Sensitivity analysis of an operational advanced Gaussian model to different turbulent regimes

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Summary. — A non-reactive air pollution model evaluating ground level concentration is presented. It relies on a new Gaussian formulation (LUPINI R. and TIRABASSI T., *J. Appl. Meteor.*, **20** (1981) 565-570; TIRABASSI T. and RIZZA U., *Atmos. Environ.*, **28** (1994) 611-615) for transport and vertical diffusion in the Atmospheric Boundary Layer (ABL). In this formulation, the source height is replaced by a virtual height expressed by simple functions of meteorological variables. The model accepts a general profile of wind $u(z)$ and eddy diffusivity coefficient K_z. The lateral dispersion coefficient is based on Taylor's theory (TAYLOR G. I., *Proc. London Math. Soc.*, **20** (1921) 196-204). The turbulence in the ABL is subdivided into various regimes, each characterized by different parameters for length and velocity scales. The model performances under unstable conditions have been tested utilizing two different data sets.

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1. – Introduction

The Gaussian plume model is the simplest and most widely used tool for estimating ground level concentration. The input parameters of such model have been generally related to the simple stability classification schemes of Pasquill-Gifford [1], each covering a broad range of atmospheric conditions. On the basis of a substantial progress in the understanding of the mean and turbulence structure of the Atmospheric Boundary Layer (ABL), advanced modelling parameterisations of the surface heat and momentum fluxes have been developed. These ones contain algorithms to computing the main factors influencing air pollution dispersion in terms of the fundamentals parameters as the Monin-Obukhov length scale and velocity scales [2-4] getting over the Pasquill-Gifford stability classes.

Within this framework, utilizing the Surface Layer Similarity Theory of Monin and Obukhov [5] and the scaling analysis from Holtslag and Nieuwstadt [6], we have developed a practical Virtual Height Dispersion Model (VHDM) to estimate the ground level concentration for positively or neutral buoyant elevated release from continuous point sources. The mathematical basis of the model together with its preliminary evaluation performances has been already described in [7].

The aim of this paper is i) to present the air quality dispersion model complete with update algorithms for plume rise calculations and the recently proposed similarity expression for the lateral dispersion parameter, ii) to evaluate its general capabilities to predict atmospheric dispersion in different turbulent conditions in view of regulatory applications.

2. – Theoretical background of VHDM model

2˙1. *Model description.* – The model is based on the well-known Gaussian plume formulation. The ground level concentration is thus given by [7]

$$C(x,y,0)=C_y\,\frac{e^{-\left(\frac{y^2}{2\sigma_y^2}\right)}}{\sqrt{2\pi}\,\sigma_y}\,,$$

where C_y is the cross-wind integrated concentration, and σ_y is the horizontal dispersion parameter. For the cross-wind integrated concentration a peculiar Gaussian formulation [8] has been proposed:

$$C_y(x,0)=\frac{Q}{\sqrt{xu_\mathrm{s}K_\mathrm{s}\pi}}\,e^{-\frac{\zeta_\mathrm{s}\mu_\mathrm{s}}{4x(K_\mathrm{s}/u_\mathrm{s})}}\,, \tag{1}$$

in which Q is the source strength, u_s and K_s are the wind speed and the eddy diffusivity at the source height respectively, μ_s and ζ_s are two virtual source heights defined [1] as

$$\mu_\mathrm{s}=\int_{z_0}^{H_\mathrm{s}}\left(\frac{u(z)}{K_z(z)}\,\frac{K_\mathrm{s}}{u_\mathrm{s}}\right)^{1/2}\mathrm{d}z\,,\qquad \zeta_\mathrm{s}=\int_{z_0}^{H_\mathrm{s}}\frac{u(z)}{u_\mathrm{s}}\,\mathrm{d}z\,, \tag{2}$$

where z_0 is the roughness length, H_s is the effective release height ($\mu_\mathrm{s}\leqslant H_\mathrm{s}\leqslant\zeta_\mathrm{s}$).

