MODELLING OF FLUCTUATING CONCENTRATION FIELDS IN COMPLEX INDUSTRIAL AREAS

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Abstract: In the framework of the new legislation related to accidental scenarios, the forecast of damage areas is a key issue. In such problems the models should reliably predict the individual exposure during a strong emission event. For the impact assessment, it should be more relevant to predict parameter related to maximum dosage rather then to average concentration. Up to now, Gaussian models are the most used to determine the impact of accidental releases. In order to overcome the simplistic limitations of this approach, the numerical model, LAGFLUM (LAGrangian FLUctuation Model), has been developed. The model utilizes a macromixing scheme, based on the so called "well-mixed" criterion, to evaluate the mean concentration. Moreover the micromixing IECM (Interaction by Exchange with the Conditional Mean) scheme is integrated to calculated the higher statistical moments of the concentration. LAGFLUM is applied to determine the mean and the fluctuation statistics of a concentration field, during a short emission episode in a complex industrial area, which includes 12 irregular shaped buildings. The model is coupled with the micro-SWIFT model, which evaluates the wind field and the turbulence parameters in the proximity of buildings. The results evidence the conditions where the fluctuations of concentration prevail respect to the averages.

Keywords: *Concentration fluctuations, Lagrangian models, Micromixing, IECM, Accidental releases.*

INTRODUCTION

The modeling systems currently used do not allow to accurately predict the effects arising from accidental release of pollutants. This can cause damages especially related to the peak values of the concentration, rather than for the average values. Both the legislation that the models refer to the average concentrations and, in general, the concentration peaks are obtained on the basis of the calculated mean concentration and using semi-empirical functions. This methodology have several limitations, including, for example, the impossibility of generalizing the empirical coefficients for the large series of type of accidents and, basically, the inherent statistical inconsistency between the requested information (relative to the single accident and then to the single embodiment of the experiment) and the obtained result, which refers, instead, to the average damage due to a very large number of similar accidents.

A rigorous assessment of the damage would require the deterministic evaluation of the turbulent dispersion of pollutants in the atmospheric boundary layer. The smaller scales of the atmospheric turbulence are of the order of millimeters. Thus, it is practically impossible to predict the flow in detail, since there is an enormous range of scales to be resolved. Therefore, a statistical approach is used, where the pollutant concentration is decomposed into its mean part and a deviation from the mean. In this way one derives only the gross characteristics of the concentration field, with a spatial resolution substantially less than the turbulence microscale. In the event of accident, this approach provides information on the average impact associated to a large number of accidents and involves, as already mentioned, an underestimation of the peak concentration. In general, the knowledge of the fluctuations is necessary in case of non-linear relationships between instantaneous concentration and consequent effect. Isolated events of exceeding the thresholds of concentration of some substances can be, for example, the cause of fire explosion, which could not be provided with the knowledge of the ensemble averages only. Moreover, even in the case of continuous release of pollutants, in the vicinity of the source or close to the edges of the plume strong differences between average and peak concentrations may occur. As a consequence, in addition to the averages, it is necessary to know the probability with which the concentration overcomes the warning level, determined a priori on the basis of the instantaneous damage.

