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VALIDATION OF THE SAFETY LAGRANGIAN ATMOSPHERIC MODEL (SLAM) AGAINST A WIND TUNNEL EXPERIMENT OVER AN INDUSTRIAL COMPLEX AREA

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Abstract: Monitoring of the emission of air pollutants, either canalized or fugitive ones, is a key issue for industrials to quantify and reduce their environmental impact. The aim of this work is to present a validation of an atmospheric dispersion modelling and operational tool for the near field of the release, which would enable the monitoring of an industrial area with almost real time calculation.

One of the main issues in the modelling of the atmospheric dispersion on industrial areas is to describe the flow around buildings or complex obstacles. Therefore we have developed a new approach (Vendel et al., 2010), based on the use of CFD detailed calculations, which are saved in a database and then coupled with the Safety Lagrangian Atmospheric Model (SLAM), a new real time lagrangian particle dispersion model. This model is able to produce a concentration field in a few minutes of calculation while a full CFD code requires 4-5 hours for the same result.

In order to validate the model, SLAM has been compared with a full CFD calculation done with Fluent and with a wind tunnel experiment, performed on a reduced scale model of an oil refinery. Numerical and experimental simulations were done for neutral atmospheric conditions. Two wind directions and two source locations were studied. Steady concentrations were measured along transverse profiles, at different downwind distances, with a Flame Ionisation Detector. The comparisons for the different configurations show that the SLAM model gives satisfactory results, which are in the uncertainty margin of the measurements and which are very close to the results obtained with the FLUENT calculations.

Key words: *Computational Fluid Dynamics (CFD), Lagrangian dispersion model, Wind tunnel experiments, model validation*

INTRODUCTION

Air pollution on an industrial site is not only due to pollutants emitted by tall chimneys, but also by various sources located near the ground: emissions of machinery or storage tanks, leaks, industrial accident. Modeling of atmospheric dispersion of ground release on an industrial site requires taking into account the effect of the many obstacles and buildings on the site.

Gaussian modeling tools (plume or puff models) usually used for regulatory studies are not very well suited to this problem and it is necessary to use models able to describe the complexity of the flow and turbulence around obstacles. CFD models (Gousseau *et al.*, 2011, Karim and Nolan, 2011), based on the RANS approach (Reynolds Averaged Navier Stokes) are well suited to describe this complexity, but their limitation lies in the computation time required, making it difficult applications of real-time monitoring or of long term studies. Alternative approaches exist, based on the use of a Mass-Consistent model coupled with a Lagrangian stochastic dispersion model: Quic-Urb (Hanna et al., 2006), MSS (Tinarelli et al., 2007).

In this paper, we present the validation of a new approach (Vendel et al., 2010), based on the use of a database of CFD simulations, coupled with the operational use of a Lagrangian particle model. In the first section, we briefly present the main features of the approach and the SLAM model. In the second part, we describe the numerical and experimental configurations used for comparison. Finally in the last section, we present the results of the comparisons.

MODEL DESCRIPTION

Flow'Air 3D Methodology

In a simulation of the flow and atmospheric dispersion with a CFD model, an important part of the computing time is devoted to modelling the flow and turbulence field. The principle of our approach, illustrated on Figure 1, is to make in advance a database of wind fields on the considered industrial site. In this way, only the dispersion is modeled in operational situations and time savings is considerable, as will be seen later.

The parameters that constitute the database are the wind direction and the inverse of the Monin-Obukhov length. As it was shown by Vendel et al. (2010), it is possible to overcome the wind speed by normalizing the velocity and turbulence fields by the friction velocity u_*. Vendel et al. have also shown that a discretization of the database in 18 wind directions (step of 20°) and 7 values of $1/L_{MO}$ can limit the interpolation error in the database to a few percents.

Once the database is done, it is used as input for the Lagrangian model SLAM. In operational situations, a point meteorological data (measurement or forecast) is used in a meteorological preprocessor toestimate the wind direction, the inverse of the Monin-Obukhov length and the friction velocity u *. From these parameters, we interpolate in the database to obtain a wind and turbulence field corresponding to the real atmospheric conditions. This field is then used to model the dispersion with the SLAM Lagrangian model.

