PROPOSAL OF A NEW LAGRANGIAN PARTICLE MODEL FOR THE SIMULATION OF DENSE GAS DISPERSION

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INTRODUCTION

In the case of accidental releases of hazardous gases and vapours, generally the emitted cloud is initially denser than the ambient air and begins to disperse under the action of its own momentum and buoyancy (and of pre-existing ventilation flows, if any). Then, its excess of density reduces as ambient air is entrained. Thus, at some distance downwind, transition to passive dispersion behaviour will take place. Real terrain dispersion simulation of these accidental releases is complicated by the presence of buildings, other obstacles, complex terrain, and possible occurrence of low wind speed and stable conditions. Dispersion simulation in these situations is generally performed by means of empirical models or, in some specific case, by computational fluid dynamics (CFD) models. However CFD models are highly computationally demanding). In this work we propose a new version of the Lagrangian Particle Dispersion (LPD) model, MicroSpray, to be used as a new simulation tool in this framework, describing the dispersion behaviour and the processes that occur in a dense gas cloud generated from accidental releases.

Besides presenting our new model, we show some preliminary comparisons of its predictions against the tracer Thorney Island field experiment No 8.

BRIEF OUTLINE OF THE MODEL

MicroSpray is part of the model system MSS that comprises MicroSWIFT (giving the 3D input wind field) and MicroSpray. MicroSWIFT is an analytically modified mass consistent interpolator over complex terrain. Given topography, meteorological data and buildings, a mass consistent 3D wind field is generated (*Brusasca et al.*, in press). MicroSWIFT (*Moussafir et al*., 2004) is also able to derive a diagnostic turbulence (namely the Turbulent Kinetic Energy (TKE) and its dissipation rate) to be considered by MicroSpray inside the flow zones modified by obstacles.

MicroSPRAY is a LPD model directly derived from SPRAY code (*Tinarelli et al.*, 1994, 2000), able to take into account the presence of obstacles. The dispersion of an airborne pollutant is simulated following the motion of a large number of fictitious particles, each representing a part of the emitted mass from sources of general shapes. Particles' movement is obtained applying a simple equation of motion where the particle velocity is split into two components: a mean one, or "transport-component" $\overline{U(t)}$, which is defined by the local wind reconstructed by MicroSwift, and a stochastic one, simulating the dispersion and reproducing the atmospheric turbulence. The stochastic component of the particle motion is obtained by solving a 3-D form of the Langevin equation for the random velocity (*Thomson*, 1987). MicroSwift derives Lagrangian time scales and wind velocity variances from the TKE and its dissipation rate ε. Obstacles or buildings are taken into account by setting as impermeable some of the cells of the terrain following grid where meteorological fields are defined.

The new version of MicroSpray model is especially oriented to deal with dense gas dispersion in urban environment and industrial sites.. The new algorithms implemented into MicroSpray to simulate dense gas dispersion regard the following cases:

1. Plume with initial momentum (horizontal, vertical or oblique in any direction)
2. Plume without initial momentum
3. Plume spread at the ground due to gravity. As far as the first two items are concerned, five conservation equations (mass, energy, vertical momentum and two horizontal momenta) are integrated for each particle at each time step, based on *Glandening et al.* (1984) and *Hurley and Manins* (1995). Concerning the third item, we recall that when a dense plume reaches the ground a horizontal momentum is generated by its weight, which thus tends to be spread. We simulate this process by an empirical method based on *Eidsvik* (1980). We notice that in this case, the movement of each particle depends on the characteristics of the 'ensemble' of particles. Thus this approach is hybrid since in LPD models each trajectory is independent on the behaviour of the other particles. The main model equations are briefly introduced in the following. Defining

$$|us| = \sqrt{u_p{}^2 + v_p{}^2 + w_p{}^2} \qquad |Ua| = \sqrt{u_a{}^2 + v_a{}^2 + w_a{}^2}$$

$$B = g\,\frac{T_p - T_a}{T_p} = g\,\frac{r_a - r_p}{r_a} \qquad E = 2\,b\,ue$$

$$ue = \left[a_1 \left| \, |us| - |Ua| \cos(y_p - y_a)\cos(f_p - f_a) \right| + a_2 \left| \, |Ua| \left[1 - \cos^2(y_p - y_a)\cos^2(f_p - f_a)\right]^{1/2} \right| \right]$$

where: a, p refer to air and plume, respectively, b is the plume radius, B is the buoyancy, E represents the entrainment rate and ue is the entrainment velocity. The following conservation equations are solved:

mass conservation
$$\frac{d}{dt}\left[\frac{r_p}{r_a}|us|b^2\right] = E|us|$$

energy conservation
$$\frac{d}{dt}\left[|us|b^2 B\right] = -\frac{r_p}{r_a} N^2 |us|\, wb\, b^2$$

vertical momentum conservation
$$\frac{d}{dt}\left[\frac{r_p}{r_a}|us|\, wp\, b^2\right] = Bb^2|us|$$

