A NEW HIGH PERFORMANCE VERSION OF THE LAGRANGIAN PARTICLE DISPERSION MODEL SPRAY, SOME CASE STUDIES

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INTRODUCTION

Lagrangian particle models are powerful tools to simulate the atmospheric dispersion of gaseous releases. Although having a quite complex mathematical basis (Thomson, 1987, Rodean, 1994), their practical implementation is generally simple and intuitive, allowing to easily take into account complex situations such as the presence of the topography or terrain inhomogeneities, low wind speeds, spatial and temporal variations of meteorological fields. In these models the atmospheric dispersion is simulated by the motion of fictitious particles splitted in a mean part due to the mean wind, and a stochastic fluctuation related to the statistical characteristics of the turbulent flow. It is quite clear that the model accuracy is strongly dependent on the number of emitted particles and the computer time often limits the kind of simulations that can be performed. For this reason, the earlier version of these models were mainly devoted to reproduce the dispersion of a limited number of emissions at local scale. The recent wide and rapid diffusion of very fast computational tools lead to the development of more sophisticated codes, able to take into account more general situations. SPRAY (Tinarelli et al., 1992) is a Lagrangian stochastic particle model designed to perform dispersion simulations in complex terrain. The version 1 of the code, based on a three dimensional form of the Langevin equation for the random velocity with coupled non-gaussian random forcing following Thomson (1984, T84 in the following) and subsequently improved (Tinarelli et al., 1992), was able to satisfactorily reproduce local to regional scale dispersion both over flat (Brusasca et al., 1989, 1992) and complex terrain (Brusasca et al., 1995, Nanni et al., 1996) taking into account the emission from single or multiple sources. The development of a better based theory (Thomson, 1987) and the further demand of more complex regional scale simulations able to cover longer periods with a variety of emissions of different kinds (i.e. main roads, industrial or urban area) called for a new version of the code. The new version 2 of SPRAY code contains some improvements regarding the

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theoretical approach, turbulence parametrizations and time response characteristics. In this paper we describe these new developments, comparing model performances with those of the previous version through simulations performed both in theoretical and real cases.

NEW DEVELOPMENTS

The version 2 of the code contains many new algorithms. They can be resumed into the following three main classes.

Langevin Equations and PDFs

A generalized form of the Ito's type Langevin equation has been added as new alternative option to the previous formulation. The equation for the vertical displacement z and for the vertical velocity w of each particle take the following form:

$$dz = w dt \tag{1}$$

$$dw = a(z,w)\, dt + \sqrt{B_0(z) dt}\, d\mu \tag{2}$$

in eq. 2 $d\mu$ is a normally distributed random variable, $B_0 = (C_0 \varepsilon) / 2$, being C_0 a constant whose value is not yet definitely established, ranging from 2 to 7 (Rodean, 1994), ε the ensemble average dissipation rate of the turbulent kinetic energy, and $a(z,w)$ is a function depending on the form of the atmospheric Eulerian PDF $P(z,w)$ of the turbulent velocity. Following Thomson (1987), the form of $a(z,w)$ can be deduced imposing the so called 'well mixed condition' leading to a solution of the following Fokker-Planck equation for stationary conditions

$$w \frac{\partial P}{\partial z} = -\frac{\partial aP}{\partial w} + B_0 \frac{\partial^2 P}{\partial w^2} \tag{3}$$

To deal with non-uniform or convective turbulence, the PDF of the vertical motion can be non-Gaussian. In this case, two different approaches have been adopted and are both present in the model, in order to give a solution of the Fokker-Planck equation with different degrees of approximation and different time responses. The first one, already presented by different authors (Baerentsen and Berkowicz, 1984, Luhar and Britter, 1989) defines P as a linear combination of two Gaussian PDFs (BG in the following)

$$P(z,w) = \alpha P_u(m_u, \sigma_u) + \beta P_d(m_d, \sigma_d) \tag{4}$$

where α and β are the weights of the two Gaussian distributions P_u and P_d whose mean and standard deviations are respectively m_u, σ_u and m_d, σ_d. The six unknown parameters in (4) are determined as a function of the first four moments of $P(z,w)$ defined as follows