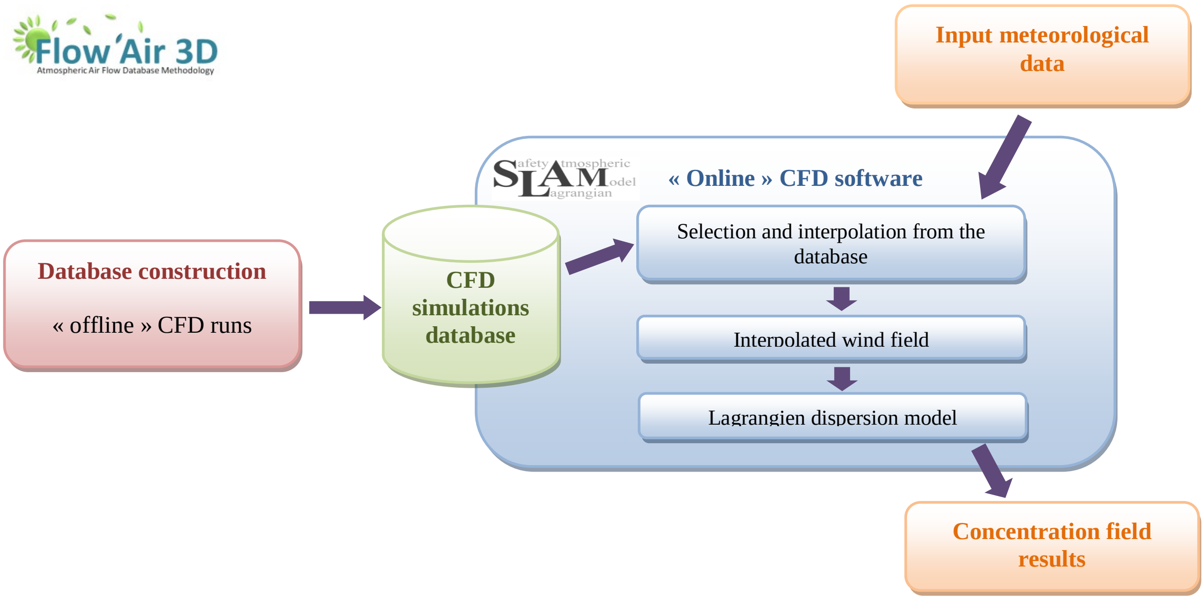

Figure 18. General description of the Flow'Air 3D methodology.

The Safety Lagrangian Atmospheric Model (SLAM)

The Safety Lagrangian Atmospheric Model is a stochastic particle dispersion model, based on the tracking of Lagrangian trajectories of individual particles. The temporal evolution of the Lagrangian velocity of each particle is given by the equation:

$$U_i(t) = \overline{U_i}(t) + U_i'(t) \quad \text{with} \quad U_i'(t+dt) = U_i'(t) + dU_i' \tag{1}$$

$\overline{U_i}$ is the mean velocity of the flow obtained from the CFD velocity field. The evolution of the fluctuating velocity U_i' is determined by the stochastic differential equation (Thomson, 1987):

$$dU_i' = a_i(\boldsymbol{X}, \boldsymbol{U}', t)\,dt + \sum_j b_j(\boldsymbol{X}, \boldsymbol{U}', t)\,d\xi_j \tag{2}$$

in which the terms a_i and b_i are expressed in terms of standard deviations of velocity fluctuations σ_{u_i} and of the Lagrangian times $T_{L,i}$. To express σ_{u_i} and $T_{L,i}$, we use the variables from the turbulence model of the CFD code. When using the *k*-*ε* turbulence model, we get σ_{u_i} and $T_{L,i}$ by the relations:

$$\begin{cases} \sigma_u = \sqrt{\dfrac{2}{3}k} \\ T_L = \dfrac{2\sigma_u^2}{C_0\varepsilon} \end{cases} \quad \text{with} \quad C_0 = 4 \tag{3}$$

It may be noted that in this case, the turbulence model imposes an assumption of turbulence isotropy. More complex turbulence models (e.g. Reynolds Stress Model) allow to take into account the anisotropy of turbulence.

From a numerical point of view, equation (2) is solved at each time step and for each particle. The time step is chosen small enough according to the Lagrangian time. At each time step, the particle is localized in the CFD mesh to assign local values of the average velocity $\overline{U_i}$ and the turbulent quantities *k* and *ε*. Concentrations are evaluated by summing the mass carried by the particles in each cell of the domain. A criterion on the number of particles is used to minimize the numerical error.

