3D SIMULATIONS OF POLLUTANTS ATMOSPHERIC DISPERSION AROUND THE BUILDINGS OF AN INDUSTRIAL SITE COMPARISON OF MERCURE CFD APPROACH WITH MICRO-SWIFT-SPRAY SEMI-EMPIRICAL APPROACH

Patrick Armand[1], Julien Commanay[2], Maxime Nibart[2], Armand Albergel[2], Pascal Achim[1]
[1] Commissariat à l'Energie Atomique – Département Analyse, Surveillance, Environnement
91 680 Bruyères-le-Châtel – France
[2] ARIA Technologies – 8-10, rue de la Ferme – 92 100 Boulogne-Billancourt – France

INTRODUCTION

All industrial installations are required by the National and European regulations to produce impact assessment studies relating to the normal operation and hypothetical on-site accidents. In both cases, these studies require dispersion simulations of atmospheric gaseous or particle releases and the health impact evaluation for workers and populations around the facilities.

For regulatory purpose, the pollutants dispersion is usually computed using Gaussian plume or puff models, as they are easy to handle and give a quick answer. But these models appear very limited when simulating the pollutants dispersion in the urban environment or around the buildings of industrial sites. At the local micro-scale, a full CFD model well adapted for the planetary boundary layer, is the reference way of investigation, but it is extremely demanding in computational resources, especially for two important applications: emergency response or preparedness and long term impact around a source near the ground. Micro-SWIFT-SPRAY (MSS) modelling system is being developed as an intermediate quick response capability to simulate flow field and dispersion processes at the micro-scale in the presence of obstacles.

MSS has been used in numerous complicated configurations with either accidental releases of toxic materials or chronic long term releases from the stacks of facilities. Some examples are commented in the paper. For accidental releases, 3D computations were carried out with MSS and MERCURE in order to compare the results and evaluate MSS solution. In the conclusion, MSS other uses and potential promising developments are discussed.

DESCRIPTION OF MICRO-SWIFT-SPRAY (MSS)

Micro-SWIFT-SPRAY (MSS) is a recent modelling system developed as an alternative where CFD codes need heavy computational resources. It is tagged as '90% of the solution for less than 10% of the CPU'.

MSS allows an exact representation of buildings, directly generated by a GIS (shape files).
Micro-SWIFT is a micro-scale analytically modified interpolator over complex terrain. A 3D mass consistent wind field is generated in the three steps below:

- According to meteorological data, a first guess of the mean flow is computed through customisable interpolation using all available and relevant data.
- This first guess is modified by creating analytical zones where the flow takes account of buildings, these being isolated or not (*Röckle*, 1990 or *Kaplan and Dinar*, 1996).
- Finally, the flow is adjusted to satisfy the continuity equation and impermeability on the ground and building walls.

Micro-SPRAY is a Lagrangian particle dispersion model directly derived from the SPRAY code (*Tinarelli et al.*, 1998), able to take obstacles into account. The dispersion of an airborne pollutant is simulated following a large number of fictitious particles, each representing a part of the emitted mass. In the motion equation, the particle velocity is split into two components: a mean one defined by the local wind reconstructed by Micro-SWIFT, and a stochastic one, reproducing the atmospheric turbulence and dispersion which is obtained applying the scheme developed by Thomson in respect of the 'well-mixed' condition (*Thomson*, 1987).

DESCRIPTION OF MERCURE

MERCURE software has been developed by EDF (French Electricity Company) on the basis of ESTET CFD code. Many validation exercises of MERCURE have been performed through systematic comparisons with experimental data and output of other 3D codes. MERCURE / ESTET fully solves Navier-Stokes equations (for averaged quantities if the flow is turbulent) by the fractional step method in finite differences and finite elements, on two- or three-dimensional domains, in transient or permanent regimes. MERCURE was fitted to the planetary boundary layer, using the virtual potential temperature as the thermal variable for the energy balance equation or other features making atmospheric releases easier to deal with.

