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APPLICATIONS OF THE MSS (MICRO-SWIFT-SPRAY) MODEL TO LONG-TERM REGULATORY SIMULATIONS OF THE IMPACT OF INDUSTRIAL PLANTS

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Abstract: The MSS (Micro-SWIFT-SPRAY) model was originally developed for emergency response purposes, in order to provide a fast dispersion solution taking into account buildings in an Urban Environment, or else in an Industrial area with buildings. The model uses a simplified CFD solution (Micro-SWIFT) to represent the flow fields with metric resolution, and a Lagrangian Particle solution (Micro-SPRAY) to compute the 3D dispersion patterns among the obstacles.
The present paper introduces first the current status of development of MSS. Then the results of the long-term applications of this modelling system to several real world cases are presented, where the model is applied sequentially, on an hourly basis, on a sequence of one to three years of meteorological data. This is exactly how a standard Long Term Gaussian or Puff model would be used.
A parallel version of this system (PMSS) has been jointly developed by ARIA Technologies and CEA and is now under test for this type of applications.
We present the advantages and disadvantages of this solution, which is being packaged as "ARIA Impact 3D". We show how it can make use of fully 3D time-dependent meteorological model solutions, and how it compares with Gaussian and Puff modeling systems. The CPU cost, the use of parallel versions, and the realistic dispersion patterns obtained by the Lagrangian Particle approach are discussed.

Key words: *air quality simulation, building effects, Lagrangian dispersion modelling*

RECENT DEVELOPMENTS OF MSS (MICRO-SWIFT-SPRAY)

Basic features: the MSS modelling system (Moussafir *et al.*, 2004 and 2007) includes Micro-SWIFT and Micro-SPRAY. Micro-SWIFT (Moussafir *et al*., 2004; Tinarelli *et al*., 2007) is an analytically modified mass consistent interpolator over complex terrain. Given topography, meteorological data and buildings, a mass consistent 3-D wind field is generated. It is also able to derive diagnostic turbulence parameters (namely the Turbulent Kinetic Energy, TKE, and its dissipation rate) to be used by Micro-SPRAY inside the flow zones modified by obstacles. Micro-SPRAY is an LPD (Lagrangian Particle Dispersion) model able to take into account the presence of obstacles. It directly derives from the SPRAY code (Anfossi *et al*., 1998; Carvalho *et. al*, 2002; Ferrero *et al*., 2001; Ferrero and Anfossi, 1998; Kerr *et al*., 2001; Trini Castelli *et al*., 2003; Tinarelli *et al*., 1994 and 2000). It is based on a 3-D form of the Langevin equation for the random velocity (Thomson, 1987).

Nested grids: SWIFT and Micro-SWIFT may run in nested mode, with multiple grids at several levels of nesting, thus allowing a smooth transition between the larger scale, where the grid cells are similar in size to the cell of a driver prognostic model such as WRF, and the smaller scale, where grid cells are metric (typically 3m to 5m).

Dense gases: a solution for dense gases simulation has been introduced into Micro-SPRAY (hence in MSS). It combines three algorithms:

1. **Dynamics of a plume with initial momentum**: the particle dynamics is described by a set of five conservation equations, integrated for each particle: this method is applicable to dense or buoyant releases, and derives from classical Plume Rise literature (Glendening *et al*., 1984)
2. **Dynamics of a plume without initial momentum**: used for instantaneous releases like the Thorney Island trials
3. **Plume spread at the ground:** this step implies a mixed algorithm. The movement of each particle depends on the characteristics of the 'ensemble', so that a Eulerian grid may be defined to proceed with a PM (particle to mesh) interaction

The dense gases solution of MSS has been validated against Thorney Island, Macdona, and Kit Fox Field experiments.

Figure 1: Thorney Island experiment – Trial 8 – Collapsing cloud photographs.