EXPERIMENTAL AND NUMERICAL SETUP

In order to validate the Flow'Air 3D approach and the SLAM model, we performed experiments in a wind tunnel and full CFD simulations (eulerian modelling of flow and dispersion) of an industrial site, representative of an oil refinery.

a) Experimental model in the wind tunnel b) CFD numerical mesh of the oil refinery

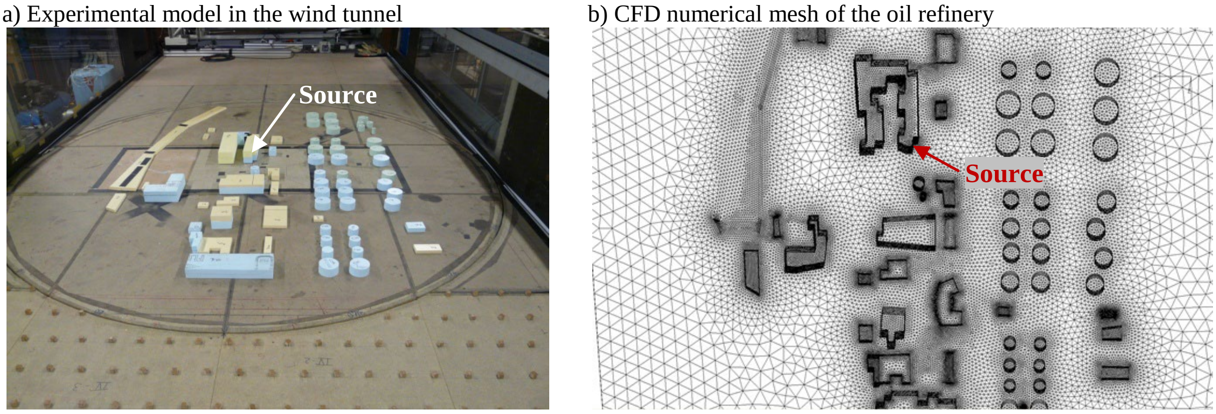

Figure 19. Experimental (a) and numerical (b) geometrical model of the oil refinery.

Wind tunnel experiments

The experiments have been performed in the atmospheric wind tunnel of the Ecole Centrale de Lyon. It is a recirculating wind tunnel with a test section of 14.0 m long, 3.8 m wide and 2.0 m high.

The industrial site is represented in the wind tunnel with a 1/250 scale model (Figure 2-a). The upstream velocity profile is defined as a neutral surface boundary layer, characterized by an aerodynamic roughness z_0 = 0.0875 m and a friction velocity u_* = 0.23 m.s^{-1}.The source of pollutants is a release of ethane (density close to the air), with momentum and buoyancy negligible compared to the external flow. The source is located very close to a building in order to get a plume significantly affected by the effects of obstacles.

The concentration measurements were performed with a Flame Ionization Detector (FID), near the ground along transverse profiles, at 4 distances downwind from the source.

CFD eulerian modelling for flow and dispersion

Eulerian CFD simulations were performed with the FLUENT model, using a RANS approach and a k-ε turbulence model. The CFD mesh (Figure 2-b) was made to reproduce at real scale the industrial site studied in wind tunnel. The numerical domain is 1000 m x 1000 m x 300 m. The mesh consists of 1.4 million of tetra elements, with grid minimum size of one meter near buildings and ten centimeters at the source. The characteristics of the upstream meteorological profile and of the source are similar to those used in wind tunnel.

CFD wind field database and SLAM Lagrangian dispersion modelling

When creating the database, the 126 CFD simulations (18 x 7) were performed with the FLUENT software, using the parameterization described above. Then, the wind fields used for SLAM are obtained by interpolation in the database. Calculations with the Lagrangian model SLAM were performed using a release of 1000 particles per second until it reaches a steady state of concentration fields.