horizontal momenta conservation
$$\frac{d}{dt}\left[\frac{\rho_p}{\rho_a}|us|b^2\, up\right] = E|us|\, ua$$

and
$$\frac{d}{dt}\left[\frac{\rho_p}{\rho_a}|us|b^2\, vp\right] = E|us|\, va$$

TRACER THORNEY ISLAND FIELD EXPERIMENT N° 8

Data and information on this experiment were found in two Data Set Reports: Rediphem (*Nielsen and Ott*, 1996) and MDA (*Hanna et al.*, 1991). For a general description of the Thorney Island experiments we refer to these two reports. In the following we only recall the main data necessary to the present work. A mixture of Freon-12 and Nitrogen (mol. weight = 47.11 g/mole) was emitted as an instantaneous puff from a cube of 14 m of side, without any initial momentum. 3958 kg were released. An array of 46 samplers, located at different heights (0.4, 2.4, 4.4 and 6.4 m) in the range 70 – 500 m downwind the source, collected some tracer for 661 s. The initial tracer concentration was 1 mol/mol. Wind speed was 2.4 ms^{-1} and the wind heading was about 18.5 degrees to the left of the array centre line. Other important data were: friction velocity u_* = 0.126 ms^{-1} and roughness length z_0 = 0.012 m. The stability was Pasquill category D. No turbulence data were given. The relative emission density, r_e / r_a , where r_e and r_a , are the emission and ambient densities, was equal to 1.63.

Figure 1 shows the map of the site and the sampler position. As it can be seen the site is an airfield and some buildings are present.

MODELLING IMPLEMENTATION

A computation domain of 200 m x 800 m x 200 m was considered. MicroSwift had horizontal grid spacing of 2 m and a stretched grid in the vertical, MicroSpray is grid free. No obstacles have been included in the MicroSwift simulation, since no exact information of their dimensions was available.

A logarithmic wind profile, horizontally homogeneous, was reconstructed on the basis of the above reported values of u_* and z_0, also used to reconstruct the turbulence fields. 20000 particles were released at t = 0 uniformly distributed within the source cube (14x14x14 m^3) centered at x = 200 m and y = 0 m and then their trajectories were calculated. Finally, concentration at sampler locations was computed.

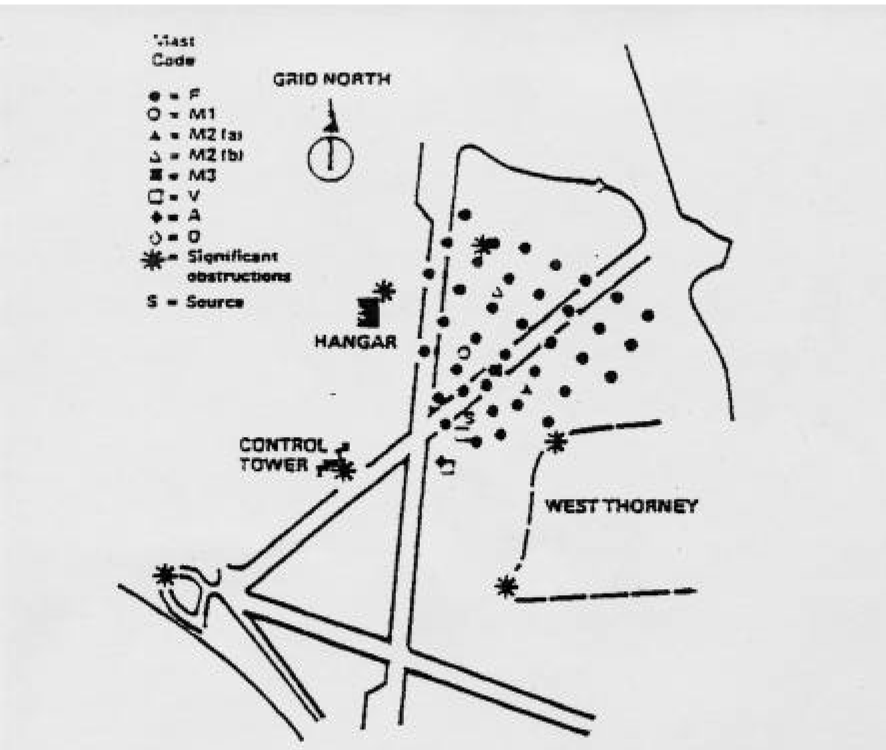

Figure 1. Map of the site (Thorney Island airfield) and the sampler position.

SOME PRELIMINARY RESULTS

Figure 2 shows, as an example, the time series of the tracer concentration at sampler 16 (distance from source = 372 m, z = 0.4 m), sampled at 3 s intervals. It clearly shows the arrival of the tracer cloud at the sampler and its passing over. A great deal of variability is also evident, due to the turbulence and wind field variation at various time scales. Since, as above mentioned, no information on the variability of wind and turbulence and on the obstacles dimensions was available and, it is hopeless to be able to reproduce such temporal details.