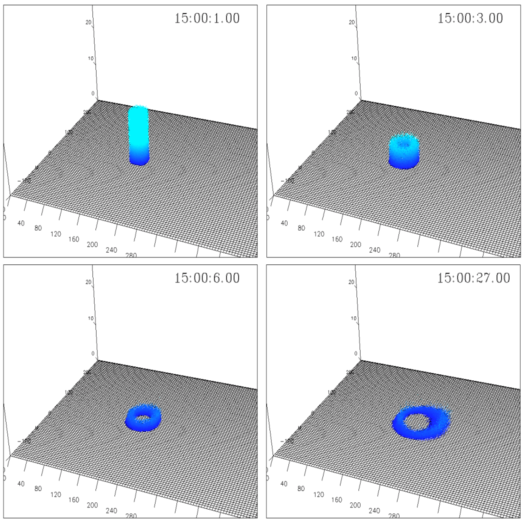

Figure 2: Thorney Island experiment – Trial 8 – Collapsing cloud simulation.

Multi-phase jets:

Air, water vapor, liquid water (several droplet size classes)

- ➪ Plume with buoyant air, water vapor, liquid water with droplets of different sizes.
- ➪ MSS represents the plume with N+1 «substances» (N classes of droplet size + water vapor)
- ➪ Condensation, evolution of droplet diameters with classical evolution with evaporation
- ➪ Each « Lagrangian particle » belonging to one of the N droplet-size classes contains a very large number of droplets of similar size, who share the same properties: plume diameter=f(t), Temperature=f(t), mass=f(water content,t)

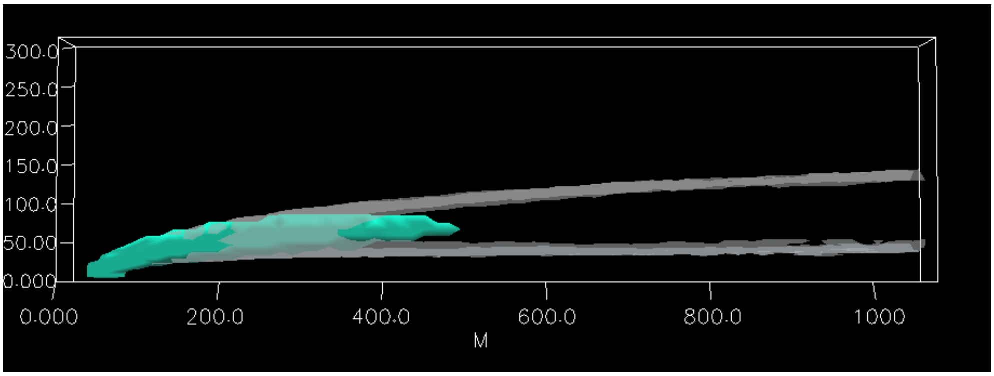

Figure 3: Cooling tower plume simulation (Outer surface: water vapor 5.E-05 kg/m3 - Inner blue surface: water droplets 1E-10 kg/m3). Distances in meters.

Air, water vapor, liquid water (total), Chlorine vapor, Chlorine in liquid phase

- ➪ « Extended» Glendening equations, with phase changes for water and Chlorine, in order to represent the thermodynamics of the jet.
- ➪ All chlorine droplets small enough not to drift / the gaseous phase

Concentration variances: MSS includes the estimate of concentration variances
Generalized geometries: arches, walkways or tunnels are coded in MSS

Pressure distributions: in MSS, Micro-SWIFT computes a diagnostic pressure field on buildings (façades and roofs), giving Delta (P) on each facet of a building (method suggested by Michael BROWN et al, LANL). The solution is obtained through the application of a Poisson solver for:

$$\frac{1}{\rho}\,\Delta\,\overline{p} = -div\left(\partial_j\left(\overline{U}_j\,\overline{U}_i\right)\right)$$