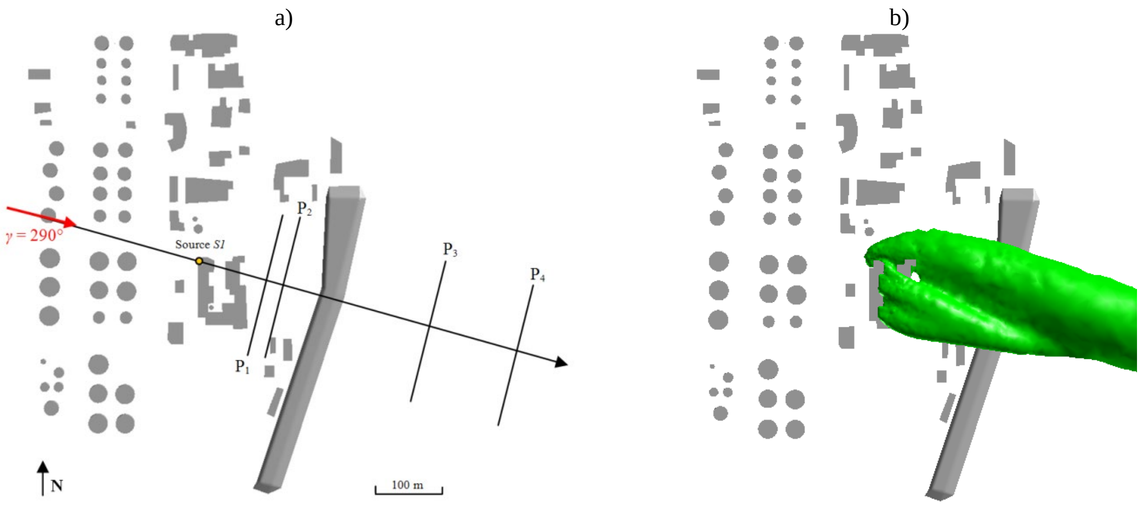

Figure 20. Configuration used for the comparison: a) wind direction and transverse measurements profiles; b) illustration of the numerical 3D plume.

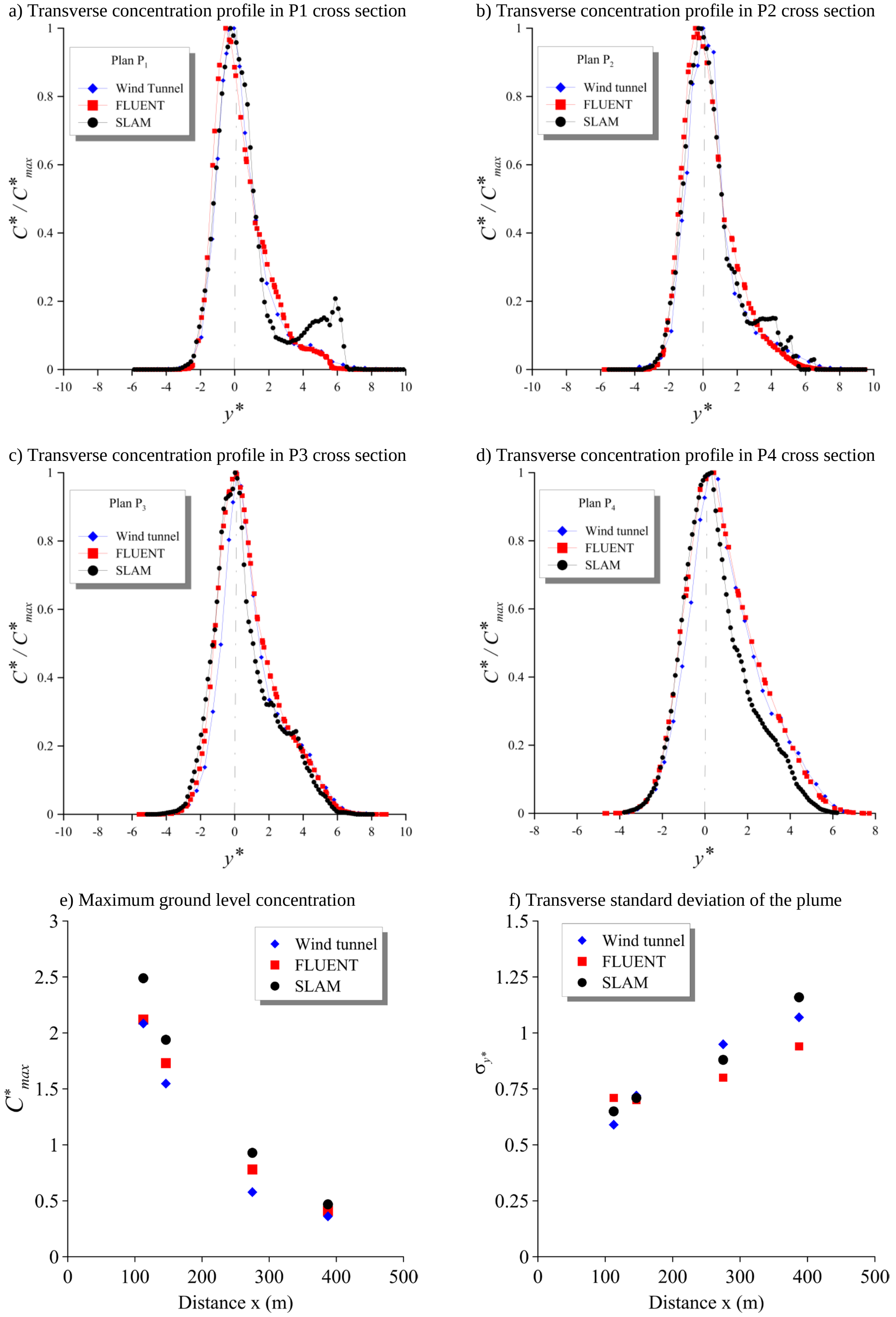

Figure 21. Transverse concentration profiles for the different cross section P1 to P4 (a to d) and longitudinal profiles of maximum ground level concentration (e) and of transverse standard deviation of the plume (f).