Until a few years ago, the most common method was found on the definition and application of correction factors of semi-empirical nature to the average concentration. Several results concerning the application of Eulerian modes for the calculation of the concentration variance based on the second order closure of the hierarchy of equations of the concentration balance are also found in the literature. However, the integration of these equations is complicated by the need of a high spatial-temporal resolution and the determination of arbitrary constants necessary for the closure. The development of numerical modeling for the calculation of concentration fluctuations had a remarkable impulse in the last years, as a consequence of the implementation of new schemes based on the Lagrangian approach, the most promising of which is based on single-particle and particle pairs Lagrangian stochastic models. The Particle-pairs approach, however, is still limited to simplified cases (i.e. homogeneous turbulence). For single-particle models, two schemes are generally used: the IECM (Interaction by Exchange with the Conditional Mean; Pope, S.B. 2004; Sawford, B.L. 2006) and the IEM (Interaction by Exchange with the Mean; Villermaux J. and J.C. Davillon, 1972; Dopazo C. and E.E. O'Brien, 1974). The IEM model is less expensive from a computational point of view, but, as pointed out by Pope S.B. (1998), it does not satisfy the physical constraint that the exchange of pollutant involves only fluid particles moving in the same realization of the experiment. In contrast, the IECM scheme allows the exchange of pollutant between neighboring particles belonging to similar realizations, i.e. they have almost the same velocity at the same particle location. The IECM scheme satisfies, in contrast to the IEM, also the balance equation of the pollutant. IECM models have been applied in several case studies: one dimensional dispersion in homogeneous turbulence for emissions from linear or areal sources (Sawford, B.L., 2004), for reactive pollutants (Sawford, B.L., 2006), for one-dimensional dispersion in convective boundary layers (Luhar, A.K. and B.L. Sawford, 2005), for one-dimensional dispersion in canopy turbulence (Cassiani, M. et al., 2005b), for two-dimensional dispersion from a point or linear source in neutral boundary layers (Cassiani, M. et al., 2005a; Dixon, N.S. and A.S. Tomlin, 2007; Cassiani, M. et al., 2007).

In the present work, the numerical code LAGFLUM (LAGrangian FLUctuation Model; Leuzzi, G. et al., 2012), a three-dimensional IECM model able to simulate the concentration fluctuations in strongly in-homogeneous turbulent flows which typically occur in urban or industrial areas, is used. The meteorological field adopted as input for the LAGFLUM comes from the numerical simulations of Gariazzo, C. et al. (2012) obtained with the micro-SWIFT model. The case analyzed in the present study refers to an area located in a plant at risk of a major accident.

THE DISPERSION MODEL

The LAGFLUM uses a macromixing scheme based on the well-mixed condition (Thomson, D.J, 1987), which states that fluid particles that are initially well-mixed must remain so. This condition is necessary to avoid the asymptotic accumulation of polluted particles in regions of smaller turbulent kinetic energy. The concentration fluctuations are calculated by the integration of the IECM equation along the particle trajectories. All the particles move according to the macromixing scheme and exchange polluted mass throughout the micromixing process. In this way, each polluted particle has its own instantaneous concentration from which the estimation of the concentration statistical moments at the end of the numerical simulation is obtained.

Although LAGFLUM is physically based (it satisfies the main balance equations), it has been developed in order to be coupled with fluid dynamic models (meteorological or CFD) of common use. In this way, the system can be considered as an integrated, operational, meteorological-dispersion model for the simulation of the statistical moments of the concentration field due to relevant accidents. LAGFLUM has been validated (Amicarelli, A., et al., 2011; Amicarelli, A. et al., 2012; Leuzzi, G. et al., 2012) by means of comparison with the MUST data base (Bezpalcova, K., 2007 and Leitl, B. et al., 2007).

NUMERICAL SETUP

The industrial area considered for the analysis consists of 12 buildings of different shapes having a number of faces varying from 4 to 10 (Figure 1). The corresponding domain is 400x300 m^2. Along the horizontal plane, it is subdivided into a regular grid of cells of 2x2 m^2.

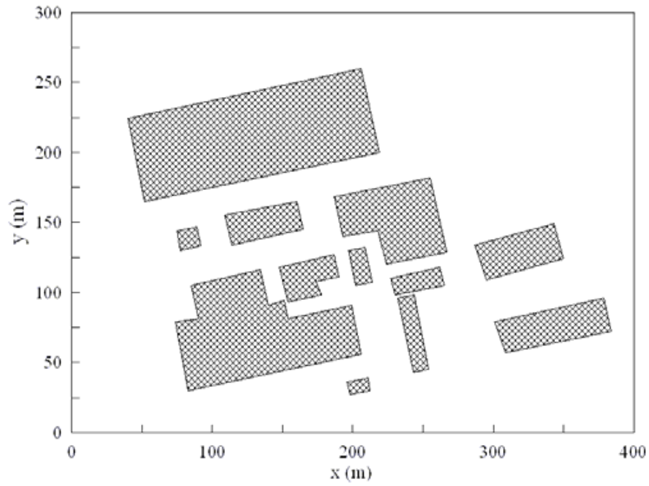

Figure 1. Plan view of the computational domain. The shaded areas are the buildings.