$$\overline{w^n} = \int w^n P(z,w) dw \qquad n=0,1,2,3 \tag{5}$$

Substituting (4) into (3) it is possible to obtain an analytical form of $a(z,w)$ (Luhar and Britter, 1989). The second method, proposed by Ferrero and Anfossi (1998) consists in the

adoption of a Gram-Charlier expansion, truncated as option to the third (GC3) or fourth (GC4) order, to approximate the PDF form with given moments (Kendall and Stuart, 1977)

$$P(x,z) = \frac{e^{-x^2/2}}{2\pi}(1 + C_3 H_3 + C_4 H_4) \qquad (6)$$

where H_3 and H_4 are Hermite polynomials and C_3 and C_4 are their coefficients, whose expressions are

$$H_3 = x^3 - 3x \qquad (7)$$

$$H_4 = x^4 - 6x^2 + 3 \qquad (8)$$

$$C_3 = \overline{\mu^3}/6 \qquad (9)$$

$$C_4 = (\overline{\mu^4} - 3)/24 \qquad (10)$$

where $x = w/\sigma_w$, $\overline{\mu^3}$ and $\overline{\mu^4}$ are the standardized moments of w. Substituting (6) into (3) the following expression for the coefficient $a(z,w)$ is found

$$a = \sigma_w \frac{\frac{1}{\tau}(T_1) + \frac{\partial \sigma_w}{\partial z}(T_2)}{T_3} \qquad (11)$$

where $\tau = \sigma_w^2/B_0$ is the Lagrangian decorrelation time scale and

$$T_1 = -3C_3 - x(15C_4 + 1) + 6C_3x^2 + 10C_4x^3 + C_3x^4 - C_4x^5 \qquad (12)$$

$$T_2 = 1 - C_4 + x^2(1 + C_4) - 2C_3x^3 - 5C_4x^4 + C_3x^5 + C_4x^6 \qquad (13)$$

$$T_3 = 1 + 3C_4 - 3C_3x - 6C_4x^2 + C_3x^3 + C_4x^4 \qquad (14)$$

Variable time step discretization

In the version 1 of the code, the T84 Lagrangian equations corresponding to (1) and (2) are numerically integrated by means of a discrete constant time step Δt. Its value is prescribed setting

$$\Delta t = \frac{\tau_{min}}{c} \qquad (15)$$

where τ_{min} is the minimum value of τ_i, i=x,y,z which represent the horizontal and vertical Lagrangian decorrelation time scales. The empirical coefficient c is generally set equal or greater than 10. Obviously, the larger is c and the lesser are the integration errors due to the discretization. On the other hand, the lesser is c and the greater is the computational time and the value 10 for c represents a good compromise between the two needs. Looking at Fig.1 showing a typical CBL τ_z profile computed according to the Weil (1990) parametrization, it is evident that, far from the domain boundaries, τ_z is much larger than τ_{min}. For the particles lying into a large portion of the domain, the restriction imposed in (15) leads to a number of time steps significantly superior to what strictly necessary to obtain an equally correct simulation.

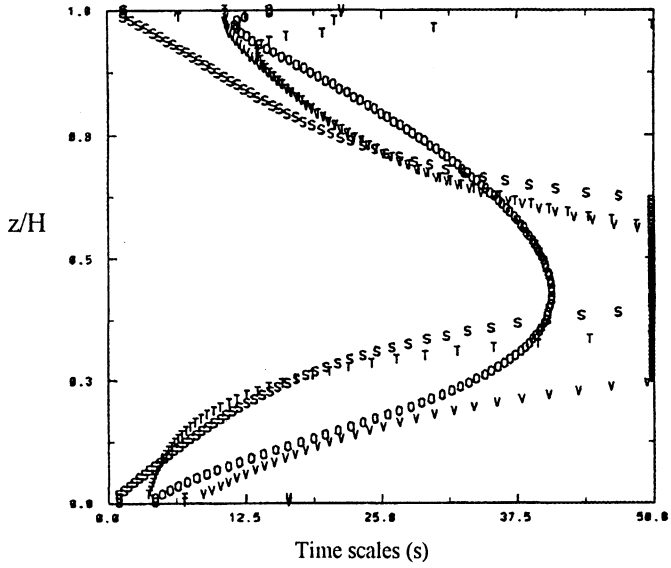

Fig. 1 Vertical profiles of τ_z (0 symbols), τ_w (V), τ_s (S) and $\tau_{\tau z}$ (T) as a function of z/H in a CBL of height H.