The model accepts both experimental and theoretical profiles for eddy diffusivity $K_z(z)$ and wind velocity $u(z)$, provided the integrals in eqs. (2) exist.

Using input of hourly meteorological and emission data, the model calculates hourly concentration data at prescribed receptor points. From the output of hourly concentrations values at each receptor point, statistics can be computed.

2˙2. *Meteorological* ABL *parameterization*

Wind speed

The wind profile is assumed to vary only in intensity as a function of height. The dependence of wind speed with height is computed using the well-known similarity functions [5] with the von Karman constant $k=0.41$:

$$u(z)=\frac{u_*}{k}\left(\ln\left(\frac{z+z_0}{z_0}\right)-\psi_m\left(\frac{z}{L_\mathrm{mo}}\right)+\psi_m\left(\frac{z_0}{l_\mathrm{mo}}\right)\right), \tag{4}$$

where u_* is the friction velocity, k the von Karman constant, L_{mo} the Monin-Obukhov length and ψ_m a universal similarity function computed using the software library from [9].

Equation (4) is only valid in the Atmospheric Surface Layer (SL) defined as the bottom 10% of the ABL. In the upper part (up to mixing layer height H) the wind is almost constant with height, hence:

$$u(z) \text{ is computed by (4)} \qquad \text{for } z \leqslant z_b ,$$

$$u(z) = u(z_b) \qquad \text{for } z \geqslant z_b ,$$

where $z_b = \max(0.1H, |L_{mo}|)$.

Turbulence

Turbulence within the ABL is described using a scaling approach [6]. Following this scheme the ABL is subdivided into various regions, each governed by different length and velocity scales. The various turbulent regimes are characterized by two dimensionless parameters H/L_{mo} and z/H.

In the SL, during calm of wind, over hot or warm surfaces, the turbulence is due to convective motions, but over rough surfaces, in the presence of fresh wind, the turbulence is mostly caused by eddy shear stress, and eddy diffusivity profile can be derived directly from the flux profile relations of the Monin-Obukhov theory:

$$K_z = \frac{k u_* z}{\Phi_c(z/L_{mo})} . \tag{5}$$

The non-dimensional concentration profile function Φ_c is assumed to be similar to that of heat ϕ_h. Based on field experimental data, Businger *et al.* [10] derived empirical functions for non-dimensional temperature profiles depending on atmospheric stability (z/L_{mo}) as

$$\phi_h = 0.74\,[1 - 9(z/L_{mo})]^{-0.5} \qquad \text{for } z/L_{mo} \leqslant 0 \text{ (unstable)},$$
$$\phi_h = 0.74 + 4.7(z/L_{mo}) \qquad \text{for } 0 < z/L_{mo} < 1 \text{ (stable)},$$
$$\phi_h = 4.7 + 0.74(z/L_{mo}) \qquad \text{for } z/L_{mo} > 1 \text{ (very stable)}.$$

Above the SL, during stable (SBL) or near neutral conditions (NNUL), *i.e.* $H/L_{mo} > 10$, the SL formulation is extended by an empirical function of z/H as recommended by Troen and Mahrt [11]:

$$K_z = \frac{k u_* z (1 - z/H)^2}{\phi_h(z/L_{mo})} . \tag{6}$$

In the Free Convection Layer (FCL), where $z/H \leqslant 0.1$ and $H/L_{mo} < -10$, and in the Mixed Layer (ML), where $z/H > 0.1$ and $H/L_{mo} < -10$, buoyant production of Turbulent Kinetic Energy is much more important than shear production. Therefore, the friction velocity is replaced by the convective velocity (w_*) as the scaling velocity to give for the vertical eddy diffusivity [12] the following relation:

$$K_z = k w_* z \left(1 - \frac{z}{H}\right). \tag{7}$$

2˙3. *Plume rise formulation.* – As far as the calculation of plume rise for buoyant effluents, and eventual plume penetration of elevated stable layers during daytime conditions are concerned, VHDM includes models suggested by Briggs [13, 14], for unstable, neutral and stable conditions separately.