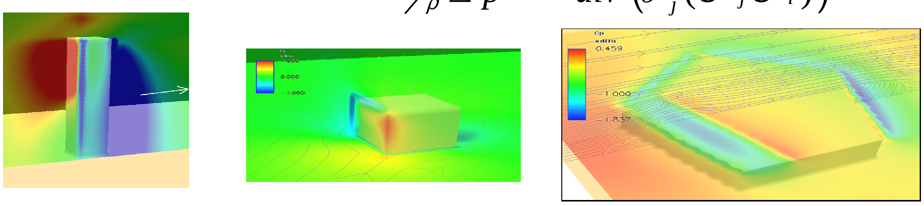

Figure 4: Examples of MSS pressure distributions on the surface of simple buildings

Infiltration: MSS infiltration into buildings is studied with two simple approaches:

- classical derivation of homogeneous concentration over all the volume of each building. This approach uses the average concentration around each building and an overall volume rate of air renewal to drive concentrations
- a more sophisticated approach using Delta(P) to control inflow and outflow of mass from the building at each facet, leading to some assumptions needed on separated domains of the buildings (e.g.: floors, walls,…)

Infiltration parameters are set for different buildings blocks exactly as texture elements in a GIS, governing transfers.

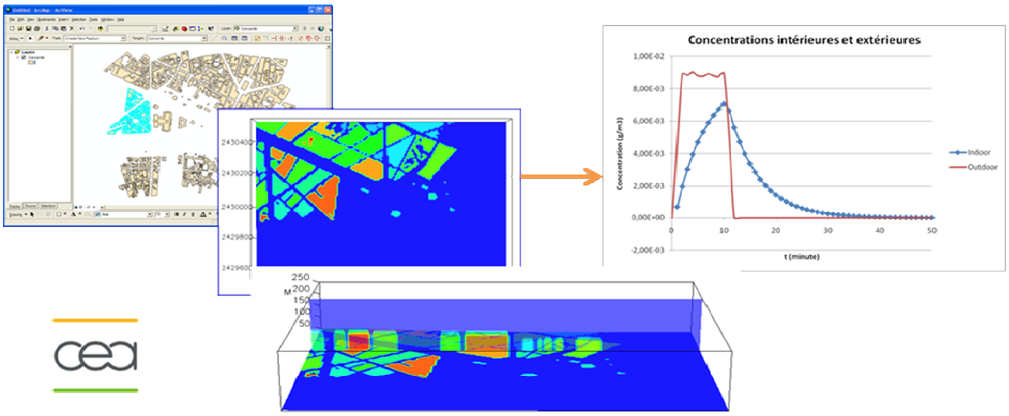

Figure 5: Schematics of building textures used to drive infiltration parameters. Chart: evolution of external forcing (stepwise red curve) and indoor concentration (slowly decaying blue curve).

Parallel version of MSS: the development of a parallel version of MSS, called PMSS, has been jointly funded by ARIA Technologies and CEA (French Atomic Energy Commission). The target configurations include: (1) Large Linux clusters (typically 2048 processors) for real-time Urban Emergency response over Paris, (2) Standard multi-core laptops (Windows). This development serves both emergency response purposes and Air Quality applications where MSS is run hourly for several years. PMSS involves a separate parallel architecture for Micro SWIFT and Micro SPRAY:

⇨ Parallel time frames and tiles (domain separation) for Micro SWIFT
⇨ Parallel particle clouds per each tile for Micro SPRAY
⇨ Simpler if no P-P interaction (dense gases in a second phase)

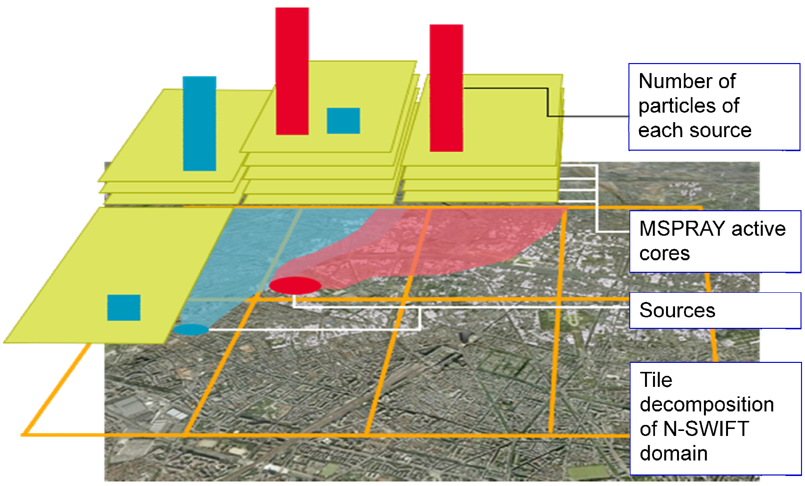

Figure 6: Stencil of MSS parallelization.

