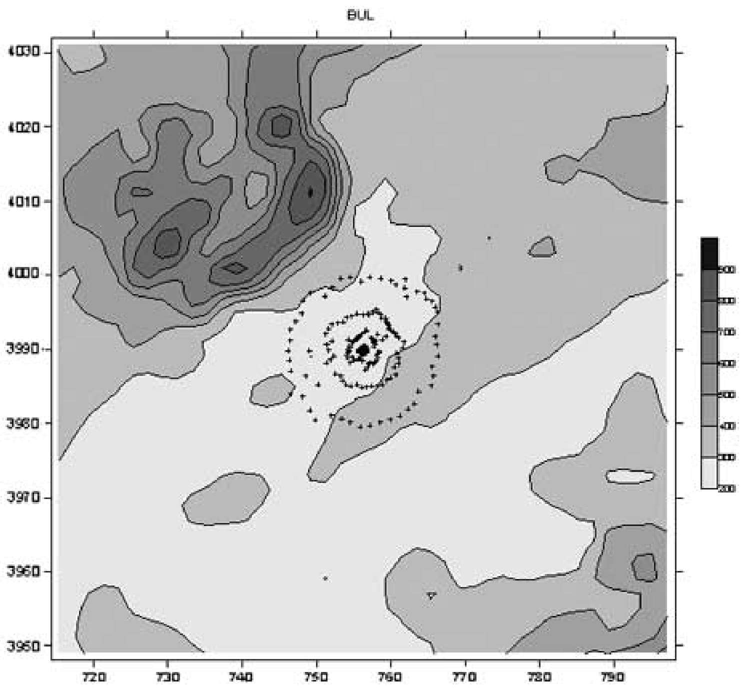

Fig. 1. – Topography, receptors positions on 4 arcs and source position (centre of the figure).

in low-wind conditions and, in this case, it is very difficult for the usual dispersion models to reproduce all the characteristics of the concentrations distribution. Moreover the single observation cannot be significant for the risk assessment. For this reason we assume that a suitable model should catch at least the cross-wind-integrated concentrations, although the single observations could not be perfectly predicted. The comparison between the three models, RAMS_SPRAY, RAMS_CALPUFF and ISC3, is performed by using

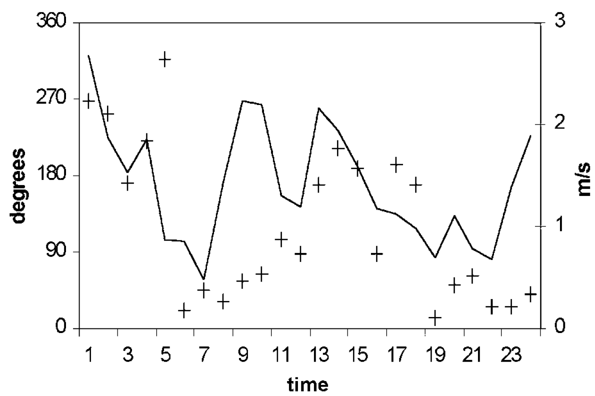

Fig. 2. – Wind direction (crosses) and wind speed (line) measured at 100 m height by the meteorological tower during 5 October 1982.

