

INTERNATIONAL ATOMIC ENERGY UNITED NATIONS EDUCATIONAL, SCIENTIFIC AND CULTURAL ORGANIZATION

INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS





I.C.T.P., P.O. BOX 586, 34100 TRIESTE, ITALY, CABLE: CENTRATOM TRIESTE

UNITED NATIONS INDUSTRIAL DEVELOPMENT ORGANIZATION



INTERNATIONAL CENTRE FOR SCIENCE AND HIGH TECHNOLOGY

c/o INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS MIND TRIESTE (ITALY) VIA GRIGNANO, 9 (ADRIATICO PALACE) P.O. BOX 386 TELEPHONE 040 224575. TELEFAX 040 224575. TELEX 46049. APH 1

SMR/760-44

"College on Atmospheric Boundary Layer and Air Pollution Modelling" 16 May - 3 June 1994

"An Intercomparison of Atmospheric Turbulence Parameters and Their Application to a Tracer Experiment Using a Monte Carlo Particle Model"

F. DESIATO Agenzia Nazionale per la Protezione dell'Ambiente A.N.P.A. (EX-ENEA/DISP) Rome, Italy

Please note: These notes are intended for internal distribution only.

AN INTERCOMPARISON OF ATMOSPHERIC TURBULENCE PARAMETERS AND THEIR APPLICATION TO A TRACER EXPERIMENT USING A MONTE CARLO PARTICLE MODEL

Franco Desiato* and Rolf Lange**

*ENEA/DISP, Rome
**Lawrence Livermore National Laboratory, CA

INTRODUCTION

Monte Carlo models simulate the dispersion of pollutants in the atmosphere by means of a large number of particles which are moved at each time step by compound velocities that take into account the mean advection component and the random turbulent fluctuations of both horizontal and vertical wind components. They are based on the solution of the Langevin equation (Gifford, 1982; Sawford, 1985) and on the assumption that wind vector fluctuations can be described by an autocorrelation process of first order (Markov process).

The approach requires the knowledge of profiles of the wind velocity variances σ_V and the Lagrangian integral time scales T_L in all three dimensions. These turbulence parameters T_L and σ_V are generally derived empirically, and their choice has a significant effect on the resulting air concentration patterns of a pollutant released into the atmosphere.

In this paper, some different methods for deriving σ_{V} and T_{L} profiles are compared, and their effect on air concentration distributions are estimated. For this purpose, a three-dimensional particle model has been applied in conjunction with a diagnostic wind field model to the SIESTA tracer data set (Gassmann et al., 1986) collected during 1985 in Switzerland. The simulated experiments are representative of near neutral stability and weak to moderate wind conditions.

THE MODEL

The model used for the present study (ARCO: Atmospheric Release in COmplex terrain) retains the basic scheme of the Monte Carlo version of ADPIC (Lange, 1978; Lange, 1990). The main new features are the following. Particles are advected by a sequence of wind fields computed in a terrain-following coordinate system; input data are allowed to vary in space (topography, roughness height) or in space and time (mixing

depth, Monin-Obukhov length, precipitation) with flexible space and time resolution; concentration are computed after assigning to each particle a Gaussian kernel density distribution.

The pseudo-velocity $U_{\rm p}$ of a particle is defined as the sum of an advection velocity $U_{\rm d}$ and a diffusive velocity $U_{\rm d}$, both interpolated to the particle position. $U_{\rm d}$ is provided by a gridded mean wind field model (Ludwig, 1988) which uses interpolated meteorological data and terrain information to produce a mass conservative wind field. $U_{\rm d}$ is computed using the Langevin equation (Legg and Raupach, 1982). The vertical component equation being,

$$w(t+\Delta t) = aw(t) + b\sigma_w \zeta + (1-a)T_L \partial \sigma_w^2/\partial z , \qquad (1)$$

where w(t) is the vertical velocity at time t, ζ is a random number from a Gaussian distribution with zero mean and unit variance, $T_{r.}$ the Lagrangian integral time scale,

$$a=\exp(-\Delta t/T_L)$$
; $b=(1-a^2)^{1/2}$. (2)

The last term in (1) allows for inhomogeneous turbulence in which \mathbf{T}_L and the standard deviation of the of the vertical wind component σ_L can vary with height. The two horizontal components of \mathbf{W}_d are computed using analogous equations without the last term, because homogeneous turbulence is assumed in the horizontal in the absence of boundaries.

ARCO incorporates several subroutines for the estimate of σ_V and $T_{_{\rm I}}$ profiles with different methods, also depending on the availability of turbulence measurements.