Consistently with the meteorological model configuration, along the vertical 15 unevenly spaced grid nodes were used. The centre of the 14 corresponding grid cells are located at z=1, 2, 4, 6, 8, 10, 19, 30, 46, 63, 85, 114, 151 and 201 m above the ground level. A routine performs the cells arrangement as a function of the building shape and position. With regard to the pollutant source, an emission of SO_2 equal to 0.018 Kg/s is considered. It derives from the instantaneous transformation of $SOCl_2$ into vapours of H_{Cl} and SO_2, in the case of crashing of a barrel of 189 litres containing thionyl chlorite. The source is located at x_s=10 m, y_s=10 m and z_s=1 m.

For the simulation, 2×10^6 particles were used both for the macromixing and the micromixing phase. The time step of the numerical integration is 0.1 s. To reduce the CPU time, the numerical runs can be conducted using a larger time step in that the Lagrangian models are intrinsically stable. However, the time step must be lesser than the integral time scale of the turbulence.

THE WIND FIELD

Figure 2a shows the velocity vectors calculated by micro-SWIFT in the horizontal plane at z=10 m, while Figure 2b depicts the velocity vectors corresponding to the vertical section passing for x=160 m. The undisturbed wind is oriented at 45° clockwise with respect to the y-axis, and has a log-form along the vertical direction. It is apparent the presence of large recirculation regions in the lee of the buildings, while canalizations between the buildings are not well-pronounced. In the vicinity of the buildings the vertical velocity assumes large values (Figure 2b), both positive and negative. Therefore, pollutants emitted near the surface can be advected at the roof top level or remain confined near the ground depending on the source location.

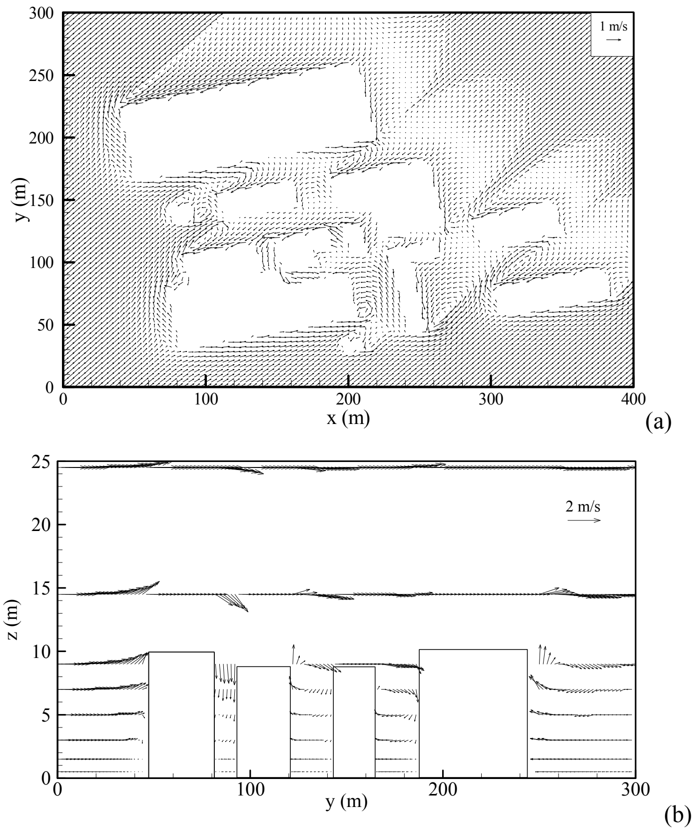

Figure 2. (a) Plane view of the velocity vectors calculated by micro-SWIFT at z=10 m. (b) As in (a), but for the vertical section at x=160 m.