LONG TERM IMPACT SIMULATIONS WITH MSS

Progress in the codes generality, and their ability to take into account the effect of buildings on the flow, suggest that the MSS model, and similar models based on Simplified CFD (such as AUSTAL or QUIC-URB), may be used to evaluate the long term impact of atmospheric releases, giving in principle a more realistic solution than standard Gaussian models, such as AERMOD.

However, even if a model like MSS has a CPU cost 50 to 100 times lower than a full-blown CFD solver with similar domains and grids the additional computational cost with respect to a straight line Gaussian solution, or to a Puff model, is not negligible, so that parallel processing is opening the way to more frequent applications of 3D Lagrangian models.

We present here (without details) two examples of studies performed with MSS for long-term impact evaluations.

Car factory
The first example we present is related to a car factory in Asia, where the evaluation of Health Impact of the plant involves the determination of the dispersion of several VOCs. The site comprises many large buildings, and it has been surrounded by the urban development with several residential tall towers. The computation of the dispersion taking into account these obstacles as well as the maximum distance of propagation for the VOCs shows the need for a high-resolution solution over the plant itself, with a very fine grid, and the possibility to use a coarser grid and a simpler model at distances above 1 kilometre from the plant. The simulation of the dispersion from the plant was made over a period of three years, with hourly input meteorological data and two grids:

- The inner grid covers a square domain of about 2x2 km size, with a resolution of 10 m. MSS is used
- The outer grid covers a square domain of 6x9 km size, with a resolution of 20 m.

On the outer grid, a transition to a puff model is used, and clusters of particles are converted into puffs when they come out of the inner domain.

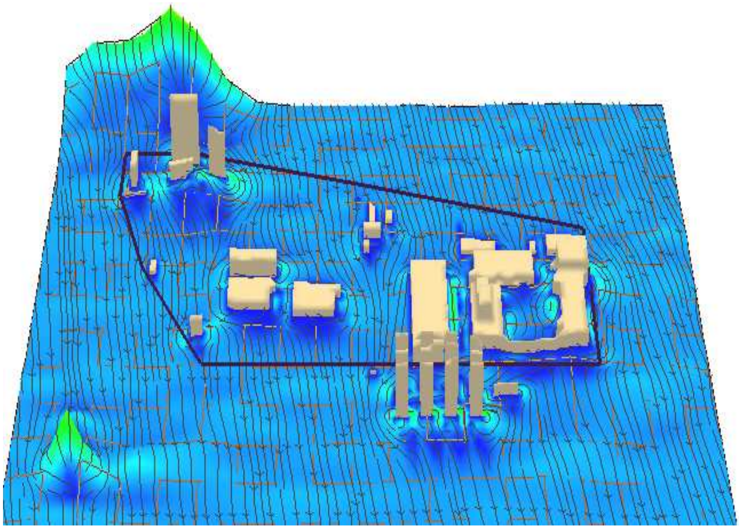

Figure 7: Car factory VOC impact study. Inner grid. Wind field streamlines at 5m and buildings. Plant limit is in black.