One approach is based on the parameterizations summarized by Hanna (1982), which, for the neutral boundary layer, are:

$$\sigma_{u} = 2 u_{\star} \exp(-3fz/u_{\star}) \tag{3}$$

$$\sigma_{v} = \sigma_{w} = 1.3 \ u_{\star} \exp(-2fz/u_{\star}), \tag{4}$$

$$T_{L} = .5 z / \sigma_{w} (1+15fz/u_{\star}),$$
 (5)

where f is Coriolis parameter and \mathbf{u}_\star is friction velocity. The last equation is assumed to be valid for all three components of turbulence in neutral conditions.

When wind fluctuation measurements σ_{v1} and σ_{w1} near the surface at height z_1 are available, as in the case of the SIESTA experiments, they can be used, in conjuction with (4), as follows:

$$\sigma_{\mathbf{v}} = \sigma_{\mathbf{v}1} \exp[-.5(\mathbf{z} - \mathbf{z}_1)/h] \tag{6}$$

$$\sigma_{\mathbf{w}} = \sigma_{\mathbf{w}1} \exp[-.5(\mathbf{z} - \mathbf{z}_1)/h] \tag{7}$$

Here it has been assumed for the neutral mixing depth h (Blackadar and Tennekes, 1968)

$$h = .25 u_{\star}/f \tag{8}$$

A different approach for the estimate of T_L is based on fitting atmospheric diffusion observation of σ_y with the

formula derived from statistical theory (Pasquill, 1971):

$$\sigma_{\mathbf{v}}(t) = \sigma_{\mathbf{v}}^{tf_1(t/T_L)} \tag{9}$$

Li and Meroney (1985) and Pasquill (1986) summarized the most recent estimates. For neutral stability, a representative value is $T_L = 750$ s (Neumann, 1978).

In conclusion, for the model application to the SIESTA data set, the following methods where used and compared, henceforth referred as model run a), b), c), respectively. Run a): σ_V from measurements of σ_Θ and σ_{ϕ} , eqs. (6),(7); T_L by Hanna (1982), eq. (5). Run b): σ_V as run a); $T_T = 750$. Run c): σ_V by Hanna (1982), eqs. (3),(4); $T_L = 750$.

EVALUATION CRITERIA

ARCO was applied to the meteorological and tracer data collected during SIESTA (SF6 International Experiments in STagnant Air). Somehow in contrast with the original aim of the campaign, the actual meteorological conditions showed well defined wind directions in 5 of the 6 experiments. The first 4 experiments were performed in a persistent "Bise" (north-east wind) regime and the last experiment took place during a west-wind situation. During all the experiments neutral or slightly stable situations were found with almost adiabatic lapse rates in the boundary layer.

For the purpose of the present study, the attention has been focused on the estimate of the following two quantities: the Crosswind Integrated Concentration (CIC), as an indicator of the vertical diffusion; the horizontal standard deviation of the plume of the plume of the plume of the horizontal diffusion.

To derive "observed" CIC and σ_y from measured SF6 concentrations, the available data were normalized to sampling intervals of 1 hour; then, groups of samplers on arcs, approximately at the same distance from the release point, and showing maximum concentration inside the arc, were selected. Within each group, concentrations were normalized the distance of the observed maximum using the Gaussian plume formula with Pasquill-Gifford σ_y and σ_z for D category.

Experiment number 5 was discarded due to the transitional situation between east and west wind that occurred during the release; experiment number 2 was discarded due to insufficient SF6 data useful for deriving CIC and $\sigma_{\rm Y}$. $\sigma_{\rm Y}$ was derived from the relationship $\sigma_{\rm Y}=\Delta {\rm Y}/4.28$, where $^{\rm Y}\Delta {\rm Y}$ is the width of the sampler arc limited by the two (interpolated) concentration values equal to 1/10 of the maximum. Finally, it was possible to obtain 7 realizations of CIC and $\sigma_{\rm Y}$ to be compared with those computed by the model, at distances from the source ranging from 5 to 17 km (Table 1).

For the model simulation, the following meteorological measurements were used. Wind speed and directions at thirty minutes interval from the 110 m meteorological tower near the release point, three small masts located downwind of the source and a tethered balloon that sounded the boundary layer up to

about 500 m; wind fluctuation σ_0 and σ_0 at 10 minutes intervals near the release point were used for model runs a) and b). The inverse of Monin-Obukhov length was set to zero in all runs; h was computed from (8); the roughness length z_0 was set to .05 m. In Table 1 the characteristic values of meteorological data for each experiment are listed.

Table 1. SIESTA tracer experiment. Average meteorological data used for model simulation.

Exp.	Date	U(10m)	σθ	σφ	h
1	15/11/85	2.7	18	7	380
3	20/11/85	1.5	19	9	250
4	24/11/85	2.2	17	6	310
6	30/11/85	3.0	21	10	420

Table 2. Comparison between observed and computed normalized CIC and $\sigma_{\rm c}$ for the 7 realizations obtained from concentrations on sampler arcs. Units of CIC are [10⁻³ s m⁻²].