Figure 3 reports the velocity variance of the vertical velocity component calculated by micro-SWIFT in the horizontal plane at z=1 m (Figure 3a) and z=10 m (Figure 3b). It is observed the presence of isolated zones of large turbulent kinetic energy, both upwind the buildings and within the recirculation regions, as a result of the perturbation produced by the buildings. The shape of these regions seems to be independent of the form of the buildings.

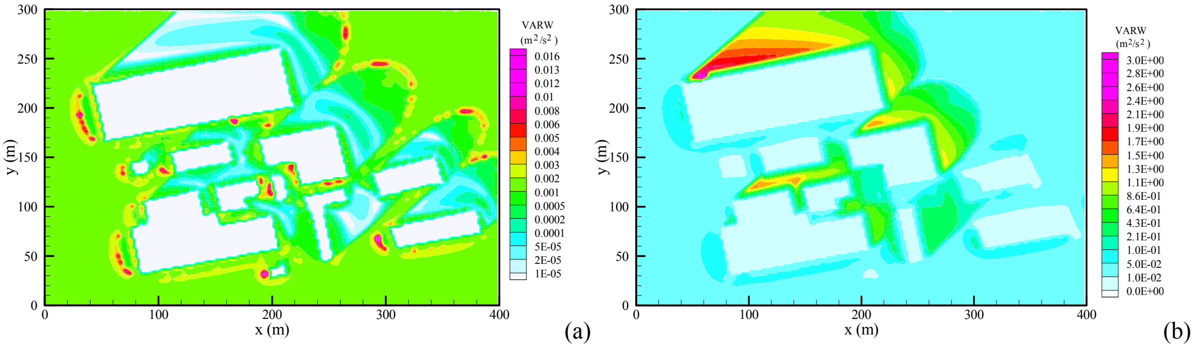

Figure 3. Horizontal section of the vertical velocity variance calculated by micro-SWIFT at (a) z=1 m and (b) z=10 m.

THE CONCENTRATION FIELD

In this section, some examples of the concentration field calculated by LAGFLUM are reported. The wind direction forms a large angle with the x-axis, therefore the polluted plume affects almost the whole domain. Figure 4a shows the mean concentration field calculated at z=1 m. High mean concentrations are present within the recirculation region in the lee of the building located at y≈150 m. This reflects the capability of LAGFUM of reproducing accurately the concentration of pollutants also in strong, in-homogeneous turbulent fields. At elevated levels (Figure 4b), it is evident that the plume goes above the building roofs and is aligned with the undisturbed wind direction. Furthermore, the mean concentration rapidly decreases as a result of the high values of the wind velocity and turbulent intensity. With regard to the standard deviation of the concentration σ_C calculated at z=1 m (Figure 5a), it is apparent their increase in the vicinity of the building where the first interaction of the plume takes places. Non-negligible values of σ_C characterize the regions close to the other buildings. For z=10 m (Figure 5b), σ_C is much smaller, also because the concentration within the plume tends to become more homogeneous.