It is worth noting that the Lagrangian decorrelation time scale cannot be the only limiting parameter to take into account. Even into the region where the condition $\tau_i >> \tau_{min}$ take place, Δt cannot become too big if strong gradients of the turbulent characteristics are present. Because of these inhomogeneities, particularly evident in the vertical direction, excessive long paths performed by the particles in a single time step could bring them into regions characterized by completely different turbulent properties. This would tend to distribute the particles in a non-uniform way thus violating the well-mixed condition. To solve this problem, three further "vertical inhomogeneity time scales" are taken into account

$$\tau_w(x,y,z) = \left(\frac{\sigma_w}{\overline{w^2}} \frac{\partial \overline{w^2}}{\partial z} \right)^{-1} \tag{16}$$

$$\tau_s(x,y,z) = \left(\frac{\sigma_w}{\overline{w^3}} \frac{\partial \overline{w^3}}{\partial z} \right)^{-1} \tag{17}$$

$$\tau_{\tau_z}(x,y,z) = \left(\frac{\sigma_w}{\tau_z} \frac{\partial \tau_z}{\partial z} \right)^{-1} \tag{18}$$

where τ_w, τ_s, and $\tau_{\tau z}$ represent the inhomogeneity time scales due to the vertical variations of variance, skewness and Lagrangian decorrelation time of the vertical velocity fluctuations respectively. The first two time scale have been proposed by Wilson and Flesch (1993) whereas the third one is proposed in this work. The model selects the time step Δt as follow

$$\Delta t = \min\left(\frac{\tau_x, \tau_y, \tau_z, \tau_w, \tau_s, \tau_{\tau z}}{c_{10}} \right) \tag{19}$$

Where c_{10} is a constant of the order 10 given by the user. Vertical profiles of τ_z, τ_w, τ_s, $\tau_{\tau z}$ are represented in Fig.1 for the Weil's CBL parametrization. It is evident that, particularly close to the boundaries, many intersections between the different curves occur. τ_s and $\tau_{\tau z}$ are also consistently greater than τ_z inside non- negligible vertical layers.

Pre-processing codes

Two meteorological pre-processors are now present in SPRAY model in order to give the turbulence variables needed by the code. The first one, already present in version 1, generates vertical profiles of turbulent variables on the basis of the wind fields coming from a diagnostic mass consistent tool, land-use characteristics and surface meteorological data. In addition, a new pre-processor is operational to interface SPRAY with the mesoscale prognostic code RAMS (Pielke at al. 1992). This new code, named MIRS (Method for Interfacing Rams and Spray) and already presented in a preliminar version (Trini Castelli and Anfossi, 1997) allows SPRAY to take as input the turbulence fields generated by the different closure schemes present in the 3b version of RAMS. In particular, TKE fields coming from the Mellor-Yamada 2.5 scheme can be used to estimate both the PBL height and σ_w profiles. Many optional turbulence parametrization models are implemented in MIRS to define all the input parameters to SPRAY code not directly given by RAMS, such as the Lagrangian decorrelation time scales and the skewness of the vertical velocity PDF.

CASE STUDIES

Some case studies have been performed in order to test the new code and compare it against the previous version. In particular, laboratory and real field simulations have been done, to check both the model consistency in controlled conditions and the performances in a real complex scenario. As regards the first case, the well-mixed condition has been tested in the convective boundary layer parametrized as in Fig. 1.