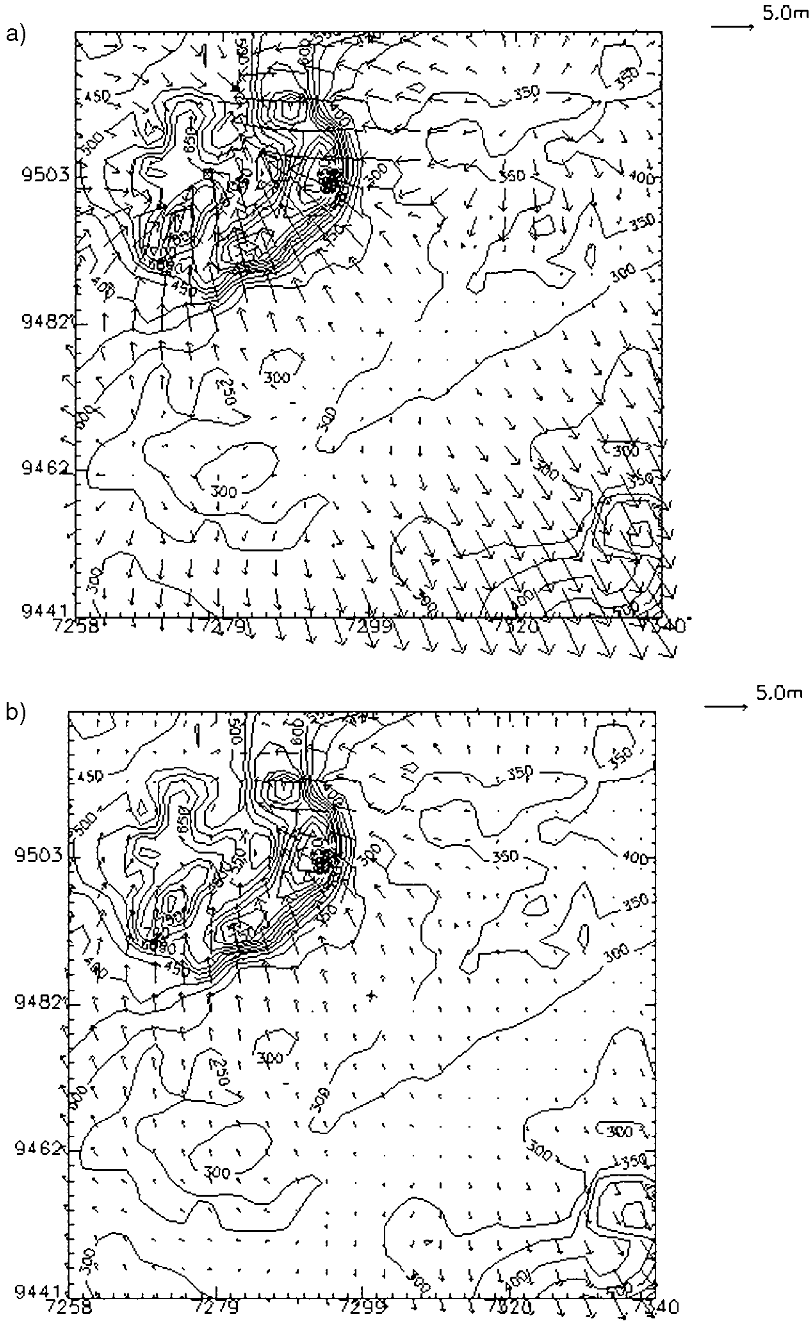

Fig. 3. – Horizontal cross-section at 250 m of the wind speed computed by RAMS at 15 LST without (a) and with (b) the assimilation of the measured data.

Table I. – *Crosswind-integrated concentrations.*

MODEL	MEAN	SIGMA	BIAS	NMSE	COR	FA2	FB
	4575.	4436.	0.00	0.00	1.0	1.00	0.00
RAMS_SPRAY	5347.	3247.	−772.	0.54	0.6	0.56	−0.16
RAMS_CALPUFF	5057.	3139.	−482.	0.93	0.3	0.36	−0.10
ISC	406.	688.	4168.	18.16	0.6	0.00	1.67
RAMS_SPRAY2	6371.	4487.	−1797.	0.44	0.8	0.53	−0.33
RAMS_CALPUFF2	3543.	3010.	1031.	1.32	0.3	0.28	0.25

the statistical indexes [11]: mean, standard deviation (SIGMA), bias, normalised mean square error (NMSE), correlation coefficient (COR), factor of two (FA2) and fractional bias (FB). The first line indicates the expected value for a "perfect model" (mean and standard deviation are calculated from the measured data). The last two simulations refer to the second runs performed using RAMS_SPRAY and RAMS_CALPUFF by initialising RAMS both with the ECMWF analysis fields and the measurements provided in the Bull Run data set.

The results displayed in table I show that the best performances are obtained by using the RAMS_SPRAY model. The NMSE, correlation and factor two are better than those obtained with the other models while FB indicates an overestimation.