In convective or neutral conditions, the effective height is given by either of two models, the "break-up" model and the "touch-down" model.

Final rise for "break-up" formulation occurs when the turbulent dissipation rate inside the plume decreases to that of the surrounding turbulent environment so the final plume rise formula is given by

$$\Delta H = 4.3 \left(\frac{f_b}{u_s w_*^2}\right)^{3/5} H^{2/5}, \tag{8}$$

where f_b is the buoyancy flux.

The "touch-down" model assumes that in strongly convective conditions a plume is eventually brought to ground by the large-scale downdrafts in the CBL,

$$\Delta H = 1.0 \left(\frac{f_b}{0.4 u_s w_*^2}\right)\left(1 + 2\frac{H_s}{\Delta H}\right). \tag{9}$$

In neutral stability, Briggs' break-up model predicts the final plume rise to be

$$\Delta H = 1.3 \left(\frac{f_b}{u_s u_*^2}\right)\left(1 + \frac{H_s}{\Delta H}\right)^{2/3}, \tag{10}$$

while in stable conditions we have

$$\Delta H = 2.6 \left(\frac{f_b}{u_s s}\right)^{1/3}, \tag{11}$$

where s is the stability parameter:

$$s = \frac{g}{T}\frac{\partial \theta}{\partial z},$$

$\partial\theta/\partial z$ is the potential temperature gradient, T the air ambient temperature and g the gravity acceleration.

2˙4. *Lateral dispersion parameter.* – In order to calculate horizontal dispersion, the model proposed by Berkowicz *et al.* [3] is used. This is based on the assumption that the turbulent intensities and related timescales can be expressed as a sum of two separate terms, the first is the contribution from convective turbulence, the other one from mechanical turbulence, that is

$$\sigma_y = (\sigma^2_{\mathrm{conv}} + \sigma^2_{\mathrm{mech}})^{1/2} x/u_{\mathrm{med}} \,, \tag{12}$$

where x is the downwind distance and u_{med} is the wind speed averaged over the layer between the ground and the source height.

The contribution from convective turbulence is

$$\sigma^2_{\mathrm{conv}} = (0.25 w^2_* /(1 + 0.9 x w_* /(H u_{\mathrm{med}})) \,, \tag{13}$$

modelled in accordance with results from convective boundary layer experiments of Deardoff and Willis [15].

The contribution from mechanical turbulence is

$$\sigma^2_{\mathrm{mech}} = u^2_* \,. \tag{14}$$

For stable conditions the convective term is zero and only the mechanical term contributes.

The internal turbulence induced by the buoyancy in thermal plumes is modelled according to Briggs [13], and the effective dispersion parameters becomes

$$\sigma_{y\,\mathrm{eff}} = (\sigma^2_y + \Delta H^2/2\pi)^{1/2} \,. \tag{15}$$

3. – Model evaluation

The model has been tested with observations from a field experiment carried out in the Copenhagen area [16] concerning passive plumes and with field data from a power plant at Kincaid [17] concerning buoyant plumes according to the protocol agreed upon at the Manno Workshop [18].

Passive plumes

The Copenhagen dataset regards dispersion experiments performed during daytime conditions under unstable conditions. The tracer SF_6 was released without buoyancy from a tower at a height of 115 meters, and collected at ground level positions in up to three cross-wind series of tracer sampling units, positioned 2–6 km far from the point of release.