Exp. r	10.	1	1	3	3	4	6	6
Sampli time	.ng	10:00/ 11:00	11:00/ 12:00	13:00/ 14:00	13:00/ 14:00	13:00/ 14:00	13:00/ 14:00	13:00 14:00
Distar (km)	ice	7.3	7.3	6.3	13.8	15.0	5.0	17.3
	Obs.	3.6	1.9	1.5	1.1	1.7	1.8	1.8
a.c. (0	Run a)	7.9	11.2	13.5	1.5	7.6	8.9	2.5
CIC/Q	Run b)	3.0	2.4	5.8	0.9	2.4	1.9	0.9
	Run c)	4.7	4.4	9.3	1.0	2.1	3.1	1.6
- -	Obs.	├ 1150	950	1140	2000	2700	960	3200
σу	Run a)	500	650	660	1230	490	690	840
(m)	Run b)	1170	950	760	1700	870	1000	1400
	Run c)	520	710	660	1000	500	700	1200

The results of the model simulations are listed in Table 2, where observed and computed $\sigma_{\rm c}$ and CIC/Q, where Q is release rate, are compared. It must be pointed out that the "observed" CIC and $\sigma_{\rm c}$ may be affected by a large uncertainty due to the inherent inaccuracy of the procedure used to derive them from the available sampling points. In addition, they provide a useful estimate of turbulence intensity only if the actual vertical distribution of the plume is not very different from the Gaussian profile.

Nevertheless, the results summarized in Table 2 seem to provide some clear indications. Run a) shows a considerable overestimation of CIC and underestimation of σ in all cases. Comparing with results of run b), which improve noticeably for both CIC and $\sigma_{\rm V}$, this seems to be due to the general underestimation of the Lagrangian time scale when computed through eq. (5). In fact, with the weak wind speed conditions of SIESTA, we obtain values of T, of the order of few tenths of seconds, which are small compared to $T_{\rm L} = 750$ s adopted for run b).

Run b) and c) also underestimate σ_{γ} , but run b) performs better; the reason of this difference is the average underestimation of σ_{γ} through eq. (4), with respect to the measured values which are actually larger then expected in typical neutral conditions. In Fig. 1 the σ_{γ} computed with run b) are compared with the observed and with Pasquill-Gifford curve for D category. The agreement with the observed σ_{γ} is good for the sampler arcs closer to the release point.

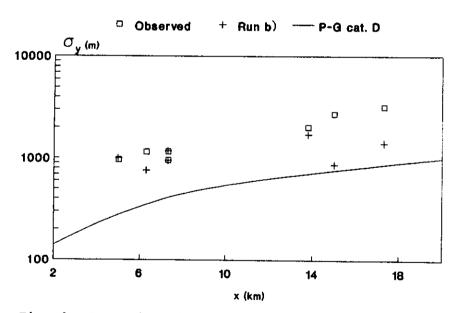


Fig. 1. Comparison between observed, computed (Run b), and Paquill-Gifford (D category) σ_y for the seven model realizations.

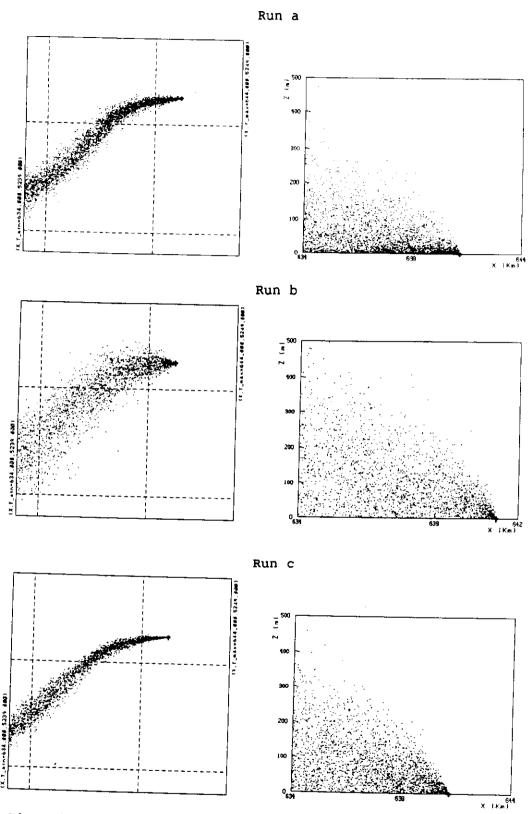


Fig. 2. Particle display on x-y (left) and x-z (right) planes, SIESTA experiment no. 1, 15/11/85, 12:00.