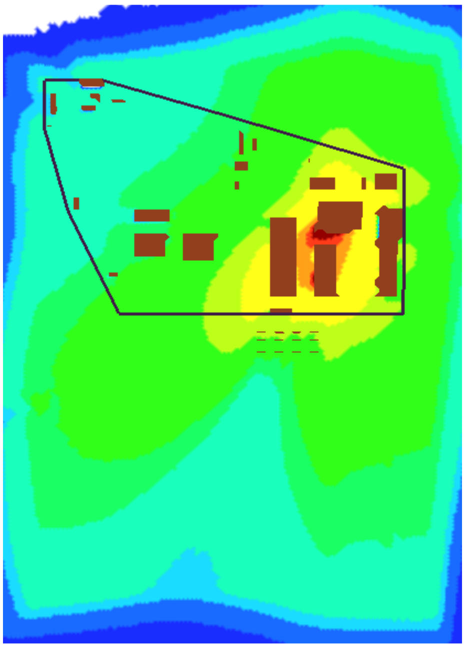

Figure 8: Car factory VOC impact study. Inner grid. Iso-contours of xylene concentration, yearly averages.

The systematic **blocking effect of the large buildings** is clearly visible on the concentration map on the right. As far as CPU is concerned this type of simulation involves about a week of elapsed time on a 10 processor machine, per year simulated.

Hospital heating system

The next example is related to a large hospital, where we studied the potential air pollution from the heating system. In this case no nesting is applied and MSS is applied at one scale only. The effect of buildings on the average concentration is striking.

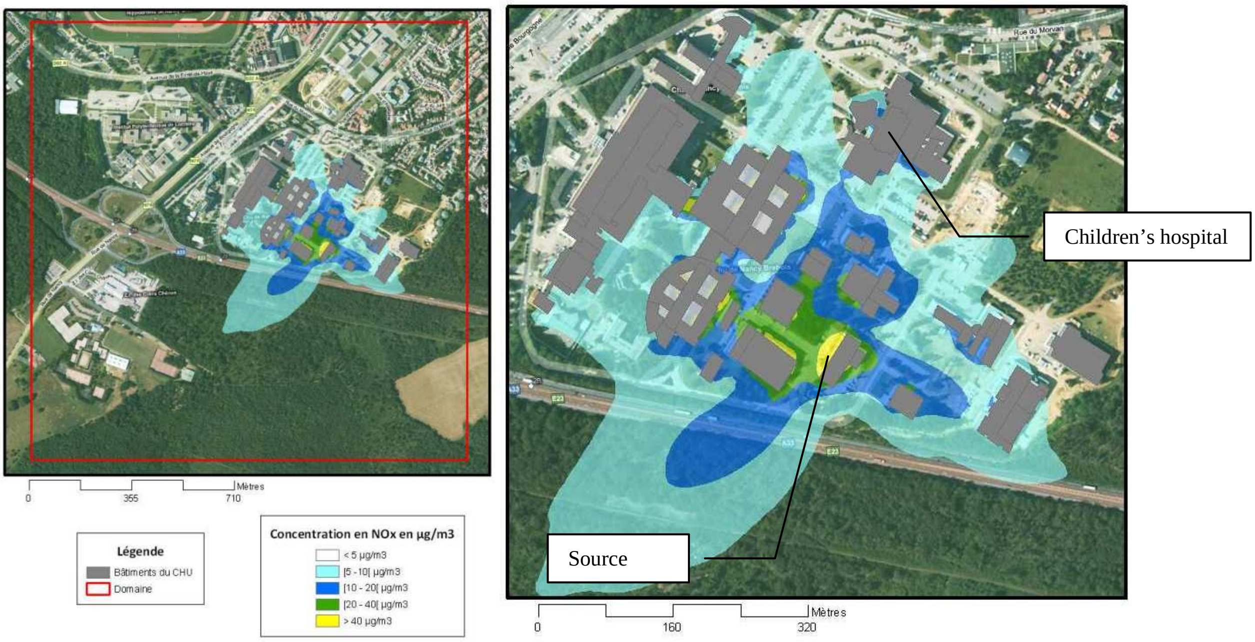

Figure 9: MSS results for a hospital area.

CONCLUSION

The MSS simulation system can be used to simulate the long term impact of releases in an environment with buildings and obstacles. The CPU demand is of course much higher than with standard Gaussian approaches, but the dispersion patterns are realistically influenced by the buildings in the output of the long-term simulations.

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