In order to evaluate the model performances in different turbulent regimes, we selected from the original data four experiments (see table I), each one corresponding

TABLE I. – *Selected meteorological experiments from Copenhagen dataset. The stability regimes are* ML *for mixed layer*, FCL *for free convection layer*, NNUL *for near neutral upper layer and* SL *for surface layer*.

u_* (m/s)	w_* (m/s)	L_{mo} (m)	H (m)	H/L_{mo}	Stability regime
0.38	1.1	− 71	1129	−15.8	Ml
0.45	—	−444	820	− 1.8	NNUL
0.64	2.1	−104	1850	−17-8	FCL
0.75	—	−289	2090	− 7.2	SL

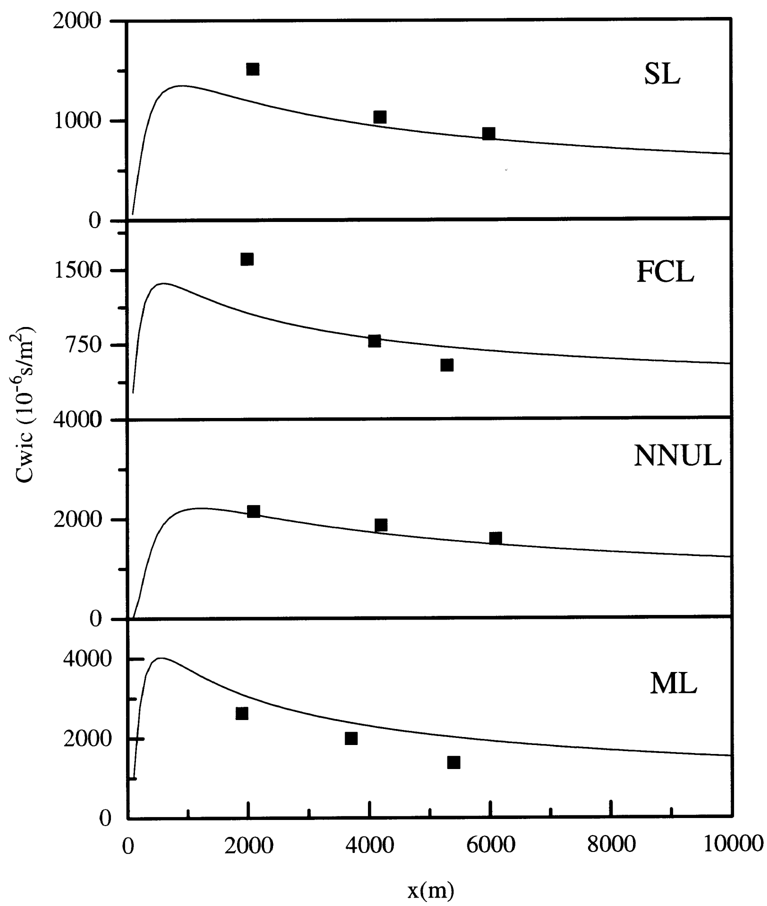

Fig. 1. – Copenhagen data set. Comparison between the predicted longitudinal cross-wind integrated concentration normalized by emission and measured data for each case considered. SL: Atmospheric Surface Layer, FCL: Free Convection Layer, NNUL: Near Neutral Upper Layer, ML: Mixed Layer.

to a stability regime as predicted by the scaling approach proposed by Holtslag and Nieuwstadt [6].

Figure 1 shows a comparison between the longitudinal profile of cross-wind integrated concentration and measurements for all cases considered. By the analysis of the curves it is of evidence that the measurements take place beyond the maximum ground level concentration; there are too few data close to the source to say whether the model correctly predicts maximum concentration.

Figure 2 shows the comparison between observed and predicted concentration for each receptor in each arc for the selected experiments. The different symbols used refer to different stability classes. There is clear correlation between data, the correlation coefficient varies from 83% in the ML case to 98% in the SL case, while the factor-two index ranges between 30% in the ML to 82% in the SL. Largest discrepancies are found in the region of lower values corresponding to concentrations