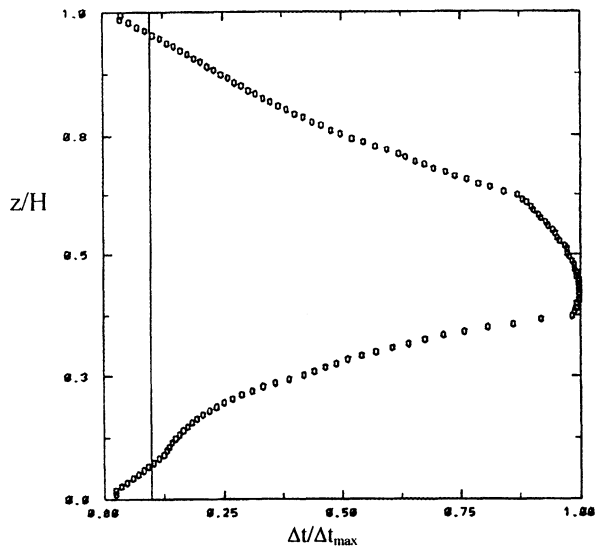

Fig.2 $\Delta t/\Delta t_{max}$ ratio as a function of z/H in the CBL indicated in Fig. 1 (O symbols). The continuous vertical line represents the $\Delta t/\Delta t_{max}$ ratio corresponding to a fixed Δt with c=10.

Fig. 2 shows the comparison between the variable Δt (normalized with the maximum value) determined by the model using the limiting rule indicated in (19) and the fixed time step following (15) with c=10, at each vertical level in the simulated CBL. The variable time step method allows an improvement into almost all the vertical domain but the two layers close to the boundaries, where vertical gradients are stronger. The actual gain depends on the vertical distribution of particles during the simulation, but an overall better time response could be expected in these conditions. The BG and GC schemes showed to be able to satisfactorily mantain well mixed an initially uniform vertical particle distribution (not shown here) both using a fixed and a variable Δt. Table 1 illustrates the speedup factor with respect to the previous T84 formulation obtained in this test case using the different models and the values of 10 and 20 for the c_{10} constant (the c constant of the fixed time step scheme was always set to 10).

Table 1 Speedup factors of the new schemes with respect to the T84 version

Δt scheme	PDF scheme	c_{10}	speedup factor
constant	T84	-	1
constant	BG	-	0.93
constant	GC4	-	1.17
variable	BG	10	2.95
variable	BG	20	1.76
variable	GC4	10	3.72
variable	GC4	20	3.00

The T84 method shows to be slightly more efficient than the BG method, but its capability to maintain the well mixed condition is only approximate. The GC method (only the GC4 results are shown in Table 1) is more efficient than the BG one, as one could expect due to its lesser mathematical complexity. In general, the GC method permits a limited speedup factor, of the order of about 20%, whereas larger factors can be obtainable using variable time steps. In this last case, better physical results have been obtained using c_{10}=20 but a reasonable performance is still reachable using c_{10}=5.

The model has been applied in a more complex situation, in order to verify the capabilities offered by the new algorithms in a real scenario. Simulations have been performed in the Valle D'Aosta regional area (Manzi et al., 1998), over a 100x80 km^2 computational domain located in Italy, adjacent to the northwestern boundary. This is a very complex topographical site where the higher summits of the Alps (more than 4400m a.s.l.) are present together with the bottom of the main valley (about 500m a.s.l.). Mean wind three dimensional fields have been reconstructed using a mass-consistent model and then used as input to the dispersion code. About 1000 emitting sources of different type have been considered, to simulate a complex network of heating systems, industrial and urban areas and main roads. Fig. 3 shows an horizontal view of the domain, with an example of the particle horizontal distribution in a typical summer diurnal condition. Two periods have been simulated, the first one lasting 11 days during summer 1996 and the second one lasting 10 days during winter of 1996. This choice was made in order to extrapolate from the obtained daily mean concentration fields some climatological aspects of the regional impact due to the considered emissions. These severe run were performed on a DEC-Alpha 600 S/333 Workstation with 256 Mbytes of central memory using the version 1 of SPRAY code. Huge peaks of the CPU time demanding were observed during the simulation and the total 21 days run took about 8 days to be completed. A 5 s fixed time step was used to disperse a mean quantity of 40000 particles with a peak number of about 85000 particles during some low wind nocturnal periods. The comparison with daily and climatological average

concentrations collected by a regional network of samplers demonstrated a rather satisfactory performance of the model, but a better time response is required to realize longer simulations of this type enhancing the climatological significance of the results.