NUMERICAL RESULTS AND COMPARISONS

4 configurations were studied in wind tunnel, corresponding to two source positions (S1 and S2) and two wind directions (290° and 335°). In this article, we detail the results for the case of the source S1 and the wind direction of 290° but the results in other situations are similar.

Thereafter, we will study four concentration profiles at the ground, made in planes perpendicular to the wind direction and at several distances from the source. To compare the experimental and numerical results, we use dimensionless quantities:

$$C^* = CU_\infty L^2 / Q \quad \text{and} \quad y^* = y/L \tag{4}$$

Where U_∞ = 5 m.s^{-1}, L is the size of the building close to the source (L = 28 m at real scale) and Q is the flow rate of the source.

Comparisons of the transverse concentration profiles downstream of the source are shown in Figure 4-a to d. There is a very good agreement between FLUENT and the measurements. For SLAM, the agreement is slightly worse but still very satisfactory taking into account the operational focus of the tool. The decay of maximum ground concentration,as a function of distance, is well reproduced by the SLAMmodel, as well as theincrease of the plume transverse standard deviation σ_{y^*}.

In terms of computational time on a workstation, the full CFD simulation (flow + dispersion) with FLUENT requires 4 h CPU while the SLAM simulation (interpolation in the database + Lagrangian dispersion) requires 6 min CPU on the same computer. The Flow'Air 3D methodology and the SLAM model can therefore generate results close to a full CFD calculation,in a computational time about 40 times lower.

CONCLUSION

In this paper, we presented a validation of the Flow'Air 3D methodology and the SLAM Lagrangian model, developed to describe dispersion in the presence of complex obstacles, in operational situations. This validation was performed by comparison with wind tunnel experiments and CFD calculations performed with the FLUENT software, on a configuration representative of an industrial oil refinery.

After reminding the principle of the Flow'Air 3D methodology, we presented the SLAM Lagrangian model. We then detailed parameterizations used in the wind tunnel, in the FLUENT code and in the SLAM model. Finally we presented comparisons of these different approaches.

The results show a good agreement between the SLAM model, the FLUENT software and the wind tunnel experiments, for different concentration profiles downstream of the source. The comparison also shows that the computational time with SLAM is about 40 times lower than with the full CFD approach.

These results are encouraging and allow to consider operational applications for real-time monitoring of the pollution around an industrial site and for crisis management.

REFERENCES

GousseauP., B. Blocken, T. Stathopoulos and G.J.F. van Heijst, 2011: CFD simulation of near-field pollutant dispersion on a high-resolution grid: A case study by LES and RANS for a building group in downtown Montreal. *Atmospheric Environment*, **45**, 428-438.

Hanna S.R., M.J. Brown, F.E. Camelli, S.T. Chan, W.J. Coirier, O.R. Hansen, A.H. Huber, S. Kim, and R.M. Reynolds, 2006: Detailed simulations of atmospheric flow and dispersion in downtown Manhattan.*Bulletin Am. Meteorol. Soc.*, **87**, 1713-1726.

Karim A.A. and P.F. Nolan, 2011: Modelling reacting localized air pollution using Computational Fluid Dynamics (CFD). *Atmospheric Environment*, **45**, 889-895.

Thomson, D.J., 1987: Criteria for the selection of stochastic models of particle trajectories lagrangian dispersion model in turbulent flows. *Journal of Fluid Mechanics*, **180**, 529-556.

Tinarelli G., G. Brusasca, O. Oldrini, D. Anfossi, S. Trini Castelli and J. Moussafir, 2007: Micro-Swift-Spray (MSS): A new modelling system for the simulation of dispersion at microscale. General description and validation. *Air Pollution Modeling and its Application XVII*, **5**, 449-458.

Vendel, F., G. Lamaison, L. Soulhac, L. Donnat, O. Duclaux and C. Puel, 2010: A new operational modelling approach for atmospheric dispersion in industrial complex area. *13th Int. Conf. on Harmo. within Atmos. Disp. Modell. for Regul. Purposes*, Paris, France.