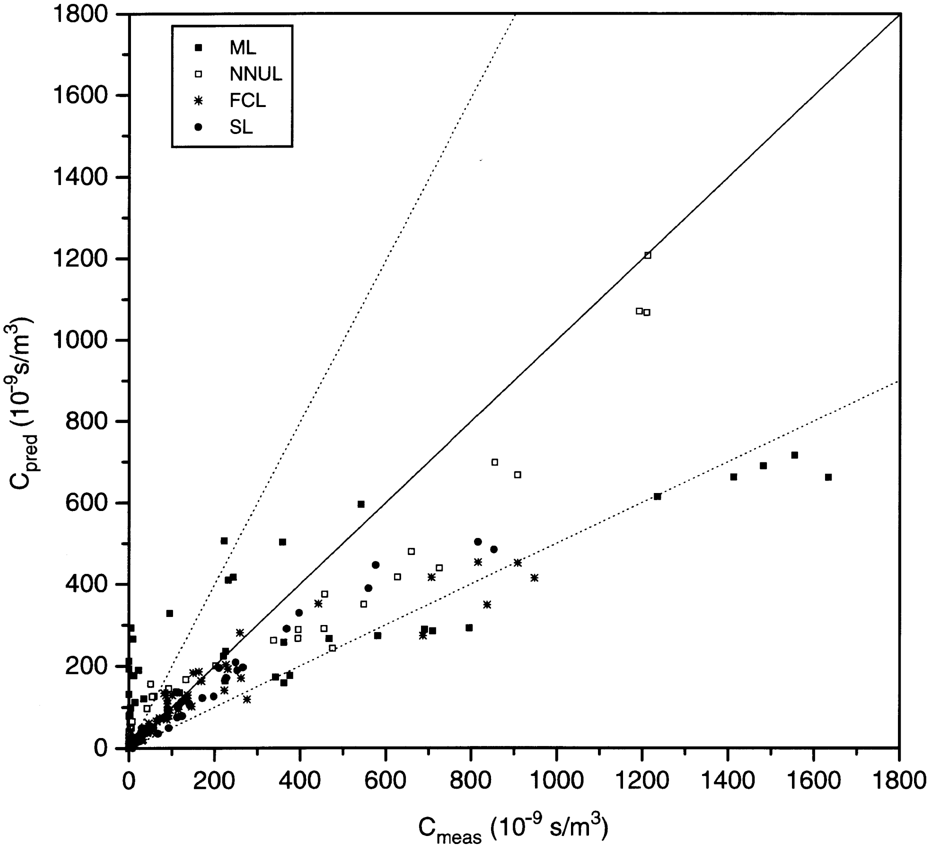

Fig. 2. – Copenhagen data set. Comparison between the measured and predicted ground level concentration normalized by emission. Data between dotted lines are in factor two. SL: Atmospheric Surface Layer, FCL: Free Convection Layer, NNUL: Near Neutral Upper Layer, ML: Mixed Layer.

measured along the arc edges for ML and NNUL regimes. This fact can be explained by the relatively large variance for the parameterisation considered and should be further investigated by using other datasets.

Buoyant plumes

The Kincaid dataset [17] is a part of the EPRI Project, Plume model Validation and Development. The power plant, located in Illinois (USA), is surrounded by flat farmland with some lakes. During the experiment, SF_6 was released from a 187 m tall stack and recorded on a network consisting of roughly 200 samplers.

Ground level concentration patterns are quite irregular, high concentration values may be found close to low values so the plumes do not even have the regular structure that a Gaussian model assumes [3]. So the evaluation presented here is focused on the model's capability to predict the maximum concentrations in the different turbulent regimes during unstable atmospheric conditions where the maximum of the observed