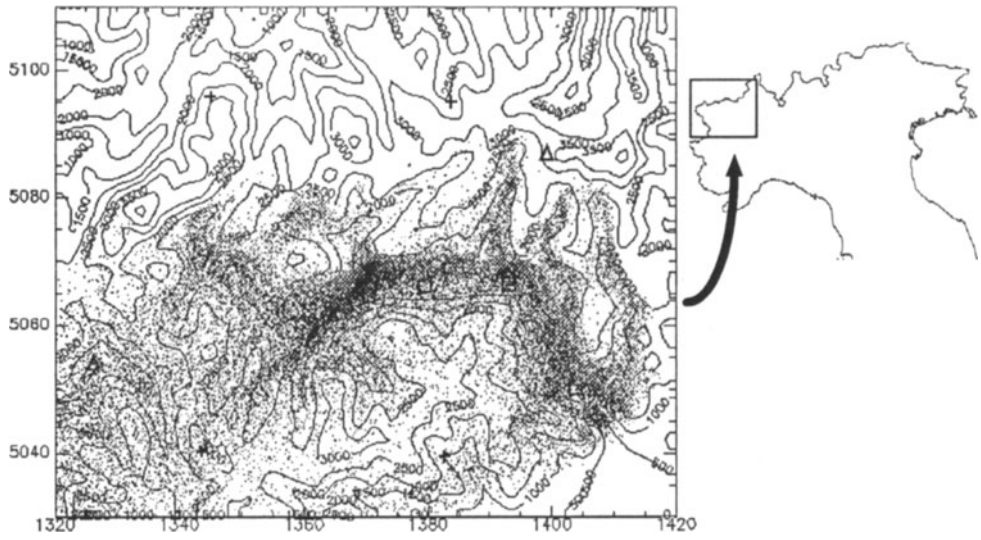

Fig.3 Computational domain used for the dispersion simulations of the Valle D'Aosta regional area (on the right side, the position with respect to the north Italian region is indicated). Contour labels indicate topography levels in meters. About 40000 particles are represented.

For this reason, some comparative simulations have been performed with the version 2 of the code. Preliminar results shows that the speedup in these conditions is, on the average, about 1.7 using variable time steps with c_{10}=5 and the BG scheme. The overall quality of the simulation results remains the same even if some differencies during peak episodes took place with respect to the T84 version. The presence of a large number of emitting points close to the ground probably does not permit the same performances listed in Table 1 due to strong gradients limiting the time step magnitude for a great number of particles. Better results can be obtained using the GC method, therefore allowing the realization of longer simulations, of the order of one month, in a reasonable time.

CONCLUSIONS

New algorithms has been added to the version 1 of the Lagrangian Particles dispersion model SPRAY in order to get better performances. These improvements involve the mathematical basis of the Langevin stochastic differential equations, the insertion of variable time stepping and the connection with a prognostic code to get input parameters. Some of these developments has been checked through controlled simulations, demonstrating an enhanced efficiency of this new version of the code and improving the physical correctness with respect to the previous one. Severe simulations in real field have also been performed and compared with those of the previous version, obtaining sensible speedup factors and showing good results, even if better performances can be expected in more simple situations such as the presence of a limited number of elevated or buoyant emissions. This new version 2 of the SPRAY code should now be able to deal with

problems requiring a large amount of CPU time, such as climatological reconstructions or real time applications, with a satisfactory degree of correctness in more than acceptable response times.

NOTICE

SPRAY is a commercial code jointly marketed by ENEL SpA/PAM, Via Reggio Emilia 39, 20090 Segrate (Milano, Italy) and Aria Technologies, le Charlebourg, 14/30 rue de Mantes, 92700 Colombes (France).

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DISCUSSION

R. YAMARTINO: How many particles do you need to use in your applications and do you use point particles or kernel estimators?

G. TINARELLI: The peak number of particles moved in the 'Valle d'Aosta' simulation in a single time step was about 150000. We did not use kernel estimators to compute concentrations but we used instead boxes. This is the main reason for which we considered such a large number of particles.

A. STOHL: It is possible to pre-calculate a large set of random numbers and then randomly select subset out of this. Although not strictly correct, it works in practice and speeds up the computations considerably.

G. TINARELLI: We will try to experiment this method in the near future.