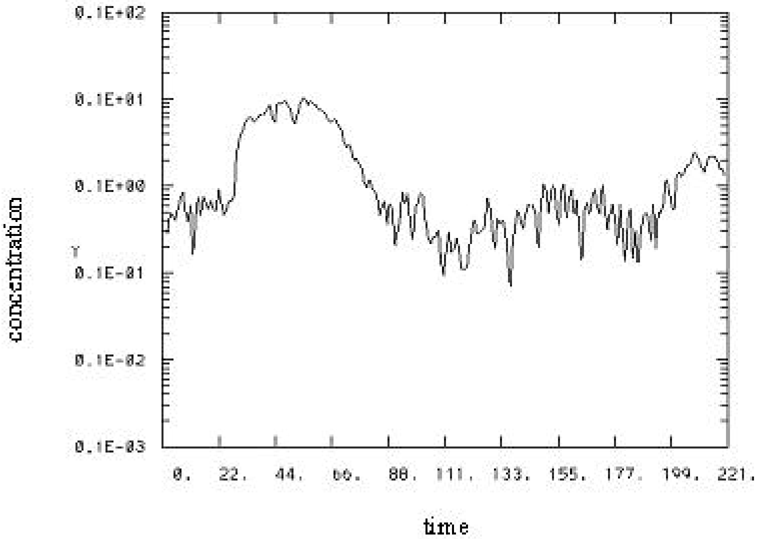

Figure 2 - Time trend of the tracer concentration at sampler 16

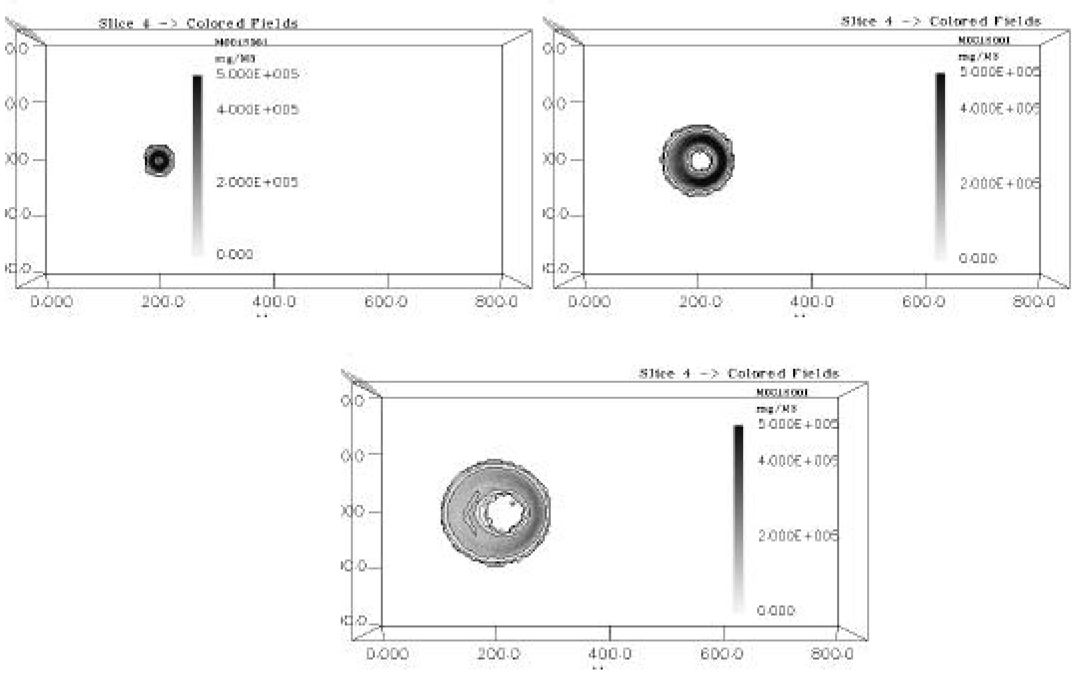

Figure 3 – Isolines of simulated tracer concentration at 1 s, 5s and 10 s, top view

To give an idea of the time evolution of the puff in the first stage of the dispersion process we show in Figure 3 the ground level concentration at three times (1, 5 and 10 s) from emission, as simulated by our LPD model MicroSpray. These three plots, in which the plume spreading effect is evident, correctly represent the observed behaviour. As time proceeds, the centre of the plume becomes empty and the edges fill themselves.

Table 1 shows the result of a statistical analysis for this preliminary comparison. To compute the statistical indexes on a consistent number of data, we decided to consider all the samplers together even if they were at different heights (0.4, 2.4, 4.4 and 6.4 m). The following indexes were computed: mean, normalised mean square error (NMSE), fractional bias (FB), correlation coefficient (CC), factor of 2 (FA2) and factor of 5 (FA5).

Table 1. Statiscal indexes

	mean (g/m^3)	NMSE	FB	CC	FA2	FA5
measured	2.56	-	-	-	-	-
calculated	2.89	3.9	-0.12	0.60	41	89

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