SIMULATIONS OF AN ACCIDENTAL RELEASE

A case study relating to an accidental chemical release among the buildings on an industrial site was carried out using both MSS and MERCURE. The hypothetical accident is a reference scenario for an emergency situation on the site.

Input conditions

Meteorological condition

The atmosphere is very stable (F Pasquill-Gifford class). The wind blows from the north-east. The wind velocity is 2 m.s^{-1} at 10 m above the ground level.

Atmospheric releases

Pressurized liquid chlorine cylinders are stored outdoor on the site. A breach in one cylinder produces a diphasic flow with a thermodynamic flash (liquid and gaseous release) followed by the evaporation of the chlorine puddle. The mass flow rate takes into account the liquid and vapor phases. It is evaluated with ATRCOD module developed by ARIA Technologies.

Toxicological reference values

'Toxicological reference values' are given by the French INERIS for the main toxic species. Concentrations combined with exposure durations are defined (1) under which no irreversible effects on human health were observed or (2) leading to the death of a fraction (1 or 5%) of exposed people. As the atmospheric concentration C is time dependant, the common practice is to calculate the dose $D = \int C^n(t)dt$ (for chlorine, n is 2.3). Introducing toxicological values in this formula, we obtain the 'irreversible effects' and 'death' doses. The computed doses are then compared to the threshold doses to determine the sanitary impact of the accident.

Computations conditions

Meshing

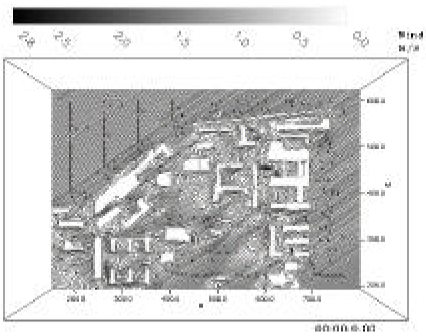
MSS calculation domain is a 645 m x 426 m x 250 m parallelepiped. The horizontal meshing is regular (3 m mesh size). The vertical meshing is refined near the ground level (28 levels). MERCURE calculation domain is slightly larger. The horizontal meshing is refined near the release location. The vertical meshing is refined near the ground level (33 levels).

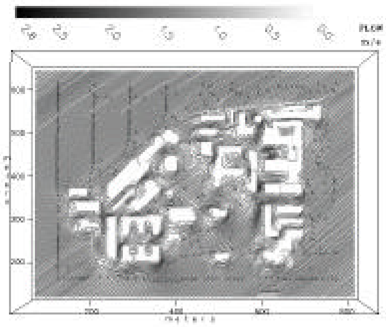
Numerical parameters

The simulated time period is 10 minutes long. In Micro-SPRAY, 250 particles are emitted at each time step of 1 s. In MERCURE, the time step is constant and equal to 1 s.

Wind fields results

Figures 1a and 1b present the wind module and the streamlines at 2 m above the ground level, simulated by MSS and MERCURE respectively. These figures illustrate the global behavior of the air flow around the buildings with the acceleration, deceleration and recirculation zones around the obstacles. The zones with low wind speeds are slightly larger according to MSS. Close to a complex ‘three-shaped’ building, MSS indicates a high speed region corresponding to a canyon in MSS modelling of the buildings.





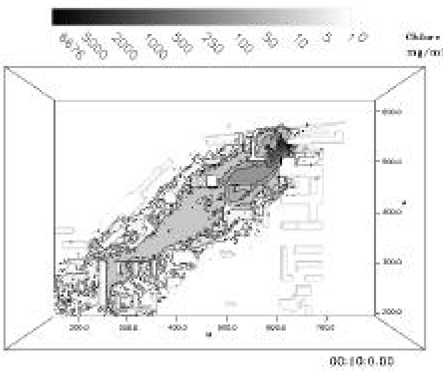
(a) *(b)*

Fig. 1; Wind module and streamlines at 2 m, (a) MSS, (b)MERCURE.