Eq. (4) performs better for the vertical component $\sigma_{\rm w}$; in fact, with the exception of the first arc of experiment no. 3, the CIC computed by run c) are in reasonable agreement with the observed and also with those computed based on $\sigma_{\rm h}$ measurements.

An example of the effect of the different parameterizations of σ_{V} and T_{L} on the horizontal and vertical diffusion of the particles is shown in Fig. 2, where the particle display on x-y and x-z sections for the three runs are compared. The reduced particle diffusion on both the horizontal and vertical planes for run a) and on horizontal plane for run (c) are evident.

The results have been summarized (Table 3) from a statistical point of view by means of two index which are frequently used in dispersion model evaluation studies, the Bias:

$$Bias = 1/N \ \Sigma_{i} \ (C_{i}-O_{i}), \tag{10}$$

and the Normalized Mean Square Error:

$$NMSE = 1/N \ \Sigma_{i} \ (C_{i} - O_{i})^{2} / (\overline{C} \ \overline{O}), \tag{11}$$

Table 3. Bias and Normalized Mean Square Error of CIC/Q and $\sigma_{_{\bf V}}$ for the three model run.

		CIC/Q Bias NMSE			Bias	Y NMSE
Run a)			3.3	+	-1005	1.35
Run b)		0.5	0.6	1	- 607	0.50
Run c)	 	1.8	1.4		- 972	1.15

where O_i and C_i are observed and computed values respectively. From Table 3 it is evident the best performance of run b), with σ_V profiles derived from σ_{θ} and σ_{ϕ} measurements and T_L is derived from Neumann (1978).

This study is limited to a particular tracer dataset, collected in weak or moderate wind regime which is not representative of most typical near neutral conditions. However, it gives the general indication that the availability of wind fluctuation measurements and the method for deriving the profiles of both $\sigma_{\rm V}$ and $T_{\rm L}$ can have a considerable effect on the results of Monte Carlo particle models.

REFERENCES

- Blackadar, A. K., and Tennekes, H., 1968, Asymptotic similarity in neutral barotropic planetary boundary layers, J. Atmos. Sci., 25:1015.
- Gassmann, F., Gaglione, P., Gryning, S. E., Hasenjaeger, H.,
 Lyck, E., Richner H., Neininger, B., Vogt, S., Thomas,
 P., 1986, "Experimental Investigation of Atmospheric
 Dispersion over Complex Terrain in a Prealpine Region
 (Experiment SIESTA)," EIR-Bericht nr. 604, Wurenlingen, Switzerland.
- Gifford, F. A., 1982, Horizontal diffusion in the atmosphere: a Lagrangian-dynamical theory, Atm. Env., 16:505.
- Gifford, F. A., 1986, The time scale of atmospheric diffusion considered in relation to the universal diffusion
- considered in relation to the universal diffusion function, f₁, Atm. Env., 21:1315.

 Hanna, S. R., 1982, Applications in air pollution modelling, in: "Atmospheric Turbulence and Air Pollution Modelling,"
 F. T. M. Niewstadt and H. van Dop ed., D. Reidel Publishing Company, Dordrecht/Boston/Lancaster.

 Lange, R., 1978, ADPIC-A three-dimensional particle-in-cell model for the dispersal of atmospheric pollutants and its
- comparison to regional tracer studies, J. Appl. Meteor., 17:320.
- Lange, R., 1990, A comparison of the Monte Carlo and the Flux Gradient Method for Atmospheric diffusion, Proceedings of the 18th NATO/CCMS International Technical Meeting on Air Modelling and Its Application, Vancouver, Pollution Canada.
- Legg, B. J., and Raupach, M. R., 1982, Markov chain simulation of particle dispersion in inhomogeneous flow: the mean drift velocity induced by a gradient in Eulerian velocity variance, <u>Boundary-Layer Met.</u>, 24:3.

 W. W., and Meroney, R. N., 1985, The estimation of atmospheric dispersion at nuclear power plants utilizing
- real time anemometer statistics, U.S. Nuclear Regulatory Commission NUREG/CR-4072.
- Ludwig, F. L., 1988, Combined objective wind analysis and adaptive volume plume model codes for microcomputer use, in: "Computer Techniques in Environmental Studies," P. Zannetti ed., Computational Mechanics Publications, Publications, Southampton/Boston.
- Neumann, J., 1978, Some observations on the simple exponential function as a Lagrangian velocity correlation function in turbulent diffusion, Atm. Env., 12:1965.
- Sawford, B. L., 1985, Lagrangian simulation of concentration mean and fluctuation field, J. Clim. Appl. Met., 24:1152.

DISCUSSION

P.J.H. BUILTJES

Would it be possible to use wind tunnel experiments to test your model?

F. DESIATO

Yes, of course it is. It is the aim of the authors to compare the schemes for deriving turbulence parameters in different stability conditions: wind tunnel data would be very useful for this purpose.