The second simulation performed with RAMS_SPRAY improves the NMSE and the correlation, while FB is worse than in the previous simulation. In the case of RAMS_CALPUFF model, the new RAMS simulation does not improve the results. The difference in the performances of the two models is due to the fact that SPRAY uses both the wind and turbulence fields produced by RAMS, while CALPUFF takes into account the wind field only.

Figures 4 a,b,c,d,e show the scatter plot for the crosswind-integrated concentrations of the five simulations. It can be observed (fig. 4a) that the RAMS_SPRAY first simulation gives rather good results except for some cases, which show either overestimation for small concentrations or underestimation of the higher values. Less satisfactory are the results of CALPUFF (fig. 4b), which exhibit a large spread of the scatter plot data. Totally unsatisfactory are the results of ISC3 (fig. 4c), which show a large number of cases with zero concentration. This fact confirms, as expected, the inability of the Gaussian model in reproducing the dispersion in low-wind conditions.

The better results obtained in the second simulation of RAMS_SPRAY model are presented in fig. 4d. It can be observed that the cases of large over and underestimation are reduced. The performance of the second simulation carried out with RAMS_CALPUFF model (fig. 4e) seems to be similar to the first one or slightly worse.

5. – Conclusions

The comparison between the performances of three different models simulating a tracer experiment in complex terrain is presented. Two models, a Lagrangian particle model (SPRAY) and a puff model (CALPUFF), use the output of the meteorological model RAMS, while the third one is a Gaussian model using directly the measurements carried out in the experimental site. Second simulations of SPRAY and CALPUFF are performed using the RAMS outputs obtained initialising the meteorological model beside