Concentrations results

Figures 2a and 2b represent sections, near the ground, of the concentration field, issued from respectively MSS and MERCURE. The figures show similar plumes with same extents of the gray areas. Chlorine plume is advected a bit more southerly by MERCURE and farther by MSS while remaining more confined close to the source and being slightly larger along with MERCURE. The difference is due to the method of taking the obstacles into account. While MSS does not consider the global effect of the buildings on the wind, MERCURE channels the flow between the buildings denoted 1 and 2 on figure 2b. Moreover, turbulence modeling is different in the two models which influences the pollutants dispersion.

(a)



(b)

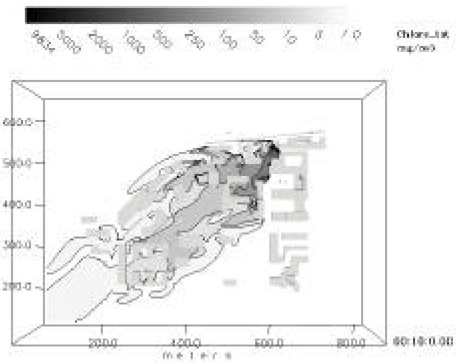


Fig.2; Chlorine concentration at 2 m – t = 10 min, (a) MSS, (b)MERCURE.

Doses results

The ‘irreversible effects’ and ‘death’ zones have been computed with MSS and MERCURE. It is worth noticing the accident impact is restricted to a small area directly near the release point. The lethal dose is obtained nowhere with MSS while it is reached up to a maximum distance of 28 m with MERCURE. The irreversible effects dose is located close to the release, up to 32 m, according to MSS while it extends to 125 m for MERCURE. The shape and the extent of the doses contours are more dissimilar than the concentrations contours. This can be explained by the doses calculation in which the concentrations are raised to the power of 2.3 with the consequence to amplify the small discrepancies between the models.

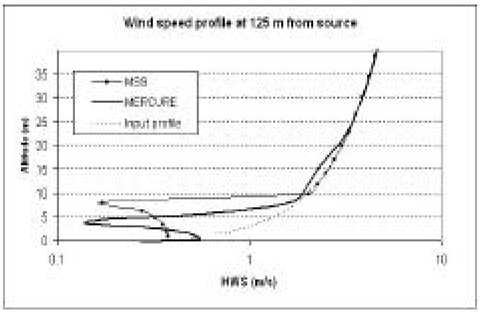
Comparison of the results on a virtual sensor

For a better assessment of MSS and MERCURE results, numerical sensors have been placed near the ground in the calculation domain. One of the detectors is located 125 m downwind of the emission source, behind the 9 m high building denoted 3 on figure 2b. This detector is used to produce the results presented on figures 3a and 3b.

Figure 3a represents the vertical profiles of the horizontal wind provided by MERCURE and MSS, compared to the input wind profile. MSS and MERCURE indicate a strong influence of building 3 on the wind below 10 m. Close to the ground, a wind reduction zone is topped by a wind acceleration zone. This corresponds to a recirculation downwind the obstacle predicted both by MSS and by MERCURE (however with different dimensions of the recirculation).

Figure 3b represents the concentration histories issued from MSS and MERCURE (for which 'instantaneous' and 'one minute-averaged' values are shown). Final concentrations are similar (difference of less than 3%), but MSS concentrations are delayed by about 50 s. The chlorine takes longer to be advected between buildings 1 and 3 where the wind is weaker in MSS.

(a)



(b

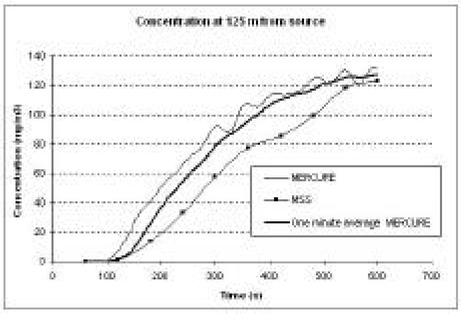


Fig. 3; Vertical profiles of the horizontal wind and concentration histories provided by MSS and MERCURE on a sensor 125 m downwind from the source. Dotted curve on figure 3a is the input wind profile. 'Smooth' curve on figure 3b is plotted with MERCURE 'one minute-averaged' concentrations.