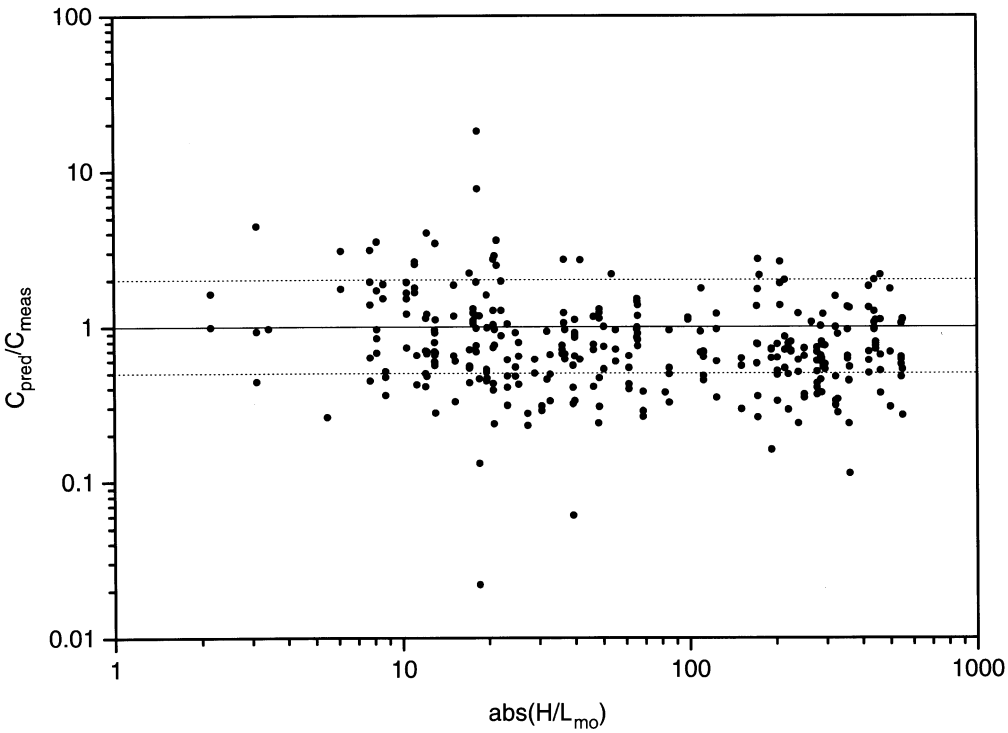

Fig. 3. – Kincaid data set. Ratio of predicted-to-measured ground level concentration as a function of the stability parameter H/L_{mo}. Data between dotted lines are in factor two.

concentration on an arc of monitoring stations is interpreted as being the centreline concentration.

Figure 3 is a residual plot of the observed and predicted concentration as a function of the stability parameter H/L_{mo}. The figure shows a large scatter of data with a general tendency of the model to underpredict the maxima, anyway 52% of data are in factor two and the model results do not seem to be dependent on the stability.

Furthermore, we compared the VHDM general performance with the advanced Gaussian model OML proposed by Berkowicz *et al.* [3] using the whole Copenhagen and Kincaid datasets. Tables II and III present the model performance evaluation statistics with the following statistical indices:

$$\text{nmse (normalized mean square)} = \overline{(C_o - C_p)^2} / \overline{C_p, C_p},$$

$$\text{cor (correlation)} = \overline{(C_o - \overline{C}_o)(C_p - \overline{C}_p)} / \sigma_o \sigma_p,$$

$$\text{fa2} = \text{fraction of } C_o \text{ values within a factor two of corresponding } C_p \text{ values},$$

$$\text{fb (fractional bias)} = (\overline{C}_o - \overline{C}_p)/(0.5(\overline{C}_o + \overline{C}_p)),$$

$$\text{fs (fractional standard deviations)} = 2(\sigma_o - \sigma_p)/(\sigma_o + \sigma_p),$$

TABLE II. – *Copenaghen dataset: statistics for cross-wind integrated concentrations normalized with emission* (10^{-6} s/m^2).

Model	nmse	cor	fa2	fb	fs
VHDM	0.12	0.75	0.91	−0.06	−0.52
OML	0.52	0.89	0.57	0.57	0.58

TABLE III. – *Kincaid dataset: statistics for maximum arcwise concentrations normalized with emission* (10^{-9} s/m^3).

Model	nmse	cor	fa2	fb	fs
VHDM	1.18	0.45	0.52	0.60	0.52
OML	1.24	0.15	0.55	0.14	−0.12

where subscripts o and p refer to observed and predicted quantities, and an overbar indicates an average. Data relative to the last model are taken from [19].