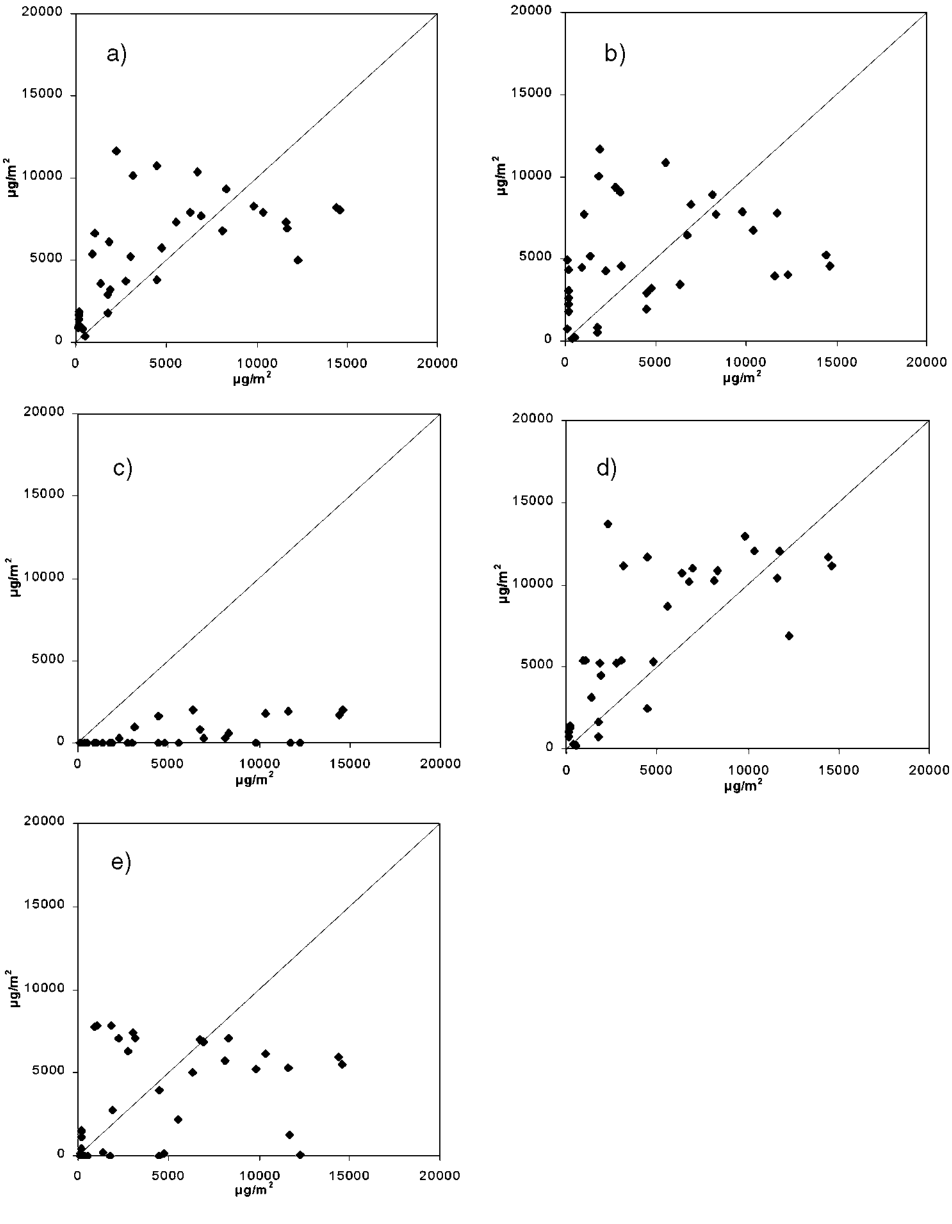

Fig. 4. – Scatter plot of crosswind-integrated concentrations (computed y-axis, measured x-axis) for the five simulations RAMS-SPRAY (a), RAMS-CALPUFF (b), ISC (c), RAMS-SPRAY2 (d), RAMS-CALPUFF2 (e).

the ECMWF data, also taking into account the experimental measurements. The best results are obtained by SPRAY and CALPUFF and the inclusion of the meteorological measurements in RAMS slightly improves the SPRAY performance.

These results demonstrate that a great improvement in the model performances is obtained by driving the dispersion model with a meteorological model providing the three-dimensional fields of flow and turbulence, even if there is a price to pay in terms of time and computer resources. However, considering the computing facilities nowadays available and their future developments, these results suggest to follow this approach. Also using a stochastic model instead of a simpler puff model gives better results, while the assimilation of local measurements to initialise the meteorological model does not produce sensible changes.

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CESI contribution to this paper has been supported by the MICA (Italian Ministry of Industry, Trade and Handicraft) in the frame of Energy Research Program for the Italian Electric System (MICA Decree of February 28, 2003), Project on SCENARI. The authors are grateful to S. R. Hanna and H. R. Olesen for providing the Bull Run data-set.

REFERENCES

[1] Pielke R. A., Cotton W. R., Walko R. L., Tremback C. J., Lyons W. A., Grasso L. D., Nicholls M. E., Moran M. D., Wesley D. A., Lee T. J. and Copeland J. H., *Meteor. Atmos. Phys.*, **49** (1992) 69.
[2] Trini Castelli S., *Rap. Int. Rep. ICGF/CNR* No 412/2000 (2000).
[3] Mellor G. L. and Yamada T., *Rev. Geophys. Space Phys.*, **20** (1982) 851.
[4] Tinarelli G., Anfossi D., Bider M., Ferrero E. and Trini Castelli S., *Air Pollution Modelling and its Applications XIII*, edited by Gryning S. E. and Batchvarova E. (Plenum Press, New York) 2000, p. 23.
[5] Thomson D. J., *J. Fluid Mech.*, **180** (1987) 529.
[6] Ferrero E. and Anfossi D., *Int. J. Environ. Pollut.*, **9** (1998) 384.
[7] Scire J. S. *et al.*, *Earth Tech Inc., Concorde, Massachusetts, USA* (2000).
[8] Londergan R. J., Minott D. H., Wackter D. J. and Bonitta D., EPA-450/4-83-003, U.S. Environmental Protection Agency, Research Triangle Park, NC, October 1982.
[9] Hanna S. R. and Paine R. J., *J. Appl. Meteorol.*, **28** (1989) 206.
[10] Brown N. E., Londergan R. L. and Murray D. R., *EA-3755, EPRI, Palo Alto, CA 94304* (1985).
[11] Hanna S. R., Strimaitis D. G. and Chang J. C., *Hazard Response Modeling Uncertainty (a quantitative method)*, Vol. **I**: *Users Guide for Software for Evaluating Hazardous Gas Dispersion Models. Sigma Research Corporation, Westford, Ma* (1991).