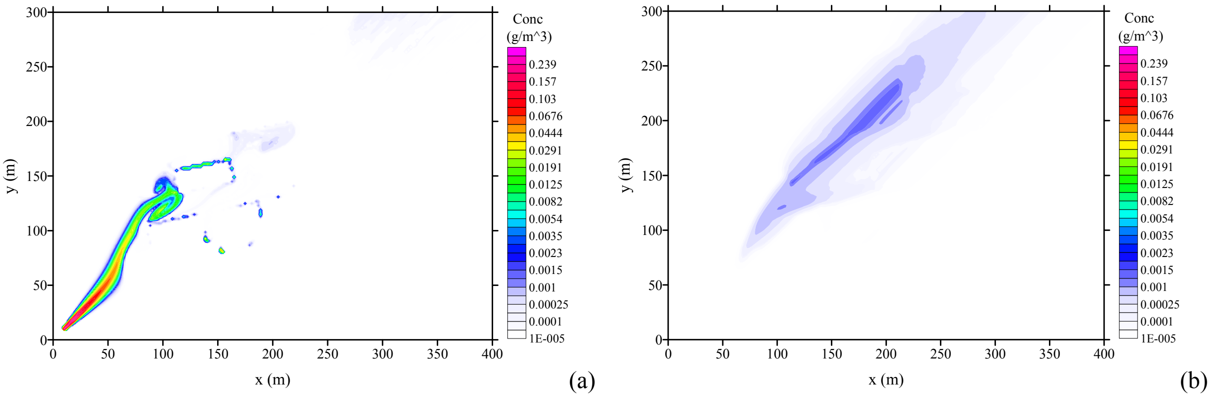

Figure 4. Horizontal section of the mean concentration field calculated by LAGFLUM at z=1 m. (b) As in a), but at z=10 m.

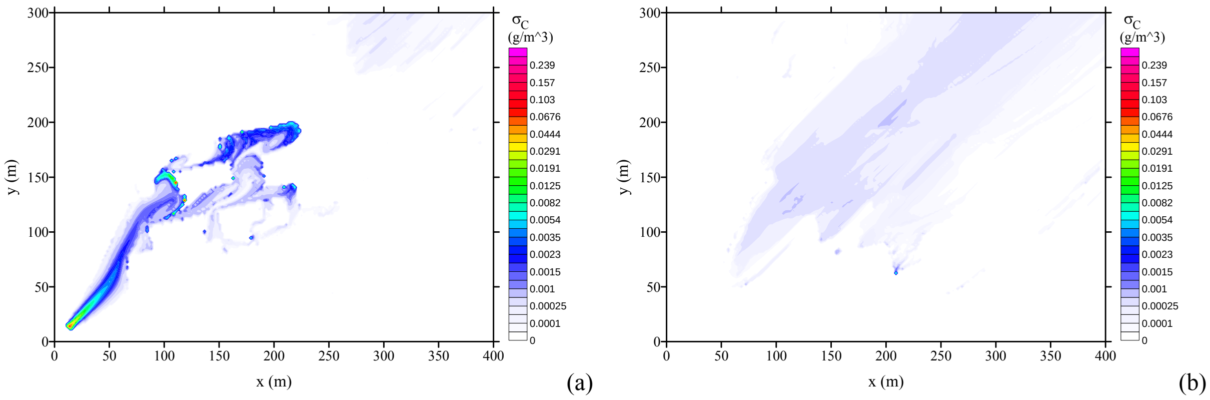

Figure 5. As in Figure 4, but for the standard deviation of the concentration σ_C.

The mean concentrations calculated by LAGFLUM are comparable with those obtained by Gariazzo, C. et al. (2012), who simulated the mean concentration fields in the same domain considered here by using a different dispersion model. With regard to the standard deviation of the concentration, no comparison with other simulation is possible. However, a qualitative agreement with the σ_C spatial distribution simulated in presence of an array of buildings performed in other contexts (Leuzzi et al. 2012) is present.

CONCLUSIONS

A models system consisting of the coupling of the meteorological model micro-SWIFT and the dispersion model LAGFLUM simulating the mean and the standard deviation of the concentration due to a pollutant emitted from a point source is presented. The system has been applied in case of a three dimensional, turbulent flow in presence of a group of buildings of irregular shapes. It seems to be, therefore, well-suited to analyze dispersion phenomena in industrial areas characterized by high risk of accident. The results show the capability of the models system of simulating the concentration field consistent with the assumed meteorological conditions and shapes of the obstacles. The values of the simulated mean concentrations are reasonably similar to those obtained by Gariazzo, C. et al. (2012) for the same meteorological filed and geometrical configuration. With regard to the standard deviation of the concentration, σ_C, there are no similar simulations to perform a quantitative comparison. However, the shape of the σ_C plume and its order of magnitude of are in qualitative agreement with those obtained by Leuzzi, G., et al. (2012) in the case of pollutant dispersion in a turbulent field in the presence of an array of obstacles.

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