The analysis of data shows a better overall behavior of VHDM with respect to OML for both datasets. Treating the lateral dispersion in the same way, the main difference between the two models relies in the description of vertical dispersion which represents the novelty of the VHDM model.

4. – Conclusions

We have presented the operational advanced-model VHDM, which may be used in regulatory air pollution applications, particularly when emission derives from industrial stacks. The model incorporates plume rise formulas, dispersion curves and stability parameters that are much more consistent with theoretical understanding of turbulence and diffusion in ABL with respect to the Pasquill-Gifford stability classes. The model has been tested using the datasets of Copenhagen and Kincaid.

Comparison between the model results and the measurements shows that the model reproduces in a realistic way the ground level concentration pattern, with a general underprediction of maxima concentrations during high convective conditions and some large overprediction in the regions far away from the plume centreline. The discrepancies and the scatter in highly turbulent conditions could be due to: i) some simplifications in the matching regions of convective ABL; ii) the well-known general difficulties of Gaussian models in reproducing positive buoyant motion. Despite these known limits, the Gaussian models are still largely utilised for regulatory applications because of their simplicity, their fast turnaround and simple input meteorological data. Moreover, incorporating advanced and realistic description of the ABL, they can give satisfactory results also in convective conditions.

REFERENCES

[1] GIFFORD F. A., *Nuclear Safety*, **2** (1961) 47.
[2] VAN ULDEN A. P., *Atmos. Environ.*, **12** (1978) 2125.
[3] BERKOWICZ R., OLESEN H. R. and TORP U., *Proceedings of the NATO-CCMS 16th International Meeting on Air Pollution Modelling and Its Applications*, edityed by C. DE WISPELAERE, F. A. SCHIERMEIER and N. V. GILLANI (Plenum Press, New York) 1986, pp. 453-481.
[4] HANNA S. R. and PAINE R. J., *J. Appl. Meteorol.*, **28** (1989) 206.
[5] MONIN A. S. and OBUKHOV A. M., *Trudy Geofiz. Inst. An. SSSR*, **24** (1954) 163.
[6] HOLSTLAG A. A. M. and NIEUWSTADT F. T. M., *Boundary Layer Meteorol.*, **36** (1986) 201.
[7] TIRABASSI T. and RIZZA U., *Atmos. Environ.*, **28** (1994) 611.
[8] LUPINI R. and TIRABASSI T., *J. Appl. Metereol.*, **20** (1981) 565.
[9] BELJAARS A. C. M. and HOLTSLAG A. A. M., *Environ. Software*, **5** (1990) 60.
[10] BUSINGER J. A., WYNGAARD J. C., IZUMI Y. and BRADLEY E. F., *J. Atmos. Sci.*, **28** (1971) 181.
[11] TROEN I. and MAHRT L., *Boundary Layer Meteorol.*, **37** (1986) 129.
[12] WYNGAARD J. C. and BROST R. A., *J. Atmos. Sci.*, **41** (1984) 102-112.
[13] BRIGGS G. A., *Atmospheric Science and power production, DOE/TIC 27601*, Department of Commerce, Springfield, USA, 1984.
[14] WEIL J. C. and BROWER R. P., *J. Air Pollut. Control Assoc.*, **34** (1984) 818.
[15] DEARDOFF J. W. and WILLIS G. E., *J. Appl. Meteorol.*, **14** (1975) 1451.
[16] GRYNING S. E., *Elevated source SF_6-tracer dispersion experiments in the Copenhagen area*, Risoe-R-446, 1981.
[17] BOWNE N. E. and LONDERGAN R. J., *Overview, results and conclusions for the EPRI plume model validation and development project: plane site,* EPRI report EA-3074, 1981.
[18] C. CUVELIER (Editor), *Workshop on Intercomparaison of Advanced Practical Short-range Atmospheric Dispersion Models, Manno, Joint Research Centre* (European Commission Institute for Safety Tecnology), EUR 15603 EN, 1993.
[19] OLESEN H. R., *Int. J. Environ. Pollut.*, **5** (1995) 761.