Computation times

Table 1 indicates the computation times for 10 minutes simulations on one processor Intel® Xeon® 3.2 GHz with 3.2 Go RAM. While the 3D numerical results obtained with MSS and MERCURE are comparable, MSS computation times are much lower than MERCURE ones.

Table 1. MSS and MERCURE computation times.

	MSS	MERCURE	Ratio
Wind and dispersion	640 s	85 680 s	0.7%

LONG TERM IMPACT ASSESSMENT

In the case of chronic atmospheric releases, a long term impact assessment is often required. The authorities demand to estimate the air concentration or soil deposition in terms of annual mean averages and other statistical figures as percentiles. These kind of studies are generally carried out with simple Gaussian approaches doing the assumption of no building effects or using empirical, not very accurate, downwash formulations. Facing the more and more severe regulations, especially for VOC (volatile organic compounds) and other species going through stacks, better solutions are necessary as provided by MSS. Moreover, to perform a long term assessment, the model must be driven with typically five years of hourly meteorological data.

This is not compatible with full CFD CPU times as in MERCURE code and faster algorithms are required.
The following application illustrates the VOC impact around an important car factory. Figure 4a shows how the plumes are affected by the wakes produced by the factory buildings. Figure 4b corresponds to the same computation with Pasquill-Gifford Gaussian approach. As the release is done through a stack, the impact is underestimated at the close vicinity of the plant while it is overestimated far from the buildings. One should notice that MSS computations can be easily dispatched on several CPUs and carried out in one or two weeks.

(a) *(b)*

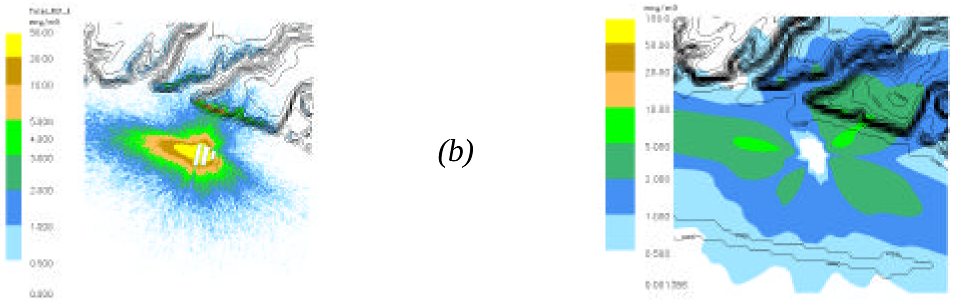


Fig. 4; Impact assessment using respectively MSS and the Gaussian approach.

CONCLUSION AND PERSPECTIVES

Gaussian plume or puff models have serious limitations when used in the frame of dispersion and impact assessment studies for industrial sites or urban environment. On the other hand, a full CFD approach needs huge CPU resources. The Micro-SWIFT-SPRAY modelling system, still under development, represents a promising compromise to quickly simulate the 3D flow field and dispersion processes at the micro-scale. 3D simulations of accidental atmospheric releases have been done with MSS and MERCURE for the same site in identical meteorological conditions. Wind fields, concentrations and doses results are comparable with minor explained discrepancies. While 3D numerical results are similar, MSS computation times are much lower than MERCURE ones. In this application, MSS goal of '90% of the solution for less than 10% of the CPU' is greatly reached. Other MSS comparisons with CFD numerical results and wind tunnel or in field experimental data also give acceptable results. The implementation of MSS in operational tools such as the new version of HPAC (US-DOD) has now been completed successfully.

Finally, it is foreseen to use MSS in near real time conditions in the framework of emergency preparedness and response to accidental or malevolent dispersal events. This would imply the development of a parallel version of MSS in order to still more decrease the CPU.

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